LOD AND ADI METHODS FOR SOLVING THREE-DIMENSIONAL DIFFUSION EQUATION

TIWAPORN PINLAOR

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หัวข้อวิทยานิพนธ์	วิธีแอลโอดีและวิธีเอดีไอสำหรับแก้ปัญหาสมการการแพร่ในปริภูมิ 3 มิติ
นักศึกษา	นางสาวทิวาภรณ์ ปิ่นละออ
รหัสประจำตัว	41065308
ปริญญา	วิทยาศาสตรมหาบัณฑิต
สาขาวิชา	คณิตศาสตร์ประยุกต์
พ.ศ.	2545
อาจารย์ผู้ควบคุมวิทยานิพนธ์	รศ.ผ่องพรรณ รัตนธนาวันต์
อาจารย์ผู้ควบคุมวิทยานิพนธ์ร่วม	รศ.ดร.ปรีชา ยุพาพิน

บทคัดย่อ

วิธีผลต่างจำกัดเป็นวิธีเชิงตัวเลขที่นิยมใช้มาเป็นเวลานานในวิทยาศาสตร์และวิศวกรรมศาสตร์สาขาต่าง ๆ เนื่องจากสามารถนำไปแก้สมการในหลายรูปแบบได้โดยไม่ยาก

งานวิจัยนี้ศึกษาวิธีแอลโอดี (Locally One-Dimensional Method) และวิธีเอดีไอ (Alternating Direction Implicit Method) ซึ่งเป็นวิธีผลต่างจำกัดที่พัฒนาเพื่อให้มีความแม่นยำสูงขึ้นโดย บี.เจ.นอย และเค.เจ.เฮย์แมน ดำเนินงานวิจัยโดยประยุกต์วิธีผลต่างจำกัดดังกล่าวสำหรับใช้แก้ปัญหาสมการการแพร่ที่เปลี่ยนแปลงตามเวลาซึ่งมีสัมประสิทธิ์เป็นค่าคงที่ในปริภูมิ 3 มิติที่อยู่ในรูป

$$u_t = \alpha\left(u_{xx} + u_{yy} + u_{zz}\right), \qquad 0 \le x \le A, 0 \le y \le B, 0 \le z \le C, 0 \le t \le T$$

โดยทำการเปรียบเทียบผลเฉลยเชิงตัวเลขที่ได้กับผลเฉลยเชิงวิเคราะห์และหาความสัมพันธ์ของความคลาดเคลื่อนกับขนาดของกริด สรุปผลเชิงเปรียบเทียบคุณสมบัติของวิธีผลต่างจำกัดต่าง ๆ แล้วนำผลที่ได้ไปอธิบายปรากฏการณ์ทางด้านวิทยาศาสตร์ความร้อน

Thesis Title	LOD and ADI Methods for Solving Three-Dimensional Diffusion Equation
Student	Miss Tiwaporn Pinlaor
Student ID.	41065308
Degree	Master of Science
Programme	Applied Mathematics
Year	2002
Thesis Advisor	Assoc.Prof.Pongpan Rattanathanawan
Thesis Co-Advisor	Assoc.Prof.Dr.Preecha Yupapin

ABSTRACT

Finite Difference Methods are numerical methods, which have been widely used for a few decades in area of science and engineering because of the various kinds of equations can be solved without difficulty.

This research is the study of LOD (Locally One-Dimensional) and ADI (Alternating Direction Implicit) Methods which are finite difference methods developing by B.J. Noye and K.J. Hayman for higher accuracy. This work will be carried out using those finite difference methods with constant-coefficient in three-dimensional time dependent diffusion equation is expressed in this form

$$u_t = \alpha\left(u_{xx} + u_{yy} + u_{zz}\right), \qquad 0 \le x \le A, 0 \le y \le B, 0 \le z \le C, 0 \le t \le T .$$

The comparison of the numerical solutions, analytic solutions and conclusion, the comparative properties of those methods using these results in the area of thermal science are also discussed.

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Tiwaporn Pinlaor

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CHAPTER 1

INTRODUCTION

1.1 Statement and Significance of the Problems

In relation to physical science, diffusion can simply be defined as the process where the flow of energy or matter from a higher concentration to a lower concentration results in a homogeneous distribution. Although the definition of diffusion may seem complicated, the process and effects of diffusion are such that encompass many aspects of daily life. Diffusion is also a process, which occurs in various forms. The distribution of thermal energy through a hot cup of tea or the distribution of odoriferous molecules throughout a room resulting from an uncorked perfume bottle are examples of the process of diffusion. Other examples of the effects of diffusion are the conduction of heat through objects or the emission of thermal rays from a concrete wall or the sun. Although these examples of diffusion demonstrate a process, which is multifaceted, these different types of diffusion do follow similar laws and properties.

Since diffusion plays an important role in the physical and engineering sciences, our intention in this research is to focus on a three-dimensional diffusion equation. An emphasis will be placed on the qualitative mathematical concepts of existence, uniqueness, and continuity of solutions. An attempt will be made to offer perspectives to the relation between analytic and numerical methods as well as between qualitative methods and results.

Many practical diffusion equations lead to problems not conveniently solvable by classical methods, such as method of separation of variables. Thus many scientists are interested in numerical methods for solving these problems. Finite difference methods (FDMs) are numerical methods which have been widely used for a few decades in teaching, modeling in thermal science and molecular diffusion. In 1994, B.J. Noye and K.J. Hayman published a journal entitled "New LOD and ADI methods for the two-dimensional diffusion equation". In this Journal, Noye and Hayman developed the FDMs, which presented new LOD and ADI methods, which are splitting methods, to solve two-dimensional diffusion equations. The two-dimensional diffusion equations are expressed in the form of

$$u_t = \alpha\left(u_{xx} + u_{yy}\right), \qquad 0 \le x \le A,\ 0 \le y \le B,\ 0 \le t \le T. \qquad (1.1)$$

1.2 Objective of the Study

This research is the study of the FDMs developed by B.J. Noye and K.J. Hayman. These methods will then be expanded to apply to three-dimensional time-dependent diffusion equations subject to a constant coefficient which is expressed in the general form as

$$u_t = \alpha\left(u_{xx} + u_{yy} + u_{zz}\right),\ 0 < x < A,\ 0 < y < B,\ 0 < z < C,\ 0 < t \le T \qquad (1.2)$$

subject to initial condition

$$u(x, y, z, 0) = F(x, y, z), \qquad 0 \le x \le A,\ 0 \le y \le B,\ 0 \le z \le C \qquad (1.3)$$

and Dirichlet boundary conditions which are expressed in the following form

$$u(0, y, z, t) = G_1(y, z), \qquad 0 < y < B,\ 0 < z < C,\ 0 < t \le T \qquad (1.4)$$

$$u(A, y, z, t) = G_2(y, z), \qquad 0 < y < B,\ 0 < z < C,\ 0 < t \le T \qquad (1.5)$$

$$u(x, 0, z, t) = G_3(x, z), \qquad 0 < x < A,\ 0 < z < C,\ 0 < t \le T \qquad (1.6)$$

$$u(x, B, z, t) = G_4(x, z), \qquad 0 < x < A,\ 0 < z < C,\ 0 < t \le T \qquad (1.7)$$

$$u(x, y, 0, t) = G_5(x, y), \qquad 0 < x < A,\ 0 < y < B,\ 0 < t \le T \qquad (1.8)$$

$$u(x,y,C,t) = G_6(x,y), \quad 0 < x < A,\ 0 < y < B,\ 0 < t \leq T. \tag{1.9}$$

Where F and G_1 to G_6 are piecewise continuous functions and all auxiliary conditions in equations (1.3)-(1.9) are linear equations. For diffusion of molecules, the function $u(x,y,z,t)$ represents chemical concentration when α is a diffusion coefficient. In diffusion of heat or heat conduction, the function $u(x,y,z,t)$ represents temperature distribution varying in time when α is thermal diffusivity.

1.3 Scope of the Study

The aim of this study is to show that the partial differential equations (1.2)-(1.9) is a well posed problem, then we will show properties of the numerical methods, a relationship between error and grid spacing by plotting a graph. We will then make a conclusion and compare the properties of each method and then solve problems in diffusion effects.

Formulating a written thesis was based on the information presented here and involved the following procedures. In chapter 2, we provided literature reviews, which involved definitions and theorems, which were later used in chapter 3-4. Chapter 3 focused on presenting information which showed that the partial differential equations (1.2)-(1.9) is a well posed problem and an analytic solution of the problem is also solved. In chapter 4 we presented properties of finite difference equations (FDEs), of the LOD and ADI methods respectively. In chapter 5 we presented examples and applications of the problems and we showed the relations between analytic and numerical methods by plotting a graph and showing the relationship between error and grid spacing. Finally, we made a conclusion and suggestion in chapter 6.

1.4 Process of the Study

1. Demonstrating equations (1.2)-(1.9) is a well posed problem.
2. Showing properties of the numerical methods.

3. Finding numerical solutions of the problem that were studied and compare the solution with analytic solution.
4. Solving the diffusion problem in thermal science area.
5. Conclude and discuss the results.

1.5 Expected Results

1. Using the numerical methods to apply in finding numerical solutions of three-dimensional diffusion equations.
2. Using the numerical methods for discussion about diffusion effects in thermal science area, for example a discussion about brick.
3. A Guideline for mathematicians in the study of various kinds of partial differential equations.

CHAPTER 2

LITERATURE REVIEW

2.1 Definitions and Theorems

We start this section by giving basic definitions and notations.

R^n denotes n-dimensional Euclidean space then point $x \in R^n$ given by $x = (x_1, x_2, \ldots, x_n)^T$.

A domain $\Omega \subset R^n$ is a connected open subset.

$\overline{\Omega}$ denotes all limit points or closure of Ω .

The boundary $\partial\Omega$ of a domain Ω is the set of limit points of Ω which are not in Ω i.e. $\partial\Omega = \overline{\Omega} \setminus \Omega$ where " \ " denotes set subtraction.

The finite cylinder $\Psi = \Omega \times (0, T)$.

$\Gamma = \{ (x,t) \in \overline{\Psi} \ : x \in \partial\Omega \text{ or } t = 0 \}$ denotes parabolic boundary.

$C(\Psi) = \{ u / u$ is continuous on $\Psi \}$.

$C^k(\Omega)$ denotes the functions having all derivatives up to the order k continuous in Ω, for $k \in N$ where N denotes the natural number .

$C^{2s,s}(\Psi)$ denotes Banach Space, where the integer $s \geq 1$ denotes the set of functions $u(x,t)$ that are continuous in the finite cylinder, Ψ together with the derivatives $\dfrac{\partial^{\alpha_1+\alpha_2+\ldots+\alpha_n+\beta} u}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n} \partial t^{\beta}}$ for all (nonnegative integer) $\alpha_1, \alpha_2, \ldots, \alpha_n, \beta$ when $\alpha_1 + \alpha_2 + \ldots + \alpha_n + 2\beta \leq 2s$.

Next, we will interpret the proof of the existence for a diffusion equation by R.C. McOwen [1]. If Ω is a bounded domain in R^n, which we view as a physical body with α as a positive constant, then the diffusion equation

$$u_t = \alpha \nabla^2 u, \qquad x \in \Omega, \ t > 0 \tag{2.1}$$

governs the distribution or diffusion of heat or molecules, i.e., $u(x,t)$ represents the temperature or the concentration distribution at the point x and time t. We generally take $\alpha = 1$ in equation (2.1) since otherwise this may be achieved by re-scaling the time variable : $t \to \alpha t$ then we can write equation (2.1) in the following form

$$u_t \quad = \quad \nabla^2 u, \qquad\qquad x \in \Omega,\ \ t > 0 \tag{2.2}$$

subject to initial and homogeneous boundary conditions

$$u(x,0) \quad = \quad f(x), \qquad\quad x \in \overline{\Omega} \tag{2.3}$$

$$u(x,t) \quad = \quad 0, \qquad\qquad x \in \partial\Omega \tag{2.4}$$

where $\nabla^2 u = \dfrac{\partial^2 u}{\partial x_1^2} + \dfrac{\partial^2 u}{\partial x_2^2} + \ldots + \dfrac{\partial^2 u}{\partial x_n^2}$.

If we assume the initial temperature distribution $f(x)$ is in $C^2(\overline{\Omega})$ with $f(x) = 0$ on $\partial\Omega$, then we can write

$$f(x) \quad = \quad \sum_{n=1}^{\infty} a_n \phi_n(x) \tag{2.5}$$

where $a_n = \int_{\Omega} f(x)\phi_n(x)\,dx$. In (2.5), ϕ_n denotes the normalized eigenfunctions of the Laplacian on Ω with Dirichlet boundary conditions. The series in (2.5) is an expansion of the eigenfunctions. It converges absolutely and uniformly on $\overline{\Omega}$ by expansion theorem [Appendix A]. Let $u(x,t) \ = \ \sum_{n=1}^{\infty} u_n(t)\phi_n(x)$, and insert this expression in (2.2), we then pass derivatives through the summation, yield $u_n'(t) + \lambda_n u_n(t) \ = \ 0$, which has the general solution $u_n(t) \ = \ A_n e^{-\lambda_n t}$. At $t = 0$ we can find $u_n(0) = A_n$, so $u(x,0) = \sum_{n=1}^{\infty} A_n \phi_n(x)$ and a comparison with (2.5) shows $a_n = A_n$. Thus the solution of (2.2), (2.3) and (2.4) is given by

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-\lambda_n t}\phi_n(x) \tag{2.6}$$

where the a_n are given in (2.5). Notice that the series (2.6) converges absolutely and uniformly on $\overline{\Omega}\times[0,\infty)$ since the factor $e^{-\lambda_n t}$ only improves the convergence of (2.5); this justifies the interchange of differentiation and summation that we performed in the derivation. Combining $a_n = \int_{\Omega} f(x)\phi_n(x)\,dx$ and (2.6) together and interchanging the integration and summation, we obtain

$$u(x,t) = \int_{\Omega}\sum_{n=1}^{\infty} e^{-\lambda_n t}\phi_n(x)\phi_n(y)f(y)\,dy\ . \tag{2.7}$$

This means that if we formally define

$$K(x,y,t) = \sum_{n=1}^{\infty} e^{-\lambda_n t}\phi_n(x)\phi_n(y) \tag{2.8}$$

we can write the solution of (2.2)-(2.4) as an integral transformation of the initial condition

$$u(x,t) = \int_{\Omega} K(x,y,t)f(y)\,dy\,. \tag{2.9}$$

This completes the proof of the existence of the problem (2.2)-(2.4).

The following theorem will be used for showing that problem (1.2)-(1.9) has unique solution. This theorem also describes that the maximum value of $u(x,t)$ is on parabolic boundary, Γ .

Theorem 2.1 (Weak Maximum Principle) Let $u \in C^{2,1}(\Psi)\cap C(\overline{\Psi})$ satisfy $\nabla^2 u \geq u_t$ in Ψ. Then u achieves its maximum on parabolic boundary Γ of Ψ,

$$\max_{(x,t)\in\overline{\Psi}} u(x,t) = \max_{(x,t)\in\Gamma} u(x,t)\ . \tag{2.10}$$

Proof [1].

Next, consider the Laplace equation which is expressed as

$$\nabla^2 u = 0, \qquad x \in \Omega \tag{2.11}$$

with its boundary condition is denoted by

$$u(x) = \chi, \qquad x \in \partial\Omega \tag{2.12}$$

Definition 2.1 A function $u(x)$ is called the classical solution of problem (2.11)-(2.12), if $u(x) \in C^2(\Omega) \cap C(\overline{\Omega})$ and satisfies the problem (2.11)-(2.12).

Lemma 2.1 If $\partial\Omega \in C^2$ and $\chi \in C(\partial\,\Omega)$, then the problem (2.11)-(2.12) has a classical solution.

Proof [2].

In studying partial differential equations, it is important to discuss the qualitative properties, which are existence, uniqueness, and continuos of solution. In the same way, for the study of difference solution, stability of the difference schemes are important. Furthermore, we can study the accuracy of a FDE by considering order of accuracy. R.F. Warming and B.J. Hyett [3] developed a technique helping consider the order of the FDE with modified differential equation (MDE). We then can consider order of the FDE by applying this technique. For considering stability we will use von Neumann's method (Fourier series method).

2.2 Numerical Methods

The splitting method is widely used for solving multi-dimensional problems. In this research, new splitting methods [4] are extended in order to solve the problem (1.2)-(1.9). First, we will discuss the LOD method, which has an explicit scheme. We then will consider the ADI method, which has an implicit scheme.

We let the Notation $U_{i,j}^{n}$ denotes an approximation of function $u(x,y,t)$ by using a FDM to approximate its values at grid point $(i\Delta x, j\Delta y, n\Delta t)$. The grid spacing Δx, Δy and Δt are computed by $\Delta x = A/I$, $\Delta y = B/J$, $\Delta t = T/N$ where I, J and N are integers. Thus we can use the notation (i,j,n) to denote grid point $(i\Delta x, j\Delta y, n\Delta t)$ for $i = 0,1,2,\ldots,I$, $j = 0,1,2,\ldots,J$ and $n = 0,1,2,\ldots,N$.

2.2.1 LOD Method

In order to solve the equation (1.1) by using LOD, we split (1.1) into one-dimensional diffusion equations,

$$\frac{1}{2}u_t = \alpha u_{xx} \qquad (2.13)$$

$$\frac{1}{2}u_t = \alpha u_{yy}. \qquad (2.14)$$

Each of these equations is then solved over half of the time step used for the complete two-dimensional equation, the formula for use in the x-sweep of the first half time step to solve (2.13) when $i = 2,3,\ldots,I-2$ is

$$\begin{aligned} U_{i,j}^{n+1/2} &= \frac{s_x}{12}(6s_x - 1)\left(U_{i-2,j}^{n} + U_{i+2,j}^{n}\right) \\ &\quad + \frac{2s_x}{3}(2 - 3s_x)\left(U_{i-1,j}^{n} + U_{i+1,j}^{n}\right) + \frac{1}{2}\left(2 - 5s_x + 6s_x^2\right)U_{i,j}^{n} \end{aligned} \qquad (2.15)$$

for each $j = 0,1,\ldots,J$.

When computing values of $U_{i,j}^{n+1}$ from the values of $U_{i,j}^{n+1/2}$ in the y-sweep used in the second stage, the formula used with $j = 2,3,\ldots,J-2$ for each $i = 1,2,\ldots,I-1$ is

$$\begin{aligned} U_{i,j}^{n+1} &= \frac{s_y}{12}(6s_y - 1)\left(U_{i,j-2}^{n+1/2} + U_{i,j+2}^{n+1/2}\right) \\ &\quad + \frac{2s_y}{3}(2 - 3s_y)\left(U_{i,j-1}^{n+1/2} + U_{i,j+1}^{n+1/2}\right) + \frac{1}{2}\left(2 - 5s_y + 6s_y^2\right)U_{i,j}^{n+1/2}. \end{aligned} \qquad (2.16)$$

This new method has fourth order and stable, in von Neumann sense, for

$$0 < s_x \le 2/3 \qquad \text{and} \qquad 0 < s_y \le 2/3 \tag{2.17}$$

when $s_x = \alpha\,\Delta t/(\Delta x)^2$ and $s_y = \alpha\,\Delta t/(\Delta y)^2$.

2.2.2 ADI Method

The difficulty with the use of the LOD method is that the restrictions on Δt require inordinately many rows of calculations. One then looks for a method in which Δt can be made larger without loss of stability. B.J. Noye and K.J. Hayman developed a new ADI method in 1994 [4], this new method is fourth-order accuracy. In order to solve (1.1) by new ADI method, the formula in y-sweep is

$$\begin{aligned}
&(6s_y - 1)U_{i,j-1}^{n+1} - 4(1+3s_y)U_{i,j}^{n+1} + (6s_y - 1)U_{i,j+1}^{n+1} \\
&= -s_x\left(U_{i-1,j-1}^{n} + U_{i-1,j+1}^{n} + U_{i+1,j-1}^{n} + U_{i+1,j+1}^{n}\right) \\
&\quad - 4s_x\left(U_{i-1,j}^{n} + U_{i+1,j}^{n}\right) + (2s_x - 1)\left(U_{i,j-1}^{n} + 4U_{i,j}^{n} + U_{i,j+1}^{n}\right)
\end{aligned} \tag{2.18}$$

and for x-sweep

$$\begin{aligned}
&(6s_x - 1)U_{i-1,j}^{n+2} - 4(1+3s_x)U_{i,j}^{n+2} + (6s_x - 1)U_{i+1,j}^{n+2} \\
&= -s_y\left(U_{i-1,j-1}^{n+1} + U_{i+1,j-1}^{n+1} + U_{i-1,j+1}^{n+1} + U_{i+1,j+1}^{n+1}\right) \\
&\quad - 4s_y\left(U_{i,j-1}^{n+1} + U_{i,j+1}^{n+1}\right) + (2s_y - 1)\left(U_{i-1,j}^{n+1} + 4U_{i,j}^{n+1} + U_{i+1,j}^{n+1}\right).
\end{aligned} \tag{2.19}$$

In order to solve equation (1.1), we first use the y-sweep equation and we then use the x-sweep equation, respectively. The double sweep of these equations is unconditionally von Neumann stable. Thus this method is solvable for all values of $s_x > 0$ and $s_y > 0$.

CHAPTER 3

THE QUALITATIVE PROPERTIES AND ANALYTIC SOLUTION OF THE THREE-DIMENSIONAL DIFFUSION EQUATION

In this chapter we will discuss the qualitative properties which are existence, uniqueness, continuity and analytic solution for the three-dimensional time-dependent diffusion equation, respectively.

3.1 Existence

From what we discussed in chapter 2, the problem which we study, can be expressed as

$$u_t = \left(u_{xx} + u_{yy} + u_{zz}\right), \quad 0 < x < A,\ 0 < y < B,\ 0 < z < C,\ \ 0 < t \le T \quad (3.1)$$

its initial condition is given by

$$u(x, y, z, 0) = F(x, y, z), \qquad 0 \le x \le A,\ 0 \le y \le B,\ 0 \le z \le C \qquad (3.2)$$

and time-independent boundary conditions are

$$u(0, y, z, t) = G_1(y, z), \qquad 0 < y < B,\ 0 < z < C,\ \ 0 < t \le T \qquad (3.3)$$

$$u(A, y, z, t) = G_2(y, z), \qquad 0 < y < B,\ 0 < z < C,\ \ 0 < t \le T \qquad (3.4)$$

$$u(x, 0, z, t) = G_3(x, z), \qquad 0 < x < A,\ 0 < z < C,\ \ 0 < t \le T \qquad (3.5)$$

$$u(x,B,z,t) = G_4(x,z), \quad 0<x<A,\ 0<z<C,\ 0<t\le T \tag{3.6}$$

$$u(x,y,0,t) = G_5(x,y), \quad 0<x<A,\ 0<y<B,\ 0<t\le T \tag{3.7}$$

$$u(x,y,C,t) = G_6(x,y), \quad 0<x<A,\ 0<y<B,\ 0<t\le T. \tag{3.8}$$

The equation (3.1) is accompanied by seven non-homogeneous auxiliary conditions (3.2)-(3.8). By the linearity of the equation (3.1), we then can decompose by letting

$$u(x,y,z,t) = u_0(x,y,z,t) + u_\infty(x,y,z) \tag{3.9}$$

here $u_\infty(x,y,z)$ is a time independent solution of the equation, which can be expressed in the form

$$\nabla^2 u_\infty(x,y,z) = 0 \tag{3.10}$$

and satisfies the boundary conditions on the edges

$$u_\infty(0,y,z) = G_1(y,z), \quad 0<y<B,\ 0<z<C \tag{3.11}$$

$$u_\infty(A,y,z) = G_2(y,z), \quad 0<y<B,\ 0<z<C \tag{3.12}$$

$$u_\infty(x,0,z) = G_3(x,z), \quad 0<x<A,\ 0<z<C \tag{3.13}$$

$$u_\infty(x,B,z) = G_4(x,z), \quad 0<x<A,\ 0<z<C \tag{3.14}$$

$$u_\infty(x,y,0) = G_5(x,y), \quad 0<x<A,\ 0<y<B \tag{3.15}$$

$$u_\infty(x,y,C) = G_6(x,y), \quad 0<x<A,\ 0<y<B. \tag{3.16}$$

When $\nabla^2 u_\infty$ denotes the Laplacian of u_∞, which equal $\frac{\partial^2 u_\infty}{\partial x^2}+\frac{\partial^2 u_\infty}{\partial y^2}+\frac{\partial^2 u_\infty}{\partial z^2}$, and $u_0(x,y,z,t)$ satisfies the original diffusion equation (3.1), with homogeneous boundary conditions

$$u_0(x,y,z,t) \;=\; 0, \qquad 0 \le t \le T \qquad \text{for all six edges} \tag{3.17}$$

and its initial condition obtained by combining (3.2) and (3.9) yields

$$u_0(x,y,z,0) \;=\; F(x,y,z) - u_\infty(x,y,z)\;. \tag{3.18}$$

Then we claim that the following sum solves the original problem (3.1)-(3.8)

$$u(x,y,z,t) \;=\; u_0(x,y,z,t) + u_\infty(x,y,z) \tag{3.19}$$

We may now turn to consider $u_0(x,y,z,t)+u_\infty(x,y,z)$ on the edge which $x=0$

$$u(0,y,z,t) \;=\; 0+G_1 \;=\; G_1 \tag{3.20}$$

on the edge $x=A$

$$u(A,y,z,t) \;=\; 0+G_2 \;=\; G_2 \tag{3.21}$$

on the edge $y=0$

$$u(x,0,z,t) \;=\; 0+G_3 \;=\; G_3 \tag{3.22}$$

on the edge $y=B$

$$u(x,B,z,t) \;=\; 0+G_4 \;=\; G_4 \tag{3.23}$$

on the edge $z=0$

$$u(x,y,0,t) \;=\; 0+G_5 \;=\; G_5 \tag{3.24}$$

on the edge $z = C$

$$u(x, y, C, t) = 0 + G_6 = G_6 \tag{3.25}$$

and inside the cube

$$\begin{aligned} \nabla^2 u(x, y, z, t) &= \nabla^2 u_0(x, y, z, t) + \nabla^2 u_\infty(x, y, z) \\ &= u_t + 0 \end{aligned} \tag{3.26}$$

In order to show existence of $u_0(x,y,z,t)$ and $u_\infty(x,y,z)$, we first consider the problem (3.10)-(3.16). This problem satisfies the Laplace's equation (2.11)-(2.12), when $\Omega \in R^3$. Thus by Lemma 2.1, we obtained the problem (3.10)-(3.16) has a classical solution. Again from chapter 2, since the problem (3.1), (3.17)-(3.18) satisfies the problem (2.2)-(2.4), there exists $u_0(x, y, z, t)$ which could be expressed as (2.9). Hence there exists $u(x,y,z,t)$ which equals $u_0(x,y,z,t) + u_\infty(x,y,z)$. Therefore the sum $u_0(x, y, z, t) + u_\infty(x, y, z)$ solves equations (3.1) through (3.8).

3.2 Uniqueness

Let $u, v \in C^{2,1}(\Psi) \cap C(\overline{\Psi})$ are two non-identical solutions of problem (3.1)-(3.8) and $u^*(x, y, z, t) = u(x, y, z, t) - v(x, y, z, t)$, we then substitute $u^*(x, y, z, t)$ in this problem to obtain

$$u^*_t = \nabla^2 u^*, \qquad (x, y, z) \in \Omega, \quad t > 0 \tag{3.27}$$

$$u^*(x, y, z, 0) = 0, \qquad (x, y, z) \in \overline{\Omega} \tag{3.28}$$

$$u^*(x, y, z, t) = 0, \qquad (x, y, z) \in \partial\Omega \tag{3.29}$$

when bounded domain $\Omega = [0, A] \times [0, B] \times [0, C]$. Applying equation (2.10) with $-u^*(x, y, z, t)$ and $u^*(x, y, z, t)$, we then obtain

$$\max_{(x,y,z,t)\in\overline{\Psi}} u^* = \max_{(x,y,z,t)\in\overline{\Psi}} -u^* . \quad (3.30)$$

Hence $u^* \equiv 0$ in $\overline{\Psi}$ thus $u \equiv v$.

3.3 Stability or Continuous Dependence

Let $u(x,y,z,t)$ be the unique solution to the model (3.1)-(3.8) in domain $\Omega \subset R^3$ and $v(x,y,z,t)$ be the unique solution to the following model

$$v_t = \nabla^2 v \quad (3.31)$$

subject to initial condition

$$v(x,y,z,0) = F(x,y,z) + \Delta_1(x,y,z) \quad (3.32)$$

and boundary conditions

$$v(0,y,z,t) = G_1(y,z) + \Delta_2(y,z) \quad (3.33)$$

$$v(A,y,z,t) = G_2(y,z) + \Delta_3(y,z) \quad (3.34)$$

$$v(x,0,z,t) = G_3(x,z) + \Delta_4(x,z) \quad (3.35)$$

$$v(x,0,z,t) = G_4(x,z) + \Delta_5(x,z) \quad (3.36)$$

$$v(x,y,0,t) = G_5(x,y) + \Delta_6(x,y) \quad (3.37)$$

$$v(x,y,C,t) = G_6(x,y) + \Delta_7(x,y). \quad (3.38)$$

When $\Delta_i \in C^1(\overline{\Psi})$ *in* $\overline{\Omega}$ for $i = 1,2,3,\ldots,7$ and for some $\varepsilon > 0$, $|\Delta_i| \le \varepsilon$. We replace $u^*(x,y,z,t) = v(x,y,z,t) - u(x,y,z,t)$ in equations (3.1)-(3.8), we then obtain

$$u^*_t = \nabla^2 u^* \quad (3.39)$$

subject to initial condition

$$u^*(x,y,z,0) \;=\; \Delta_1(x,y,z) \tag{3.40}$$

and boundary conditions

$$u^*(0,y,z,t) \;=\; \Delta_2(y,z) \tag{3.41}$$

$$u^*(A,y,z,t) \;=\; \Delta_3(y,z) \tag{3.42}$$

$$u^*(x,0,z,t) \;=\; \Delta_4(x,z) \tag{3.43}$$

$$u^*(x,B,z,t) \;=\; \Delta_5(x,z) \tag{3.44}$$

$$u^*(x,y,0,t) \;=\; \Delta_6(x,y) \tag{3.45}$$

$$u^*(x,y,C,t) \;=\; \Delta_7(x,y)\,. \tag{3.46}$$

Similarly, setting $-u^*(x,y,z,t) = u(x,y,z,t) - v(x,y,z,t)$ and replacing into equations (3.1)-(3.8). According to theorem 2.1, $u^*(x,y,z,t)$ is bounded by the maximum and minimum values of Δ_i (for some i). Thus

$$\left|u^*(x,y,z,t)\right| \le |\Delta_i| \le \varepsilon \qquad \text{or} \qquad |v-u| \;\le\; \varepsilon\,. \tag{3.47}$$

This shows a small change, ε, in the boundary and/or initial values produces an equally small change in the solution. This proves that $u(x,y,z,t)$ is continuous with respect to small changes in data functions (initial and/or boundary conditions) that the change in $u(x,y,z,t)$ is the same as the change in those functions.

3.4 Analytic Solution

In this part, we will find analytic solution by using the methods of separation of variables. In the same manner as section 3.1, using linearity property with the problem (1.2)-(1.9), setting

$$u(x,y,z,t) = u_0(x,y,z,t) + u_\infty(x,y,z) \tag{3.48}$$

when $u_\infty(x,y,z)$ is a solution of the diffusion equation in problem1, which is expressed in the form

Problem 1 $\quad \alpha \nabla^2 u_\infty(x,y,z) = 0 \qquad (3.49)$

which satisfies the boundary conditions on the edges

$$u_\infty(0,y,z) = G_1(y,z), \quad 0<y<B, 0<z<C \tag{3.50}$$

$$u_\infty(A,y,z) = G_2(y,z), \quad 0<y<B, 0<z<C \tag{3.51}$$

$$u_\infty(x,0,z) = G_3(x,z), \quad 0<x<A, 0<z<C \tag{3.52}$$

$$u_\infty(x,B,z) = G_4(x,z), \quad 0<x<A, 0<z<C \tag{3.53}$$

$$u_\infty(x,y,0) = G_5(x,y), \quad 0<x<A, 0<y<B \tag{3.54}$$

$$u_\infty(x,y,C) = G_6(x,y), \quad 0<x<A, 0<y<B\,. \tag{3.55}$$

and $u_0(x,y,z,t)$ satisfies the following problem.

Problem 2 $\quad u_t = \alpha \nabla^2 u(x,y,z,t) \qquad (3.56)$

with homogeneous boundary conditions

$$u_0(x,y,z,t) = 0, \qquad 0 < t \le T \quad \text{for all six edges} \tag{3.57}$$

which an initial condition

$$u_0(x,y,z,0) = F(x,y,z) - u_\infty(x,y,z) \tag{3.58}$$

Since the problem (3.49)-(3.55) has six non-homogeneous boundary conditions, again we takes advantage of linearity of problem (3.49), by dividing the problem into the following six problems.

Problem 1.1

$$\alpha \nabla^2 u_1(x,y,z) = 0 \quad \text{inside the cube} \tag{3.59}$$

$$u_1(0,y,z) = G_1(y,z) \quad \text{on the edge } x = 0 \tag{3.60}$$

$$u_1(x,y,z) = 0 \quad \text{on the other five edges} \tag{3.61}$$

Problem 1.2

$$\alpha \nabla^2 u_2(x,y,z) = 0 \quad \text{inside the cube} \tag{3.62}$$

$$u_2(A,y,z) = G_2(y,z) \quad \text{on the edge } x = A \tag{3.63}$$

$$u_2(x,y,z) = 0 \quad \text{on the other five edges} \tag{3.64}$$

Problem 1.3

$$\alpha \nabla^2 u_3(x,y,z) = 0 \quad \text{inside the cube} \tag{3.65}$$

$$u_3(x,0,z) = G_3(x,z) \quad \text{on the edge } y = 0 \tag{3.66}$$

$$u_3(x,y,z) = 0 \quad \text{on the other five edges} \tag{3.67}$$

Problem 1.4

$$\alpha \nabla^2 u_4(x,y,z) = 0 \quad \text{inside the cube} \tag{3.68}$$

$$u_4(x,B,z) = G_4(x,z) \quad \text{on the edge } y = B \tag{3.69}$$

$$u_4(x,y,z) = 0 \quad \text{on the other five edges} \tag{3.70}$$

Problem 1.5 $\alpha \nabla^2 u_5(x, y, z) = 0$ inside the cube (3.71)

$u_5(x, y, 0) = G_5(x, y)$ on the edge $z = 0$ (3.72)

$u_5(x, y, z) = 0$ on the other five edges (3.73)

Problem 1.6 $\alpha \nabla^2 u_6(x, y, z) = 0$ inside the cube (3.74)

$u_6(x, y, C) = G_6(x, y)$ on the edge $z = C$ (3.75)

$u_6(x, y, z) = 0$ on the other five edges (3.76)

Here we only show the work for finding a solution of Problem 1.1 by using separation of variables method.

Solution of Problem 1.1 The equation (3.59) is a three-dimensional Laplace's equation which can be expressed as a product of factors, each depending as a single variable

$$u_1(x, y, z) = X(x)Y(y)Z(z) \tag{3.77}$$

If we insert equation (3.77) into equation (3.59) we can manipulate equation (3.59) into a form where only one variable occurs on each side of the equation

$$\begin{aligned} \alpha\nabla^2 u_1(x, y, z) &= 0 \\ &= \alpha \frac{\partial^2}{\partial x^2}(X(x)Y(y)Z(z)) + \alpha \frac{\partial^2}{\partial y^2}(X(x)Y(y)Z(z)) \\ &\quad + \alpha \frac{\partial^2}{\partial z^2}(X(x)Y(y)Z(z)) \\ &= \alpha(X''(x)Y(y)Z(z) + X(x)Y''(y)Z(z) + X(x)Y(y)Z''(z)) \end{aligned} \tag{3.78}$$

thus

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} = 0. \tag{3.79}$$

Using orthogonality in the two homogeneous directions, we set the y-dependent term of equation (3.79) equal to $-\lambda^2$ and the z-dependent term to $-\beta^2$, we obtained

$$X'' - \left(\lambda^2 + \beta^2\right)X = 0 \tag{3.80}$$

$$Y'' + \lambda^2 Y = 0 \tag{3.81}$$

$$Z'' + \beta^2 Z = 0. \tag{3.82}$$

Next, we will solve the above ordinary differential equations. We first consider the equation (3.81), its general solution is

$$Y(y) = A_3 \sin(\lambda y) + A_4 \cos(\lambda y) \tag{3.83}$$

with its boundary conditions are $Y(0) = Y(B) = 0$, now we apply the boundary condition $Y(0) = 0$ implies that $A_4 = 0$. The cosine term vanishes in the equation (3.83), thus $Y(y) = A_3 \sin(\lambda y)$. Only the boundary condition at $y = B$ has not been satisfied. $Y(B) = 0$ implies that

$$Y(B) = 0 = A_3 \sin(\lambda B). \tag{3.84}$$

Either $A_3 = 0$ or $\sin(\lambda B) = 0$. If $A_3 = 0$, then $Y(y) \equiv 0$. This is the trivial solution but we need λ that have nontrivial solutions. Thus, the eigenvalues λ must satisfy

$$\sin(\lambda B) = 0. \tag{3.85}$$

Thus λB must be zero of the sine function. Hence $\lambda B = m\pi$, λB must equal an integral multiple of π, where m is a positive integer. The eigenvalues λ are

$$\lambda_m = \frac{m\pi}{B} \quad \text{for } m = 1,2,3\ldots \tag{3.86}$$

The eigenfunction corresponding to this eigenvalue is

$$Y(y) = A_3 \sin\left(\frac{m\pi y}{B}\right) \tag{3.87}$$

where A_3 is an multiplication constant. Similarly, solving equations (3.80) and (3.82) and substituting the solution into the expression (3.77) to obtain

$$u_1(x,y,z) = \left\{A_1 \sinh\left(\left(\sqrt{\lambda^2+\beta^2}\right)(x-A)\right) + A_2 \cosh\left(\left(\sqrt{\lambda^2+\beta^2}\right)(x-A)\right)\right\} \times \left[A_3 \sin(\lambda y) + A_4 \cos(\lambda y)\right]\left[A_5 \sin(\beta z) + A_6 \cos(\beta z)\right]. \tag{3.88}$$

To find the constants A_1, A_2, A_5, A_6 and β we may now apply the boundary conditions (3.61) yield

$$A_2 = A_6 = 0 \tag{3.89}$$

$$\beta_n = \frac{n\pi}{C} \quad \text{for} \quad n = 1,2,3\ldots \tag{3.90}$$

Combining equations (3.87)-(3.90), we get

$$u_{1,mn} = H_{mn} \sinh\left(\pi\sqrt{\left(\frac{m}{B}\right)^2 + \left(\frac{n}{C}\right)^2}(x-A)\right) \times \sin\frac{m\pi y}{B} \sin\frac{n\pi z}{C}. \tag{3.91}$$

The constant H_{mn} is obtained by combining the constants A_1, A_3 and A_5. The subscript m,n accounts for all values of $m = 1,2,3,\ldots$ and $n = 1,2,3,\ldots$. The general solution is the linear combination of all these solutions (Principle of Superposition, Appendix A). Based on the above, we obtained the expression for the general solution for the diffusion is

$$u_1 = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} H_{mn}\, sinh\left(\pi\sqrt{\left(\frac{m}{B}\right)^2+\left(\frac{n}{C}\right)^2}\,(x-A)\right) sin\frac{m\pi\, y}{B}\, sin\frac{n\pi\, z}{C}. \qquad (3.92)$$

Next , we will apply the boundary condition (3.60), $u_1(0,y,z) = G_1(y,z)$,

$$G_1(y,z) = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} H_{mn}\, sinh\left(\pi\sqrt{\left(\frac{m}{B}\right)^2+\left(\frac{n}{C}\right)^2}\,(-A)\right) sin\frac{m\pi\, y}{B}\, sin\frac{n\pi\, z}{C}. \qquad (3.93)$$

We notice that the quantity $\sum_{m=1}^{\infty} H_{mn}\, sinh\left(\pi\sqrt{\left(\frac{m}{B}\right)^2+\left(\frac{n}{C}\right)^2}\,(-A)\right) sin\frac{m\pi\, y}{B}$ depends only on index n (after the summation is carried out), we then let

$$I_n(y) = \sum_{m=1}^{\infty} H_{mn}\, sinh\left(\pi\sqrt{\left(\frac{m}{B}\right)^2+\left(\frac{n}{C}\right)^2}\,(-A)\right) sin\frac{m\pi\, y}{B} \qquad (3.94)$$

thus equation (3.93) becomes

$$G_1(y,z) = \sum_{n=1}^{\infty} I_n(y)\, sin\left(\frac{n\pi\, z}{C}\right). \qquad (3.95)$$

Utilizing the orthogonality property of $sin(n\pi/C)z$ in equation (3.95), we multiply both side of the equation (3.95) by $sin(p\pi/C)z$, we obtained

$$\int_0^C G_1(y,z)\, sin\left(\frac{p\,\pi\, z}{C}\right) dz = \sum_{n=1}^{\infty} I_n(y) \int_0^C sin\left(\frac{p\pi\, z}{C}\right) sin\left(\frac{n\pi\, z}{C}\right)\, dz$$

$$= I_n(y)\frac{C}{2} \qquad (3.96)$$

thus

$$I_n(y) = \frac{2}{C}\int_0^C G_1(y,z)\, sin\left(\frac{n\pi}{C}z\right)\, dz \qquad (3.97)$$

Using definition of $I_n(y)$ from equation (3.94) and substituting it in equation (3.97), we again apply the orthogonality property of the function $sin(m\pi/B)y$ yields

$$H_{mn} = \frac{4}{BC} \frac{\int_0^B \left[\int_0^C G_1(y,z) sin\left(\frac{n\pi\, z}{C}\right) dz \right] sin\left(\frac{m\pi\, y}{B}\right) dy}{sinh\left(\pi(-A)\sqrt{\left(\frac{m}{B}\right)^2 + \left(\frac{n}{C}\right)^2}\right)}. \tag{3.98}$$

The solution of Problem 1.1, $u_1(x,y,z)$ is completed, by combining equation (3.92) and (3.98). The result is expressed in the following form

$$u_1(x,y,z) = \frac{4}{BC}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^B \left[\int_0^C G_1\, sin\left(\frac{n\pi z}{C}\right) dz \right] sin\left(\frac{m\pi y}{B}\right) dy}{sinh\left(\pi(-A)\sqrt{\left(\frac{m}{B}\right)^2 + \left(\frac{n}{C}\right)^2}\right)}\right\}$$
$$\times\, sinh\left(\pi\sqrt{\left(\frac{m}{B}\right)^2 + \left(\frac{n}{C}\right)^2}\,(x-A)\right) sin\left(\frac{m\pi y}{B}\right) sin\left(\frac{n\pi z}{C}\right). \tag{3.99}$$

Similarly, by using separation of variable method to solve Problem 1.2 to Problem 1.6, we obtained

$$u_2(x,y,z) = \frac{4}{BC}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^B \left[\int_0^C G_2\, sin\left(\frac{n\pi\, z}{C}\right) dz \right] sin\left(\frac{m\pi\, y}{B}\right) dy}{sinh\left(\pi\, A\sqrt{\left(\frac{m}{B}\right)^2 + \left(\frac{n}{C}\right)^2}\right)}\right\}$$
$$\times\, sin\left(\frac{m\pi\, y}{B}\right) sin\left(\frac{n\pi\, z}{C}\right) sinh\left(\pi\sqrt{\left(\frac{m}{B}\right)^2 + \left(\frac{n}{C}\right)^2}\; x\right) \tag{3.100}$$

$$u_3(x,y,z)=\frac{4}{AC}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^A\left[\int_0^C G_3\,sin\left(\frac{n\pi\,z}{C}\right)dz\right]sin\left(\frac{m\pi\,x}{A}\right)dx}{sinh\left(\pi(-B)\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{C}\right)^2}\right)}\right\}$$

$$\times\,sin\left(\frac{m\pi\,x}{A}\right)sin\left(\frac{n\pi\,z}{C}\right)sinh\left(\pi(y-B)\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{C}\right)^2}\right)\qquad(3.101)$$

$$u_4(x,y,z)=\frac{4}{AC}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^A\left[\int_0^C G_4\,sin\left(\frac{n\pi\,z}{C}\right)dz\right]sin\left(\frac{m\pi x}{A}\right)dx}{sinh\left(\pi\,B\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{C}\right)^2}\right)}\right\}$$

$$\times\,sin\left(\frac{m\pi\,x}{A}\right)sin\left(\frac{n\pi\,z}{C}\right)sinh\left(\pi\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{C}\right)^2}\;y\right)\qquad(3.102)$$

$$u_5(x,y,z)=\frac{4}{AB}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^A\left[\int_0^B G_5\,sin\left(\frac{n\pi y}{B}\right)dy\right]sin\left(\frac{m\pi x}{A}\right)dx}{sinh\left(\pi(-C)\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{B}\right)^2}\right)}\right\}$$

$$\times\,sin\left(\frac{m\pi x}{A}\right)sin\left(\frac{n\pi y}{B}\right)sinh\left(\pi(z-C)\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{B}\right)^2}\right)\qquad(3.103)$$

$$u_6(x,y,z)=\frac{4}{AB}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^A\left[\int_0^B G_6\,sin\left(\frac{n\pi y}{B}\right)dy\right]sin\left(\frac{m\pi x}{A}\right)dx}{sinh\left(\pi C\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{B}\right)^2}\right)}\right\}$$

$$\times\,sin\left(\frac{m\pi x}{A}\right)sin\left(\frac{n\pi y}{B}\right)sinh\left(\pi\sqrt{\left(\frac{m}{A}\right)^2+\left(\frac{n}{B}\right)^2}\;z\right)\qquad(3.104)$$

In order to find $u_0(x,y,z,t)$, using the same procedure as finding $u_1(x,y,z)$, to obtain

$$u_0(x,y,z,t) = \frac{8}{ABC}\sum_{p=1}^{\infty}\sum_{q=1}^{\infty}\sum_{r=1}^{\infty}\left\{\int_0^A\left\langle\int_0^B\left[\int_0^C u_0(x,y,z,0)\,sin\left(\frac{r\pi z}{C}\right)dz\right]sin\left(\frac{q\pi y}{B}\right)dy\right\rangle sin\left(\frac{p\pi x}{A}\right)dx\right\}$$
$$\times\, sin\left(\frac{p\pi x}{A}\right)sin\left(\frac{q\pi y}{B}\right)sin\left(\frac{r\pi z}{C}\right)exp\left[-\alpha\pi^2\left(\frac{p^2}{A^2}+\frac{q^2}{B^2}+\frac{r^2}{C^2}\right)t\right]. \quad (3.105)$$

When $u_0(x,y,z,0) = F(x,y,z) - u_\infty(x,y,z)$ (Appendix C).

CHAPTER 4

NUMERICAL METHODS FOR THE THREE-DIMENSIONAL DIFFUSION EQUATION

In principle, we can extend the numerical methods in chapter 2 to higher space dimensions. We then extend the LOD method in section 4.1 and the ADI Method in section 4.2, respectively. We also discuss stability in von Neumann sense of both methods.

4.1 The LOD Method

In order to solve the equation (1.2) by using new LOD method we split this equation into three one-dimensional heat equations,

$$\frac{1}{3}\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{4.1}$$

$$\frac{1}{3}\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial y^2} \tag{4.2}$$

$$\frac{1}{3}\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial z^2}. \tag{4.3}$$

Each of these equations is then solved one third of the time step used for the complete three-dimensional equation. First of all we introduce some basic notations. We let the Notation $U_{i,j,k}^n$ denote an approximation of function $u(x,y,z,t)$ by using FDM to approximate its values at grid point $(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$. The grid spacing $\Delta x,\ \Delta y, \Delta z$, and Δt are computed by $\Delta x = A/I$, $\Delta y = B/J$, $\Delta z = C/K$, $\Delta t = T/N$ where I, J, K and N are integers. Thus we can use the notation (i,j,k,n) to denote grid point $(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$ for $i = 0,1,2,\ldots,I$, $j = 0,1,2,\ldots,J$, $k = 0,1,2,\ldots,K$ and $n = 0,1,2,\ldots,N$.

Next, we shall now show the formula used in solving equation (4.1) where $i = 2,3,4\ldots,I-2$ is

$$U_{i,j,k}^{n+1/3} = \frac{s_x}{12}(6s_x - 1)\left(U_{i-2,j,k}^{n} + U_{i+2,j,k}^{n}\right) + \frac{2s_x}{3}(2 - 3s_x)\left(U_{i-1,j,k}^{n} + U_{i+1,j,k}^{n}\right) + \frac{1}{2}\left(2 - 5s_x + 6s_x^2\right)U_{i,j,k}^{n} \quad (4.4)$$

for all $j = 0,1,2,\ldots,J$ and $k = 0,1,2,\ldots,K$. The problem in finding values of $U_{1,j,k}^{n+1/3}$ which can not be derived by using (4.4) can be overcome by using a re-arrangement of the unconditionally stable inverted version of the equation (4.4), which is obtained by setting Δt for $-\Delta t$ in (4.4). Putting $i = 3$ and re-arranging gives

$$U_{1,j,k}^{n+1/3} = \frac{8(2+3s_x)}{(6s_x+1)}\left(U_{2,j,k}^{n+1/3} + U_{4,j,k}^{n+1/3}\right) - \frac{6\left(2+5s_x+6s_x^2\right)}{s_x(6s_x+1)}U_{3,j,k}^{n+1/3} - U_{5,j,k}^{n+1/3} + \frac{12}{s_x(6s_x+1)}U_{3,j,k}^{n}. \quad (4.5)$$

This gives values of $U_{1,j,k}^{n+1/3}$ for all $j = 0,1,2,\ldots,J$ and $k = 0,1,2,\ldots,K$, because all the values on its right hand side are known. The values of $U_{I-1,j,k}^{n+1/3}$ may be calculated using a similar formula obtained by replacing Δt by $-\Delta t$ and setting $i = I-3$ in the equation (4.4) to obtain

$$U_{I-1,j,k}^{n+1/3} = \frac{8(2+3s_x)}{(6s_x+1)}\left(U_{I-2,j,k}^{n+1/3} + U_{I-4,j,k}^{n+1/3}\right) - \frac{6\left(2+5s_x+6s_x^2\right)}{s_x(6s_x+1)}U_{I-3,j,k}^{n+1/3} - U_{I-5,j,k}^{n+1/3} + \frac{12}{s_x(6s_x+1)}U_{I-3,j,k}^{n} \quad (4.6)$$

for all $j = 0,1,2,\ldots,J$ and $k = 0,1,2,\ldots,K$. Similarly, for computing values of $U_{i,j,k}^{n+2/3}$ from the values of $U_{i,j,k}^{n+1/3}$ in the y-sweep used in the second stage, the formula used with $j = 2,3,4,\ldots,J-2$ for each $i = 1,2,\ldots,I-1$ and $k = 1,2,\ldots,K-1$ is

$$U_{i,j,k}^{n+2/3} = \frac{s_y}{12}\left(6s_y - 1\right)\left(U_{i,j-2,k}^{n+1/3} + U_{i,j+2,k}^{n+1/3}\right) + \frac{2s_y}{3}\left(2 - 3s_y\right)\left(U_{i,j-1,k}^{n+1/3} + U_{i,j+1,k}^{n+1/3}\right) + \frac{1}{2}\left(2 - 5s_y + 6s_y^2\right)U_{i,j,k}^{n+1/3} \quad (4.7)$$

The formulas for computing the values $U_{i,1,k}^{n+2/3}$ and $U_{i,J-1,k}^{n+2/3}$ are

$$U_{i,1,k}^{n+2/3} = \frac{8\left(2+3s_y\right)}{\left(6s_y+1\right)}\left(U_{i,2,k}^{n+2/3} + U_{i,4,k}^{n+2/3}\right) - \frac{6\left(2+5s_y+6s_y^2\right)}{s_y\left(6s_y+1\right)}U_{i,3,k}^{n+2/3} - U_{i,5,k}^{n+2/3} + \frac{12}{s_y\left(6s_y+1\right)}U_{i,3,k}^{n+1/3} \quad (4.8)$$

and

$$U_{i,J-1,k}^{n+2/3} = \frac{8\left(2+3s_y\right)}{\left(6s_y+1\right)}\left(U_{i,J-2,k}^{n+2/3} + U_{i,J-4,k}^{n+2/3}\right) - \frac{6\left(2+5s_y+6s_y^2\right)}{s_y\left(6s_y+1\right)}U_{i,J-3,k}^{n+2/3} - U_{i,J-5,k}^{n+2/3} + \frac{12}{s_y\left(6s_y+1\right)}U_{i,J-3,k}^{n+1/3}. \quad (4.9)$$

For computing values of $U_{i,j,k}^{n+1}$ from the values of $U_{i,j,k}^{n+2/3}$ in the z-sweep used in the third stage, the formula used with $k = 2,3,4,\ldots,K-2$ for each $i = 1,2,3,\ldots,I-1$ and $j = 1,2,3,\ldots,J-1$ is

$$U_{i,j,k}^{n+1} = \frac{s_z}{12}\left(6s_z - 1\right)\left(U_{i,j,k-2}^{n+2/3} + U_{i,j,k+2}^{n+2/3}\right) + \frac{2s_z}{3}\left(2 - 3s_z\right)\left(U_{i,j,k-1}^{n+2/3} + U_{i,j,k+1}^{n+2/3}\right) + \frac{1}{2}\left(2 - 5s_y + 6s_y^2\right)U_{i,j,k}^{n+2/3} \quad (4.10)$$

as in x and y-sweep, the formula for computing values of $U_{i,j,1}^{n+1}$ is

$$U_{i,j,1}^{n+1} = \frac{\left(6s_z+1\right)}{8\left(2+3s_z\right)}\left(U_{i,j,0}^{n+1} + U_{i,j,4}^{n+1}\right) + \frac{3\left(2+5s_z+6s_z^2\right)}{4s_z\left(2+3s_z\right)}U_{i,j,2}^{n+1} - U_{i,j,3}^{n+1} - \frac{3}{2s_z\left(2+3s_z\right)}U_{i,j,2}^{n+2/3}. \quad (4.11)$$

At the end of the complete procedure involving diffusion in those x, y and z directions, the known boundary values $U_{i,j,0}^{n+1}$ are used. We include the values on the right hand side of equation (4.11), which all values are known. The values of $U_{i,j,K-1}^{n+1}$ are found by using similar equation

$$U_{i,j,K-1}^{n+1} = \frac{(6s_z+1)}{8(2+3s_z)}\left(U_{i,j,K}^{n+1}+U_{i,j,K-4}^{n+1}\right)+\frac{3(2+5s_z+6s_z^2)}{4s_z(2+3s_z)}U_{i,j,K-2}^{n+1} - U_{i,j,K-3}^{n+1}-\frac{3}{2s_z(2+3s_z)}U_{i,j,K-2}^{n+2/3}. \quad (4.12)$$

4.1.1 MDE

Before considering stability of finite-difference approximation, we must find modified differential equations (MDEs) of the above equations by using a technique in [3]. The technique involves determining the actual partial differential equation which is solved numerically, by the application of a given difference method to solve a problem. The MDE is derived by expanding each term of a finite-difference equation into Taylor's series and then eliminating time derivatives which are higher than first order and mixed time and space derivatives by a method described below.

In order to obtain the MDE of equation (4.1), first let us expand each term of the given difference algorithm in a Taylor's series at grid point (x_i, y_j, z_k, t^n). The terms which appear in equation (4.4) are

$$U_{i,j,k}^{n+1/3} = u_{i,j,k}^n + \frac{1}{3}\frac{\partial u}{\partial t}\Big|_{i,j,k}^n \Delta t + \frac{1}{18}\frac{\partial^2 u}{\partial t^2}\Big|_{i,j,k}^n \Delta t^2 + \frac{1}{162}\frac{\partial^3 u}{\partial t^3}\Big|_{i,j,k}^n \Delta t^3 + \frac{1}{1944}\frac{\partial^4 u}{\partial t^4}\Big|_{i,j,k}^n \Delta t^4 + \ldots \quad (4.13)$$

$$U_{i\pm1,j,k}^n = u_{i,j,k}^n \pm \frac{\partial u}{\partial x}\Big|_{i,j,k}^n \Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{i,j,k}^n \Delta x^2 \pm \frac{1}{6}\frac{\partial^3 u}{\partial x^3}\Big|_{i,j,k}^n \Delta x^3 + \frac{1}{24}\frac{\partial^4 u}{\partial x^4}\Big|_{i,j,k}^n \Delta x^4 + \ldots \quad (4.14)$$

and

$$U_{i\pm2,j,k}^{n} = u_{i,j,k}^{n} \pm 2\frac{\partial u}{\partial x}\Big|_{i,j,k}^{n}\Delta x + 2\frac{\partial^2 u}{\partial x^2}\Big|_{i,j,k}^{n}\Delta x^2 \pm \frac{4}{3}\frac{\partial^3 u}{\partial x^3}\Big|_{i,j,k}^{n}\Delta x^3 + \frac{2}{3}\frac{\partial^4 u}{\partial x^4}\Big|_{i,j,k}^{n}\Delta x^4 + \ldots \quad (4.15)$$

Placing the values in right hand side of equations (4.13)-(4.15) into equation (4.4), by manipulating and not write the symbol $\Big|_{i,j,k}^{n}$ to obtain

$$\frac{1}{3}\frac{\partial u}{\partial t} - \alpha\frac{\partial^2 u}{\partial x^2} + \frac{1}{3^2\cdot 2!}\frac{\partial^2 u}{\partial t^2}\Delta t - \frac{1}{3^3\cdot 3!}\frac{\partial^3 u}{\partial t^3}\Delta t^2 - \frac{\alpha^2}{2}\frac{\partial^4 u}{\partial x^4}\Delta t + \frac{1}{3^4\cdot 4!}\frac{\partial^4 u}{\partial t^4}\Delta t^3 + \frac{1}{3^5\cdot 5!}\frac{\partial^5 u}{\partial t^5}\Delta t^4 + \frac{\alpha}{90}\frac{\partial^6 u}{\partial t^6}\Delta x^4 - \frac{\alpha^2}{12}\frac{\partial^6 u}{\partial x^6}\Delta t\Delta x^2 + \frac{1}{3^6\cdot 6!}\frac{\partial^6 u}{\partial t^6}\Delta t^5 + \frac{1}{3^7\cdot 7!}\frac{\partial^7 u}{\partial t^7}\Delta t^6 + \frac{\alpha}{1008}\frac{\partial^8 u}{\partial t^8}\Delta x^6 - \frac{\alpha^2}{160}\frac{\partial^8 u}{\partial x^8}\Delta t\Delta x^4 + \frac{1}{3^8\cdot 8!}\frac{\partial^8 u}{\partial t^8}\Delta t^7 + \ldots = 0. \quad (4.16)$$

In considering the above equation, we need to eliminate all the time derivatives appearing in the above equation (except $\frac{\partial u}{\partial t}$). The procedure requires repeated use of equation (4.16) itself. To eliminate the $\frac{\partial^2 u}{\partial t^2}$ term, we multiply equation (4.16) by the operator $-\frac{\Delta t}{6}\frac{\partial}{\partial t}$ and then add the result to (4.16). Which results as

$$\alpha\Delta t\frac{\partial^3 u}{\partial t\partial x^2} - \frac{(\Delta t)^2}{2^2\cdot 3^4}\frac{\partial^3 u}{\partial t^3} + \alpha^2\frac{(\Delta t)^2}{2^2\cdot 3}\frac{\partial^5 u}{\partial t\partial x^4}\Delta t^4 - \frac{(\Delta t)^4}{2^4\cdot 3^5\cdot 5}\frac{\partial^5 u}{\partial t^5}^4 + \left(\frac{\alpha(\Delta x)^4}{2\cdot 3^2\cdot 5} - \frac{\alpha^2\Delta t(\Delta x)^2}{2^2\cdot 3}\right)\frac{\partial^6 u}{\partial x^6} + \ldots = 0. \quad (4.17)$$

The result of new equation has term $\frac{\partial^3 u}{\partial t\partial x^2}$ which can be removed by applying the operator $-\frac{\alpha\,\Delta t}{2}\frac{\partial^2}{\partial x^2}$ to equation (4.16) and adding the result to the new equation (4.17). The calculation can be conveniently organized into table 4.1. The first two rows list the derivatives through sixth order and their coefficients appearing in equation (4.16). The subsequent rows show the coefficients of the derivative terms obtained after operation on equation (4.16) with the differential operator shown on the left-most column. The table is continued until the desired numbers of time derivatives are deleted. The final equation is obtained by adding the coefficients in each column and multiplying by the derivative at the top of the column. Hence, the MDE of equation (4.4) is

$$\frac{1}{3}\frac{\partial u}{\partial t}-\alpha\frac{\partial^2 u}{\partial x^2} = -\frac{\alpha}{6}\left(\alpha^2\Delta t^2-\frac{\alpha\Delta t\Delta x^2}{2}+\frac{\Delta x^4}{15}\right)\frac{\partial^6 u}{\partial x^6}+\ldots \tag{4.18}$$

then

$$\frac{1}{3}\frac{\partial u}{\partial t}-\alpha\frac{\partial^2 u}{\partial x^2} = -\frac{\alpha(\Delta x)^4}{180}\left(30s_x{}^2-15s_x+2\right)\frac{\partial^6 u}{\partial x^6}+O\{(\Delta x)^6\}\,. \tag{4.19}$$

Following the same procedure MDE of equation (4.5) and (4.6), respectively are

$$\frac{1}{3}\frac{\partial u}{\partial t}-\alpha\frac{\partial^2 u}{\partial y^2} = -\frac{\alpha(\Delta y)^4}{180}\left(30s_y{}^2-15s_y+2\right)\frac{\partial^6 u}{\partial y^6}+O\{(\Delta y)^6\} \tag{4.20}$$

$$\frac{1}{3}\frac{\partial u}{\partial t}-\alpha\frac{\partial^2 u}{\partial z^2} = -\frac{\alpha(\Delta z)^4}{180}\left(30s_z{}^2-15s_z+2\right)\frac{\partial^6 u}{\partial z^6}+O\{(\Delta z)^6\}\,. \tag{4.21}$$

Terms appearing in the MDE which are not in the original partial differential equation represent a type of truncation error. These error terms allow one to determine the order of accuracy of a finite-difference approximation.

Combining equation (4.19) through (4.21), gives

$$\frac{\partial u}{\partial t}-\alpha\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right) = -\frac{\alpha(\Delta x)^4}{180}\left(30s_x{}^2-15s_x+2\right)\frac{\partial^6 u}{\partial x^6}$$
$$-\frac{\alpha_y(\Delta y)^4}{180}\left(30s_y{}^2-15s_y+2\right)\frac{\partial^6 u}{\partial y^6}-\frac{\alpha_z(\Delta z)^4}{180}\left(30s_z{}^2-15s_z+2\right)\frac{\partial^6 u}{\partial z^6}$$
$$+O\{(\Delta x)^6\}+O\{(\Delta y)^6\}+O\{(\Delta z)^6\}\,. \tag{4.22}$$

Since the lowest-order terms (truncation error) of the preceding equation is of $O\left\{(\Delta x)^4 + (\Delta y)^4 + (\Delta z)^4\right\}$. Thus we determined the order of accuracy is fourth-order by consider the right hand side of the preceding equations.

Table 4.1 Procedure for calculation the MDE of equation (4.4).

Partial Derivatives	$\frac{\partial u}{\partial t}$	$\frac{\partial^2 u}{\partial x^2}$	$\frac{\partial^2 u}{\partial t \partial x}$	$\frac{\partial^2 u}{\partial t^2}$	$\frac{\partial^3 u}{\partial x^3}$	$\frac{\partial^3 u}{\partial t \partial x^2}$	$\frac{\partial^3 u}{\partial t^2 \partial x}$	$\frac{\partial^3 u}{\partial t^3}$	$\frac{\partial^4 u}{\partial x^4}$	$\frac{\partial^4 u}{\partial t \partial x^3}$
Coefficient of (4.16)	$\frac{1}{3}$	$-\alpha$	0	$\frac{\Delta t}{2 \cdot 3^2}$	0	0	0	$\frac{\Delta t^2}{2 \cdot 3^4}$	$\frac{-\alpha^2 \Delta t}{2}$	0
$-\frac{\Delta t}{6}\frac{\partial}{\partial t}(4.16)$				$-\frac{\Delta t}{2 \cdot 3^2}$	0	$\frac{\alpha \Delta t}{6}$	0	$\frac{-\Delta t^2}{2^2 \cdot 3^3}$	0	0
$-\frac{\alpha \Delta t}{2}\frac{\partial^2}{\partial x^2}(4.16)$						$-\frac{\alpha \Delta t}{6}$	0	0	$\frac{\alpha^2 \Delta t}{2}$	0
$\frac{\Delta t^2}{2^2 \cdot 3^3}\frac{\partial^2}{\partial t^2}(4.16)$								$\frac{\Delta t^2}{2^2 \cdot 3^4}$	0	0
$\frac{\alpha \Delta t^2}{3^2}\frac{\partial^3}{\partial t \partial x^2}(4.16)$										
$\frac{\alpha^2 \Delta t^2}{2^2 \cdot 3}\frac{\partial^4}{\partial x^4}(4.16)$										
$-\frac{\alpha \Delta t^3}{2^2 \cdot 3^3}\frac{\partial^4}{\partial t^2 \partial x^2}(4.16)$										
$-\frac{\Delta t^4}{2^4 \cdot 3^6 \cdot 5}\frac{\partial^4}{\partial t^4}(4.16)$										
⋮										
Sum of coefficients in each column	$\frac{1}{3}$	$-\alpha$	0	0	0	0	0	0	0	0

Table 4.1 (cont.)

$\frac{\partial^4 u}{\partial t^2 \partial x^2}$	$\frac{\partial^4 u}{\partial t^3 \partial x}$	$\frac{\partial^4 u}{\partial t^4}$	$\frac{\partial^5 u}{\partial x^5}$	$\frac{\partial^5 u}{\partial t \partial x^4}$	$\frac{\partial^5 u}{\partial t^2 \partial x^3}$	$\frac{\partial^5 u}{\partial t^3 \partial x^2}$	$\frac{\partial^5 u}{\partial t^4 \partial x}$	$\frac{\partial^5 u}{\partial t^5}$	$\frac{\partial^6 u}{\partial x^6}$	...
0	0	$\frac{\Delta t^3}{2^3 \cdot 3^5}$	0	0	0	0	0	$\frac{\Delta t^4}{2^3 \cdot 3^6 \cdot 5}$	$\frac{\alpha\ \Delta x^4}{2 \cdot 3^2 \cdot 5}$ $\frac{-\alpha^2 \Delta t \Delta x^2}{2^2 \cdot 3}$	
0	0	$\frac{-\Delta t^3}{2^2 \cdot 3^5}$	0	$\frac{\alpha^2 \Delta t^2}{2^2 \cdot 3}$	0	0	0	$\frac{-\Delta t^4}{2^4 \cdot 3^6}$	0	
$-\frac{\alpha \Delta t^2}{2^2 \cdot 3^2}$	0	0	0	0	0	$\frac{-\alpha \Delta t^3}{2^2 \cdot 3^4}$	0	0	$\frac{\alpha^3 \Delta t^2}{2^2}$	
$-\frac{\alpha \Delta t^2}{2^2 \cdot 3^3}$	0	$\frac{\Delta t^3}{2^3 \cdot 3^5}$	0	0	0	0	0	$\frac{\Delta t^4}{2^3 \cdot 3^7}$	0	
$\frac{\alpha \Delta t^2}{3^3}$	0	0	0	$\frac{-\alpha^2 \Delta t^2}{3^2}$	0	$\frac{\alpha \Delta t^3}{2 \cdot 3^4}$	0	0	0	
				$\frac{\alpha^2 \Delta t^2}{2^2 \cdot 3^2}$	0	0	0	0	$-\frac{\alpha^3 \Delta t^2}{2^2 \cdot 3}$	
						$\frac{-\alpha \Delta t^3}{2^2 \cdot 3^4}$	0	0	0	
								$\frac{-\Delta t^4}{2^4 3^7 \cdot 5}$	0	
0	0	0	0	0	0	0	0	0	$\frac{\alpha^3 \Delta t^2}{6}$ $-\frac{\alpha^2 \Delta t \Delta x^2}{12}$ $+\frac{\alpha \Delta x^4}{90}$	

4.1.2 Stability

In this section we will determine von Neumann stability (Appendix B), which is applied with the problem (4.4), first let $U^n_{p,q,r} = e^{\gamma s a} e^{i\beta_1 b_1 h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h}$, when $e^{\gamma s} = \xi$, then substitute in (4.4) yields

$$\begin{aligned}
\xi^{a+\frac{1}{3}} e^{i\beta_1 b_1 h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h} &= \frac{s_x}{12}(6s_x - 1)\left(\xi^a e^{i\beta_1 (b_1-2)h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h} + \xi^a e^{i\beta_1 (b_1+2)h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h}\right) \\
&+ \frac{2s_x}{3}(2 - 3s_x)\left(\xi^a e^{i\beta_1 (b_1-1)h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h} + \xi^a e^{i\beta_1 (b_1+1)h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h}\right) \\
&+ \frac{1}{2}\left(2 - 5s_x + 6s_x^2\right)\xi^a e^{i\beta_1 b_1 h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h}. \qquad (4.23)
\end{aligned}$$

Cancelling all common terms, by dividing (4.23) with $\xi^{a} e^{i\beta_1 b_1 h} e^{i\beta_2 b_2 h} e^{i\beta_3 b_3 h}$

$$\xi^{\frac{1}{3}} = \frac{s_x}{12}(6s_x - 1)\left(e^{-2i\beta_1 h} + e^{2i\beta_1 h}\right) + \frac{2s_x}{3}(2 - 3s_x)\left(e^{-i\beta_1 h} + e^{i\beta_1 h}\right) + \frac{1}{2}\left(2 - 5s_x + 6s_x^2\right). \quad (4.24)$$

Then using the definition, $\dfrac{e^{i\beta h} + e^{-i\beta h}}{2} = \cos \beta h$, thus the amplification factor is

$$\xi^{\frac{1}{3}} = \frac{s_x(6s_x - 1)}{3}\cos^2 \beta_1 h + \frac{4s_x(2 - 3s_x)}{3}\cos \beta_1 h + \frac{3 - 7s_x + 6s_x^{\,2}}{3} \quad (4.25)$$

where $\beta_1 = m\pi\,; m \in I$ and let $\xi^{\frac{1}{3}} = G$, the condition

$$|G| \le 1 \qquad \text{for all } \beta_1 \quad (4.26)$$

is required for stability. For all positive values of s_x we obtain the FDE (4.4) is stable over the interval $(0, 2/3]$ (Appendix B).

In the same procedure as above to apply with (4.7) and (4.10), we obtain that the FDEs is stable over all s_y and s_z in the interval $(0, 2/3]$.

4.2 The ADI Method

In order to solve problem (1.2)-(1.9) by the new ADI method, we use three stages procedure. The first stage for use in the z–direction sweep is

$$\begin{aligned}
(6s_z - 1)U_{i,j,k-1}^{n+1} - 4(1 + 3s_z)U_{i,j,k}^{n+1} + (6s_z - 1)U_{i,j,k+1}^{n+1} \\
= -s_x\left(U_{i-1,j,k-1}^{n} + U_{i-1,j,k+1}^{n} + U_{i+1,j,k-1}^{n} + U_{i+1,j,k+1}^{n}\right) - 4s_x\left(U_{i-1,j,k}^{n} + U_{i+1,j,k}^{n}\right) \\
- s_y\left(U_{i,j-1,k-1}^{n} + U_{i,j-1,k+1}^{n} + U_{i,j+1,k-1}^{n} + U_{i,j+1,k+1}^{n}\right) - 4s_y\left(U_{i,j-1,k}^{n} + U_{i,j+1,k}^{n}\right) \\
+ (2s_x + 2s_y - 1)\left(U_{i,j,k-1}^{n} + 4U_{i,j,k}^{n} + U_{i,j,k+1}^{n}\right) \quad (4.27)
\end{aligned}$$

then for second stage in the next time step where the formula use in y–direction sweep is

$$(6s_y-1)U_{i,j-1,k}^{n+2}-4(1+3s_y)U_{i,j,k}^{n+2}+(6s_y-1)U_{i,j+1,k}^{n+2}$$
$$=-s_x\left(U_{i-1,j-1,k}^{n+1}+U_{i-1,j+1,k}^{n+1}+U_{i+1,j-1,k}^{n+1}+U_{i+1,j+1,k}^{n+1}\right)-4s_x\left(U_{i-1,j,k}^{n+1}+U_{i+1,j,k}^{n+1}\right)$$
$$-s_z\left(U_{i,j-1,k-1}^{n+1}+U_{i,j-1,k+1}^{n+1}+U_{i,j+1,k-1}^{n+1}+U_{i,j+1,k+1}^{n+1}\right)-4s_z\left(U_{i,j,k-1}^{n+1}+U_{i,j,k+1}^{n+1}\right)$$
$$+(2s_x+2s_z-1)\left(U_{i,j-1,k}^{n+1}+4U_{i,j,k}^{n+1}+U_{i,j+1,k}^{n+1}\right) \tag{4.28}$$

finally, the formula for use in the x–direction sweep is

$$(6s_x-1)U_{i-1,j,k}^{n+3}-4(1+3s_x)U_{i,j,k}^{n+3}+(6s_x-1)U_{i+1,j,k}^{n+3}$$
$$=-s_y\left(U_{i-1,j-1,k}^{n+2}+U_{i-1,j+1,k}^{n+2}+U_{i+1,j-1,k}^{n+2}+U_{i+1,j+1,k}^{n+2}\right)-4s_y\left(U_{i,j-1,k}^{n+2}+U_{i,j+1,k}^{n+2}\right)$$
$$-s_z\left(U_{i-1,j,k-1}^{n+2}+U_{i-1,j,k+1}^{n+2}+U_{i+1,j,k-1}^{n+2}+U_{i+1,j,k+1}^{n+2}\right)-4s_z\left(U_{i,j,k-1}^{n+2}+U_{i,j,k+1}^{n+2}\right)$$
$$+(2s_y+2s_z-1)\left(U_{i-1,j,k}^{n+2}+4U_{i,j,k}^{n+2}+U_{i+1,j,k}^{n+2}\right). \tag{4.29}$$

The recursive procedure is carried on by using (4.27) then (4.28) and (4.29) respectively, then start at (4.27) again with the same procedure. The equations (4.27)-(4.29) can be expressed in a tridiagonal form of matrix equations, $Ax=B$. The elements of matrix A occur only on the main diagonal and on one subdiagonal above and below. This phenomenon of the matrix can be solved by the efficiency Thomas algorithm (Appendix D).

In order to show stability of the ADI method, we replace $U_{p,q,r}^{n}=\xi^n e^{i\beta_1 pk}e^{i\beta_2 qk}e^{i\beta_3 rk}$ into (4.27) to obtain

$$(6s_z-1)\xi^{n+1}e^{i\beta_1 pk}e^{i\beta_2 qk}\left(e^{i\beta_3(r-1)k}+e^{i\beta_3(r+1)k}\right)-4(1+3s_z)\xi^{n+1}e^{i\beta_1 pk}e^{i\beta_2 qk}e^{i\beta_3 rk}$$
$$=-s_x\left\{\xi^n e^{i\beta_2 qk}\left(e^{i\beta_1(p-1)k}e^{i\beta_3(r-1)k}+e^{i\beta_1(p-1)k}e^{i\beta_3(r+1)k}+e^{i\beta_1(p+1)k}e^{i\beta_3(r-1)k}+e^{i\beta_1(p+1)k}e^{i\beta_3(r+1)k}\right)\right\}$$
$$-s_y\left\{\xi^n e^{i\beta_1 qk}\left(e^{i\beta_2(q-1)k}e^{i\beta_3(r-1)k}+e^{i\beta_2(q-1)k}e^{i\beta_3(r+1)k}+e^{i\beta_2(q+1)k}e^{i\beta_3(r-1)k}+e^{i\beta_2(q+1)k}e^{i\beta_3(r+1)k}\right)\right\}$$
$$-4s_x\left\{\xi^n e^{i\beta_1 qk}e^{i\beta_3 rk}\left(e^{i\beta_1(p-1)k}+e^{i\beta_1(p+1)k}\right)\right\}-4s_y\left\{\xi^n e^{i\beta_1 pk}e^{i\beta_3 rk}\left(e^{i\beta_2(q-1)k}+e^{i\beta_2(q+1)k}\right)\right\}$$
$$+(2s_x+2s_y-1)\left\{\xi^n e^{i\beta_1 qk}e^{i\beta_2 qk}\left(4e^{i\beta_3 rk}+e^{i\beta_3(r-1)k}+e^{i\beta_3(r+1)k}\right)\right\}. \tag{4.30}$$

Dividing the preceding equation by $\xi^n e^{i(\beta_1 p+\beta_2 q+\beta_3 r)k}$, we get

$$
\begin{aligned}
&(6s_z-1)\xi\left(e^{-i\beta_3 k}+e^{i\beta_3 k}\right)-4(1+3s_z)\xi \\
&\quad=-s_x\left\{e^{-i\beta_1 k}e^{-i\beta_3 k}+e^{-i\beta_1 k}e^{i\beta_3 k}+e^{i\beta_1 k}e^{-i\beta_3 k}+e^{i\beta_1 k}e^{i\beta_3 k}\right\}-4s_x\left\{e^{-i\beta_1 k}+e^{i\beta_1 k}\right\} \\
&\qquad-s_y\left\{e^{-i\beta_2 k}e^{-i\beta_3 k}+e^{-i\beta_2 k}e^{i\beta_3 k}+e^{i\beta_2 k}e^{-i\beta_3 k}+e^{i\beta_2 k}e^{i\beta_3 k}\right\}-4s_y\left\{e^{-i\beta_2 k}+e^{i\beta_2 k}\right\} \\
&\qquad+(2s_x+2s_y-1)\left\{4+e^{-i\beta_3 k}+e^{i\beta_3 k}\right\} \\
&\quad=-s_x\left\{e^{-i\beta_1 k}\left(e^{-i\beta_3 k}+e^{i\beta_3 k}\right)+e^{i\beta_1 k}\left(e^{-i\beta_3 k}+e^{i\beta_3 k}\right)\right\}-4s_x\left\{e^{-i\beta_1 k}+e^{i\beta_1 k}\right\} \\
&\qquad-s_y\left\{e^{-i\beta_2 k}\left(e^{-i\beta_3 k}+e^{i\beta_3 k}\right)+e^{i\beta_2 k}\left(e^{-i\beta_3 k}+e^{i\beta_3 k}\right)\right\}-4s_y\left\{e^{-i\beta_2 k}+e^{i\beta_2 k}\right\} \\
&\qquad+(2s_x+2s_y-1)\left\{4+e^{-i\beta_3 k}+e^{i\beta_3 k}\right\}. \qquad (4.31)
\end{aligned}
$$

Using $e^{-i\beta_i k}+e^{i\beta_i k}=2\cos\beta_i k$, for $i=1,2,3$, to obtain

$$
\begin{aligned}
\xi &= -\frac{4s_x(\cos\beta_1 k\cos\beta_3 k)}{2(6s_z-1)\cos\beta_3 k-(4+12s_z)}-\frac{4s_y(\cos\beta_2 k\cos\beta_3 k)}{2(6s_z-1)\cos\beta_3 k-(4+12s_z)} \\
&\quad+\frac{\left(-8s_x\cos\beta_1 k-8s_y\cos\beta_2 k+(2s_x+2s_y-1)(4+2\cos\beta_3 k)\right)}{2(6s_z-1)\cos\beta_3 k-(4+12s_z)}. \qquad (4.32)
\end{aligned}
$$

We then apply $\cos\beta k=1-2\sin^2\dfrac{\beta k}{2}$, $a_i=\sin^2\dfrac{\beta_i k}{2}$; $i=1,2,3$ and let $\xi=\xi_z$ in (4.32) to obtain

$$
\begin{aligned}
\xi_z &= \left\{\frac{(24-16a_3)(a_1s_x+a_2s_y)+2(2a_3-3)}{-24a_3s_z+2(2a_3-3)}\right\} \\
&= \left\{\frac{(2a_3-3)\left(1-4(a_1s_x+a_2s_y)\right)}{-12a_3s_z+(2a_3-3)}\right\}. \qquad (4.33)
\end{aligned}
$$

Using the same procedure apply with (4.28) yields

$$
\begin{aligned}
\xi_y &= \left\{\frac{(24-16a_2)(a_1s_x+a_3s_z)+2(2a_2-3)}{-24a_2s_y+2(2a_2-3)}\right\} \\
&= \left\{\frac{(2a_2-3)\left(1-4(a_1s_x+a_3s_z)\right)}{-12a_2s_y+(2a_2-3)}\right\}. \qquad (4.34)
\end{aligned}
$$

Similarly, for (4.29)

$$\xi_x = \left\{\frac{(24-16a_1)(a_2 s_y + a_3 s_z) + 2(2a_1 - 3)}{-24a_1 s_x + 2(2a_1 - 3)}\right\}$$
$$= \left\{\frac{(2a_1 - 3)(1 - 4(a_2 s_y + a_3 s_z))}{-12a_1 s_x + (2a_1 - 3)}\right\}. \tag{4.35}$$

Thus

$$G = \xi_x \xi_y \xi_z$$
$$= \left\{\frac{(2a_3 - 3)(1 - 4(a_1 s_x + a_2 s_y))}{-12a_3 s_z + (2a_3 - 3)}\right\} \times \left\{\frac{(2a_2 - 3)(1 - 4(a_1 s_x + a_3 s_z))}{-12a_2 s_y + (2a_2 - 3)}\right\}$$
$$\times \left\{\frac{(2a_1 - 3)(1 - 4(a_2 s_y + a_3 s_z))}{-12a_1 s_x + (2a_1 - 3)}\right\}. \tag{4.36}$$

Let $s = s_x = s_y = s_z$ yields

$$G = \left\{\frac{(2a_3 - 3)(1 - 4(a_1 + a_2)s)}{-12a_3 s + (2a_3 - 3)}\right\} \times \left\{\frac{(2a_2 - 3)(1 - 4(a_1 + a_3)s)}{-12a_2 s + (2a_2 - 3)}\right\}$$
$$\times \left\{\frac{(2a_1 - 3)(1 - 4(a_2 + a_3)s)}{-12a_1 s + (2a_1 - 3)}\right\}. \tag{4.37}$$

The condition

$$|G| \le 1 \qquad \text{for all } \beta_i \ ; i = 1,2,3 \tag{4.38}$$

is required for stability. In order to find the values of s which satisfy the condition in (4.38), we must substitute $G = \xi_x \xi_y \xi_z$ into (4.38) yields

$$|\xi_x \xi_y \xi_z| = |\xi_z||\xi_y||\xi_z| \le 1 \tag{4.39}$$

let us consider the case $|\xi_z| \le 1$, $|\xi_y| \le 1$ and $|\xi_z| \le 1$ which satisfy (4.39).

Consider $a_i = sin^2 \dfrac{\beta_i k}{2}; i = 1,2,3$ when $\beta_i = m\pi\,; m \in I$, if $k \in I$ we then obtain $sin^2 \dfrac{\beta_i k}{2} = 0$ and $sin^2 \dfrac{\beta_i k}{2} = 1$. Hence we can divide values of a_1, a_2 and a_3 into 8 cases. Next, we will show the values of s which satisfy the condition $|\xi_z| \le 1$.

Case 1 Let $a_1 = 1, a_2 = 1$ and $a_3 = 1$

$$|\xi_z| = \left|\frac{(1-8s)}{12s+1}\right| \le 1 \qquad \text{thus} \quad s \ge 0. \tag{4.40}$$

Case 2 Let $a_1 = 1, a_2 = 1$ and $a_3 = 0$

$$|\xi_z| = |1-8s| \le 1 \qquad \text{thus} \quad 0 \le s \le 1/4\ . \tag{4.41}$$

Case 3 Let $a_1 = 1, a_2 = 0$ and $a_3 = 1$

$$|\xi_z| = \left|\frac{-(1-4s)}{-12s-1}\right| \le 1 \quad \text{thus} \quad s \ge 0. \tag{4.42}$$

Case 4 Let $a_1 = 1, a_2 = 0$ and $a_3 = 0$

$$|\xi_z| = |1-4s| \le 1 \qquad \text{thus} \quad 0 \le s \le 1/2. \tag{4.43}$$

Case 5 Let $a_1 = 0, a_2 = 1$ and $a_3 = 0$

$$|\xi_z| = |1-4s| \le 1 \qquad \text{thus} \quad 0 \le s \le 1/2. \tag{4.44}$$

Case 6 Let $a_1 = 0, a_2 = 1$ and $a_3 = 1$

$$|\xi_z| = \left|\frac{(1-4s)}{12s+1}\right| \le 1 \quad \text{thus} \quad s \ge 0. \tag{4.45}$$

Case 7 Let $a_1 = 0, a_2 = 0$ and $a_3 = 1$

$$|\xi_z| = \left|\frac{1}{12s+1}\right| \le 1 \quad \text{thus} \quad s \ge 0. \tag{4.46}$$

Case 8 Let $a_1 = 0, a_2 = 0$ and $a_3 = 0$

$$\xi_z = 1 \quad \text{satisfies } |\xi_z| \le 1 \text{ for all values of } s. \tag{4.47}$$

Considering the values of ξ_z when $k \notin I$. $\left\{\frac{(2a_3-3)(1-4(a_1+a_2)s)}{-12a_3 s+(2a_3-3)}\right\}$ can be expressed as a function of $sin\,\frac{\beta_3 k}{2}$ as

$$\xi_z\left(sin\,\frac{\beta_3 k}{2}\right) = \left\{\frac{\left(2\,sin^2\,\frac{\beta_3 k}{2}-3\right)(1-4(a_1+a_2)s)}{-12s\,sin^2\,\frac{\beta_3 k}{2}+\left(2\,sin^2\,\frac{\beta_3 k}{2}-3\right)}\right\} \tag{4.48}$$

its extremum of $\xi_z\left(sin\,\frac{\beta_3 k}{2}\right)$ occurs at $sin\,\frac{\beta_3 k}{2} = 0$, we then substitute this value into (4.33) to obtain

$$\xi_z\left(sin\,\frac{\beta_3 k}{2}\right) = (1-4(a_1+a_2)s). \tag{4.49}$$

Hence the condition $\left|\xi_z\left(sin\,\frac{\beta_3 k}{2}\right)\right| = |(1-4(a_1+a_2)s)| \le 1$ is required for stability, from this condition requires that $0 \le s \le \frac{1}{2(a_1+a_2)}$. Choosing the minimum value of $\frac{1}{2(a_1+a_2)}$ we obtain $0 \le s \le 1/4$. Combining all the results leads to the conclusion that $0 \leq s \leq 1/4$. Since $s = \alpha\, \Delta t/(\Delta x)^2$ and α is a positive constant thus $0 < s \leq 1/4$.

Similarly, apply the above procedure with ξ_x in (4.35) and ξ_y in (4.34), we obtain that $0 < s \leq 1/4$. Hence the FDEs (4.27)-(4.29) are stable over the interval $(0, 1/4]$. This shows the method is conditionally stable in three-dimensional problem since we need to use the values of s in the interval $(0, 1/4]$ to make the problem stable.

In chapter 2, we discussed the advantages of the ADI method for solving two-dimensional diffusion equations over the LOD method. Although the ADI method is difficult and requires the solving of simultaneous equations, it proves useful since Δt can be made larger without loss of stability. Here we apply the ADI method for solving three-dimensional equations and presented them as conditionally stable. The result of our findings is that the ADI method loses its advantage over the LOD method in solving three-dimensional equations.

CHAPTER 5

EXAMPLES OF DIFFUSION PROBLEMS

In this chapter we will discuss easy examples of heat diffusion problems which involve heat conduction in different mediums. All problems are considered as conduction problems when convection and radiation heat transfer are neglected. As part of our discussion, a comparison of exact solution and numerical solution will be made by using different values of s in example 5.1. We will compare analytic solutions and numerical solutions by using examples 5.2-5.4 to demonstrate the differences in the sequel.

Example 5.1 In this example, using $u(x,y,z,t) = exp\,(-3\alpha\pi^2 t)\,sin\,\pi x\,sin\,\pi y\,sin\,\pi z + 100xyz$, which is the exact solution of equations (1.2)-(1.9) to verify theoretical predictions, numerical tests were carried out on the region $0 \le x,y,z \le 1$. Using this function to define both initial and boundary conditions. The initial condition is given by setting $t = 0$ then we obtained

$$u(x,y,z,0) = sin\,\pi x\,sin\,\pi y\,sin\,\pi z + 100xyz\,, \qquad 0 \le x,y,z \le 1 \tag{5.1}$$

while Dirichlet boundary conditions are obtained by setting $x = 0,1$, $y = 0,1$ and $z = 0,1$ respectively, we obtained

$$u(0,y,z,t) = 0\,, \qquad 0 < y,z < 1 \tag{5.2}$$

$$u(1,y,z,t) = 100yz\,, \qquad 0 < y,z < 1 \tag{5.3}$$

$$u(x,0,z,t) = 0\,, \qquad 0 < x,z < 1 \tag{5.4}$$

$$u(x,1,z,t) = 100xz\,, \qquad 0 < x,z < 1 \tag{5.5}$$

$$u(x,y,0,t) = 0\,, \qquad 0 < x,y < 1 \tag{5.6}$$

$$u(x,y,1,t) = 100xy\,, \qquad 0 < x,y < 1\,. \tag{5.7}$$

In order to compare exact solutions (u) and numerical solutions (U) when using different values of s, in table 5.1-5.2, let $s = 1/6$, $s = 2/3$ respectively. We let grid spacing $\Delta x = \Delta y = \Delta z = 0.05$, $\alpha = 1$ and percentage error = $\frac{(u-U)}{u} \times 100$. From table 5.1, we can observe that the LOD method gives a better approximation than the ADI method, only at the grid point $(1,10,10,10)$, the ADI method gives a better approximation than the LOD method.

Table 5.1 Compares exact solutions with numerical solutions when $s = 1/6$.

i	Exact Solution, $u_{i,10,10}^{10}$ when $s = 1/6$	Numerical Solution of LOD Method		Numerical Solution of ADI Method	
		$U_{i,10,10}^{10}$ when $s = 1/6$	$\lvert percentage\ error \rvert$	$U_{i,10,10}^{10}$ when $s = 1/6$	$\lvert percentage\ error \rvert$
1	1.38827813302170	1.38832600744485	0.00344847491373	1.38825467311414	0.00168985644893
2	2.77315139948959	2.77316533040336	0.00050234955698	2.77310505733525	0.00167110076820
3	4.15129877196453	4.15130227124451	0.00008429361922	4.15123068866105	0.00164004826490
4	5.51956483683943	5.51956562160373	0.00001421786543	5.51947668882370	0.00159701024148
5	6.87503749109451	6.87503769805865	0.00000301037108	6.87493144886323	0.00154242404375
6	8.21511964793835	8.21511976349965	0.00000140669042	8.21499832260317	0.00147685414673
7	9.53759318570389	9.53759329707803	0.00000116773842	9.53745956469724	0.00140099293447
8	10.84067356536549	10.84067368266467	0.00000108202852	10.84053093888000	0.00131566073482
9	12.12305377181218	12.12305389351812	0.00000100392148	12.12290565178529	0.00122180458552
10	13.38393649689751	13.38393662011573	0.00000092064259	13.38378653053585	0.00112049516743

Table 5.2 Compares exact solutions with numerical solutions when $s = 2/3$.

i	Exact Solution $u_{i,,10,10}^{10}$	Numerical Solution of LOD Method		Numerical Solution of ADI Method	
		$U_{i,10,10}^{10}$	$\lvert percentage\ error \rvert$	$U_{i,10,10}^{10}$	$\lvert percentage\ error \rvert$
1	1.34550293199057	1.34492311539666	0.04309292682493	1.33465779688558	0.80602835171422
2	2.68865426483948	2.68865595906736	0.00006301397329	2.66697110038191	0.80646904814533
3	4.02716030358043	4.02719892660702	0.00095906355044	3.99465035710176	0.80726725603067
4	5.35884173580491	5.35884495841785	0.00006013637086	5.31551072241442	0.80858916024663
5	6.68168729356644	6.68168898451013	0.00002530713599	6.62750687610675	0.81087927463858
6	7.99390327747238	7.99390771301856	0.00005548661306	7.92872907550554	0.81529885594822
7	9.29395772351594	9.29396277065046	0.00005430554636	9.21730048561454	0.82480725845608
8	10.58061812511436	10.58062333941163	0.00004928159404	10.49103269805211	0.84669369977174
9	11.85298178151138	11.85298719812452	0.00004569831659	11.74653804623688	0.89803339983643
10	13.11049802526580	13.11050350790240	0.00004181867531	12.97731513830304	1.01584918212945

In Chapter 4, we showed stability of the ADI method requires $0 < s \le 1/4$. This results in the error of the ADI method to increases when s increases from $1/6$ to $2/3$.

In order to study the relation between an error and spatial grid separation, we let $\alpha = 1$, $\Delta x = \Delta y = \Delta z$, $s = 1/5$, $s = 1/3$ and numbers of grid spacing to be 10, 20, 30, 40, 50.

Table 5.3 The relation between error and spatial grid separation when $s = 1/5$.

Number of Grid Spacing	Exact Solution	Numerical Solution from LOD Method		Numerical Solution from ADI Method	
	$u(0.5,0.5,0.5,10\Delta t)$	$U(0.5,0.5,0.5,10\Delta t)$	$\lvert percentage\ error\rvert \times 10^{-3}$	$U(0.5,0.5,0.5,10\Delta t)$	$\lvert percentage\ error\rvert$
10	13.05312223391429	13.05319265905484	0.53952716666109	12.99098138341709	0.47606120117184
20	13.36239311187577	13.36239319853764	0.00064855052417	13.36216164754841	0.00173220713851
30	13.43632057856776	13.43632058681168	0.00006135549575	13.43627167503284	0.00036396522868
40	13.46366551906545	13.46366552057457	0.00001120883416	13.46364960939574	0.00011816744622
50	13.47659128563391	13.47659128603470	0.00000297397542	13.47658468464187	0.00000489811697

Table 5.4 The relation between error and spatial grid separation when $s = 1/3$.

Number of Grid spacing	Exact Solution $u(0.5,0.5,0.5,10\Delta t)$	Numerical Solution of LOD Method		Numerical Solution of ADI Method	
		$U(0.5,0.5,0.5,10\Delta t)$	$\lvert percentage\ error \rvert \times 10^{-3}$	$U(0.5,0.5,0.5,10\Delta t)$	$\lvert percentage\ error \rvert$
10	12.91136917350630	12.91144198683225	0.56394736275843	12.34838491964704	12.06784788561494
20	13.30086242635995	13.30086262801868	0.0001516327157	13.29950163650164	0.13788199778285
30	13.40601805578892	13.40601807572237	0.00014869031477	13.40588103696658	0.00255106716743
40	13.44599639118161	13.44599639488429	0.00002753740924	13.44595126238977	0.00078676924056
50	13.46509322523905	13.46509322622907	0.00000735249651	13.46507438747228	0.00033070416130

In this example, it is evident in table 5.1-5.2 that numerical solutions of ADI methods give a bad approximation when compare with the LOD solution but it is also notice in tables 5.3-5.4 that as grid spacing decrease so does the error of the numerical solution.

In order to present a relation between errors and spatial grid separations we then use data in tables 5.3-5.4 to plot a graph, which is showed in the following figures.

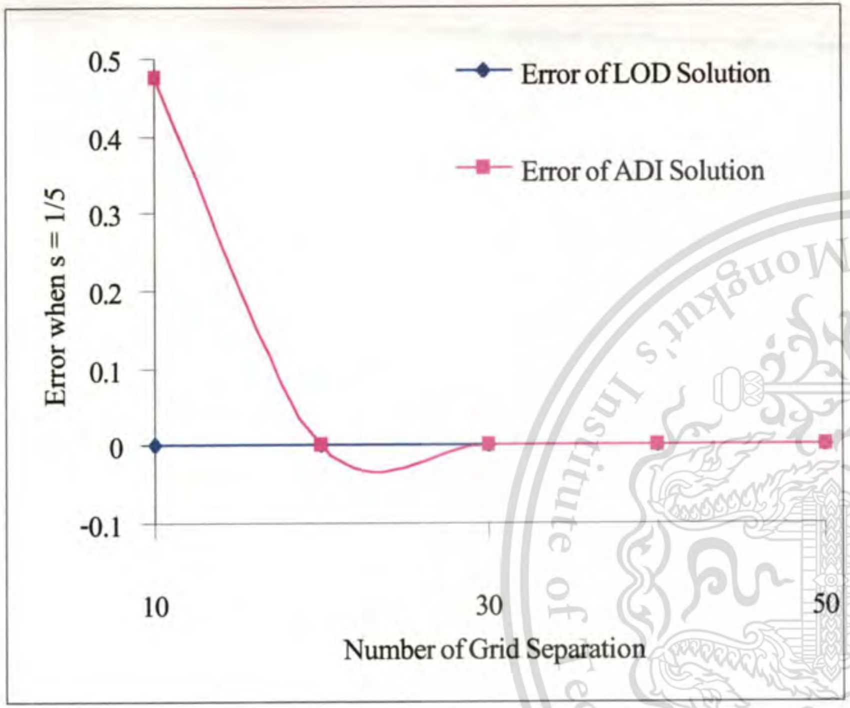

Figure 5.1 The relation between error and spatial grid separation when $s = 1/5$.

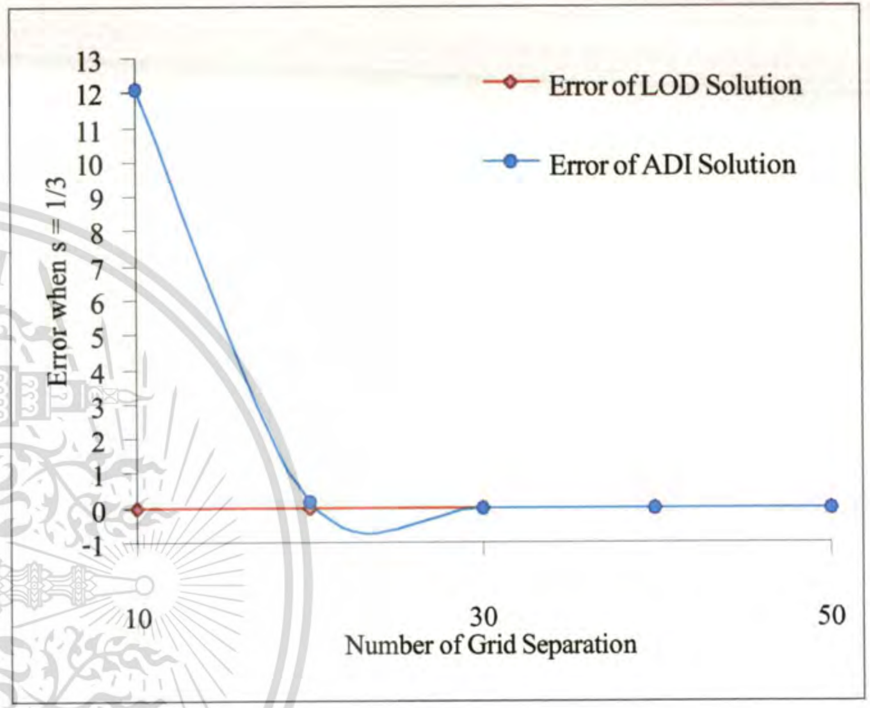

Figure 5.2 The relation between error and spatial grid separation when $s = 1/3$.

Although the error of the ADI method when $s = 1/5$ is smaller than when $s = 1/3$, similar results are observed in both figures as the number of spatial separation increases, resulting in an error decrease and a convergence to 0. It is noticed that the ADI method requires 30 grids to converge to 0 in comparison to 10 grids required in the LOD method.

The physical interpretation is shown by some selected thermal diffusivity values, α, as following example. For simplicity homogeneous boundary conditions will be considered in this example.

Example 5.2 The thermal diffusivity values of clay brick, paving brick and finally building brick will be discussed. For all three kinds of bricks, placing the bricks in an oven with temperature $300^\circ C$ starts the experiment. In order to assure that all sides of the bricks are uniformly heated $300^\circ C$ throughout the experiment, we will put the bricks on a grid in the oven. After the bricks are uniformly heated, $300^\circ C$, we will take them in a large well-stirred bath of liquid, $0^\circ C$. All the brick's dimension are the same, which is $0.2\,m \times 0.2\,m \times 0.1\,m$. We neglect some parameters to obtain the mathematical problem (the problem is considered ideal since the brick's sudden temperature changes may cause the brick damage)

$$u_t = \alpha(u_{xx} + u_{yy} + u_{zz}), \qquad 0<x<0.2, 0<y<0.2, 0<z<0.1, 0<t\le T \quad (5.8)$$

subject to initial condition as

$$u(x,y,z,0) = 300, \qquad 0 \le x \le 0.2,\ 0 \le y \le 0.2,\ 0 \le z \le 0.1 \quad (5.9)$$

boundary conditions are

$$u(0,y,z,t) = u(0.2,y,z,t) = u(x,0,z,t) = u(x,0.2,z,t) = u(x,y,0,t) = u(x,y,0.1,t) = 0 \quad (5.10)$$

when the thermal diffusivity values of clay brick, paving brick and building brick are $1.01183 \times 10^{-6}\ m^2/s$, $5.75 \times 10^{-7}\ m^2/s$ and $4 \times 10^{-7}\ m^2/s$ respectively [7-8]. By using separation of variables method. The analytic solution of this problem (when initial condition is a constant and all boundary values are equal 0, Appendix C) is

$$u(x,y,z,t)=\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\sum_{r=0}^{\infty}A_{(2p+1)(2q+1)(2r+1)}\,sin\left(\frac{(2p+1)\pi x}{0.2}\right)sin\left(\frac{(2q+1)\pi y}{0.2}\right)sin\left(\frac{(2r+1)\pi z}{0.1}\right)$$
$$\times exp\left[-1.01183\times10^{-6}\pi^2\left(\frac{(2p+1)^2}{0.2^2}+\frac{(2q+1)^2}{0.2^2}+\frac{(2r+1)^2}{0.1^2}\right)t\right] \quad (5.11)$$

when $A_{(2p+1)(2q+1)(2r+1)} = \dfrac{4.8\times10^6}{(2p+1)(2q+1)(2r+1)\pi^3}$.

The initial-boundary value problem from equation (5.8) to (5.10) are considered, where the solution to the problem for the heat diffusion with zero boundary conditions (5.10), and initial temperature distribution is equal to $300^\circ C$, while the solution is expressed in equation (5.11). Though we have certain form of the analytic solution but the solution is complicated, involving infinite series. Thus it is difficult to determine, which value of p,q,r will give a good approximation of $u(x,y,z,t)$ in (5.11). We notice that the temperature distribution approaches a steady state i.e. $u(x,y,z,t) = 0$ (since all of edges are at $0^\circ C$). We expect all the initial heat energy contained in the brick ($300^\circ C$) to flow out those six edges and note that each term in (5.11) decays at a different rate i.e. decay as exponential function, $exp\left[-1.01183\times10^{-6}\pi^2\left(\frac{(2p+1)^2}{0.2^2}+\frac{(2q+1)^2}{0.2^2}+\frac{(2r+1)^2}{0.1^2}\right)t\right]$. The rate is depends on time, t since $\lim_{t\to\infty} u(x,y,z,t) = 0$.

We first analyze the analytic solutions of a clay brick at the point $(0.1,0.1,0.05,n)$. The table 5.5 gives the values of $u(0.1,0.1,0.05,n\Delta t)$ when $n = 1,2,3,4$, $\Delta x = \Delta y = \Delta z = 0.01\,m$, $\Delta t = 49.41541563306090\ s$ and $s = 1/2$. We let $p = q = r$ in (5.11). The values of p are in the most left-handed column in the table, notice that for higher level of time step n, we only need a smaller value of p since an analytic solution is achieved to fourteen decimal places.

Table 5.5 Results of $u(x,y,z,t)$ in different values of p and n.

p-th term	$u(0.1,0.1,0.05,\Delta t)$ $\times 10$	$u(0.1,0.1,0.05,2\Delta t)$ $\times 10$	$u(0.1,0.1,0.05,3\Delta t)$ $\times 10$	$u(0.1,0.1,0.05,4\Delta t)$ $\times 10$
1	57.50488192010932	53.40197947767882	49.59181406713178	46.05349926208144
3	21.72346590650390	23.91177590752528	25.19057499412581	25.78612538407251
5	34.49140192060174	32.45009699881517	31.20111570741473	30.07292762190778
7	27.90110288348629	29.10757520982114	29.41545299631155	29.11891193279624
9	31.07305739345171	30.25268878806385	29.83467807695766	29.27078941026494
11	29.49590909273160	29.90156058193377	29.75641231705127	29.25350799840342
13	30.22541484255444	29.99225687061042	29.76761287714015	29.25487652728908
15	29.90774452839557	29.97250474059183	29.76639107145767	29.25480172020290
17	30.03479545714233	29.97609762890607	29.76649197928484	29.25480452540461
19	29.98800136475217	29.97555321525354	29.76648569413636	29.25480445352824
21	30.00377679887646	29.97562157913812	29.76648598854828	29.25480445478310
23	29.99891252930610	29.97561446161032	29.76648597819774	29.25480445476820
25	30.00028162891072	29.97561507452699	29.76648597847044	29.25480445476833
27	29.99993023514037	29.97561503092204	29.76648597846506	29.25480445476833
29	30.00001239785648	29.97561503348259	29.76648597846515	⋮
31	29.99999490889117	29.97561503335857	29.76648597846515	⋮
33	29.99999829578406	29.97561503336352	⋮	⋮
35	29.99999769933431	29.97561503336335	⋮	⋮
37	29.99999779481235	29.97561503336335	⋮	⋮
39	29.99999778092432	⋮	⋮	⋮
41	29.99999778275942	⋮	⋮	⋮
43	29.99999778253921	⋮	⋮	⋮
45	29.99999778256320	⋮	⋮	⋮
47	29.99999778256082	⋮	⋮	⋮
49	29.99999778256104	⋮	⋮	⋮
51	29.99999778256102	⋮	⋮	⋮
52	29.99999778256102	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮

Next, using data from the preceding table to plot a graph, which is expressed as

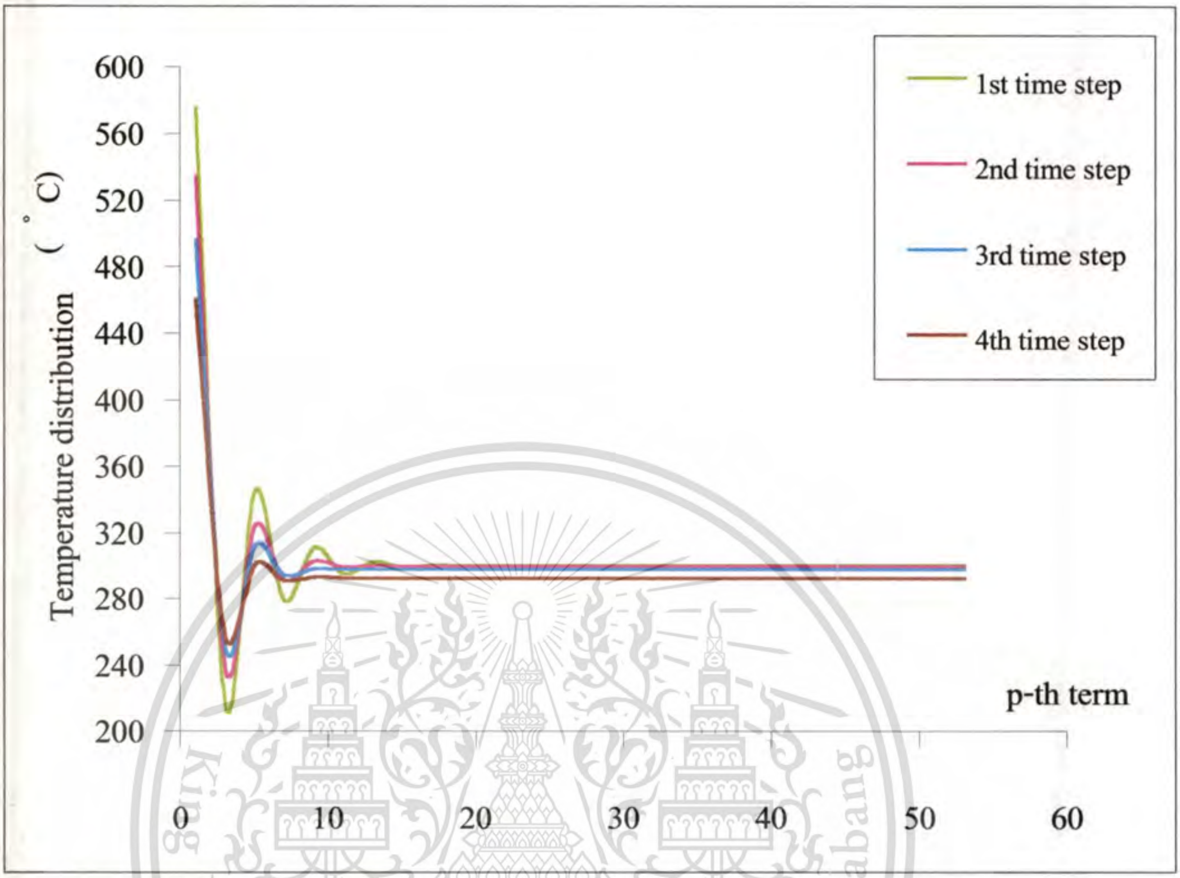

Figure 5.3 Results of $u(0.1,0.1,0.05,n\Delta t)$ when p and n are difference.

The above figure shows the oscillation of the multiple summation of the series solution (5.11) in different values of p. The graphs show that more than 20 terms of p is needed to make the series solution (5.11) smooth. Thus for high accuracy we need to use more than 20 terms of p to approximate the values of $u(0.1,0.1,0.05,n\Delta t)$ when $n = 1,2,3,4$.

For studying the decay of temperature distribution and comparing percentage error when time is varying; table 5.6 presents values of temperature distribution of $u(0.1,0.1,0.05,n\Delta t)$. Let all spatial grid separation are equal $0.005\,m$, $s = 1/2$ and $\Delta t = 12.35385390826522\,s$. To study the characteristic of p, we present analytic solution when using $p = 20$ which is showed in the most-right column and $p = 100$ in the most-left column.

Table 5.6 Decay of temperature distribution varies in time t when $s = 1/2$.

n	$u(0.1,0.1,0.05,n\Delta t)$ when use $p = 100$	Analytic Solution when use $p = 20$	
		$u(0.1,0.1,0.05,n\Delta t)$	$\lvert percentage\ error \rvert$
0	300.0000000000000	300.0000000000000	0.00000000000000
1	300.00032163322900	294.47759839252300	1.84090577324711
2	300.00032163230600	298.44465369048400	0.51855542466007
3	300.00031697480200	299.56515555459200	0.14505365347548
4	299.99997765097400	299.88001347295400	0.03998806231899
5	299.99567509838900	299.96303161330200	0.01088131856443
6	299.97358735020400	299.96480528905200	0.00292761147060
7	299.90609016161500	299.90375051621100	0.00078012600635
8	299.75615015914000	299.75553197804200	0.00020622799490
9	299.48544865004500	299.48528643643600	0.00005416410370

Using data in the preceding table to plot a graph as showed in figure 5.4. The peak of figure 5.4 occurs at $t = 0$ when temperature, $u(0.1,0.1,0.05,n\Delta t)$ decays as

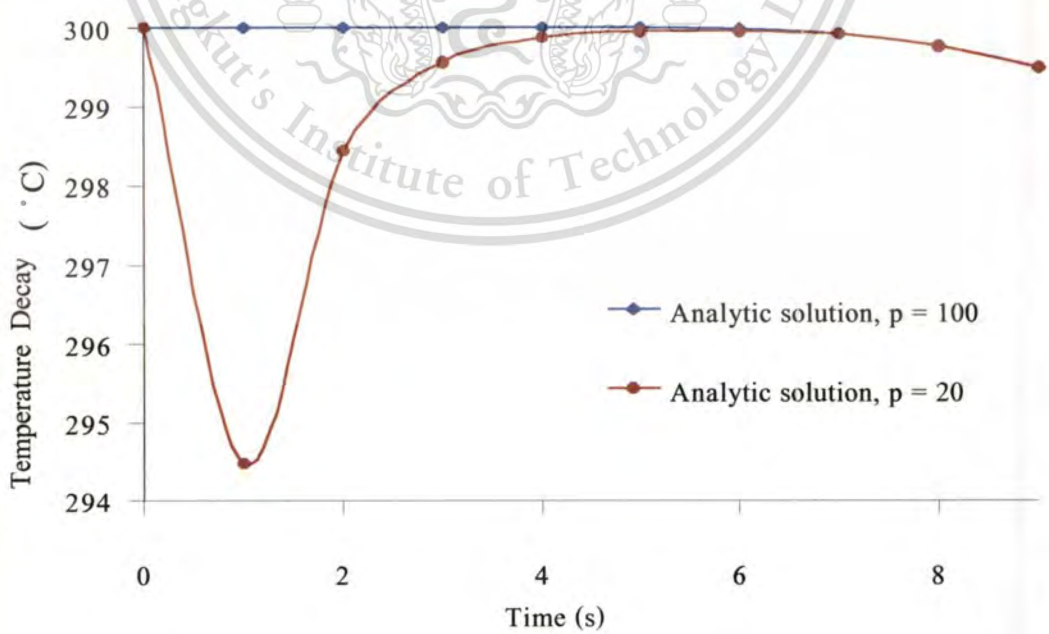

Figure 5.4 Decay of temperature distribution varies in time t when $s = 1/2$.

Because the time step separation is quite small ($\Delta t = 12.35385390826522\ s$) we need value of $p > 20$ in analytic solutions calculation. We can observe from Figure 5.4 that the analytic solutions when $p = 20$ produces a bad approximation when compared with analytic solutions when $p = 100$.

Table 5.7 presents values of temperature distribution at the grid point $(0.1, 0.1, z, n\Delta t)$ when $\Delta x = \Delta y = \Delta z = 0.01$ m, $s = 1/2$ and $\Delta t = 49.41541563306090\ s$.

Table 5.7 Characteristic of temperature distribution varies in z-direction when $s = 1/2$.

z (m)	Analytic Solution, $U(0.1, 0.1, z, n\Delta t)$		LOD Solution, $U(0.1, 0.1, z, n\Delta t)$		ADI Solution, $U(0.1, 0.1, z, n\Delta t)$	
	$n = 36$	$n = 72$	$n = 36$	$n = 72$	$n = 36$	$n = 72$
0.00	0.0000000000000	0.0000000000000	0.0000000000000	0.0000000000000	0.0000000000000	0.0000000000000
0.01	13.06780862456555	0.92680211851370	13.54281897057050	0.96156053471981	10.96625335925131	0.63410814309061
0.02	24.85644352001205	1.76288238825695	25.76238040276436	1.82916822485858	20.52430318544386	1.18681795007079
0.03	34.21194998821542	2.42639944711346	35.45933766947896	2.51766777417393	29.10786326539686	1.68327343007961
0.04	40.21855029452073	2.85240362236738	41.68531989182472	2.95972291918758	34.54401803861352	1.99776705607081
0.05	42.28828272729974	2.99919465719952	43.83062005496344	3.11204290506294	36.43090680856309	2.10700651751398
0.06	40.21855029452074	2.85240362236738	41.68531989182472	2.95972291918758	34.67704769639251	2.00566717549246
0.07	34.21194998821542	2.42639944711346	35.45933766947896	2.51766777417393	29.46378105184984	1.70420399282304
0.08	24.85644352001205	1.76288238825695	25.76238040276436	1.82916822485858	21.26299123898172	1.22988965391750
0.09	13.06780862456555	0.92680211851370	13.54281897057050	0.96156053471981	10.98120151346475	0.63517789301653
0.10	0.0000000000000	0.0000000000000	0.000000000000	0.0000000000000	0.0000000000000	0.0000000000000

Using data from table 5.7 to plot this following graph. We can notice that the peak of this graph is at the middle of z-length, $z = 0.05$ m, which shown in the following figure.

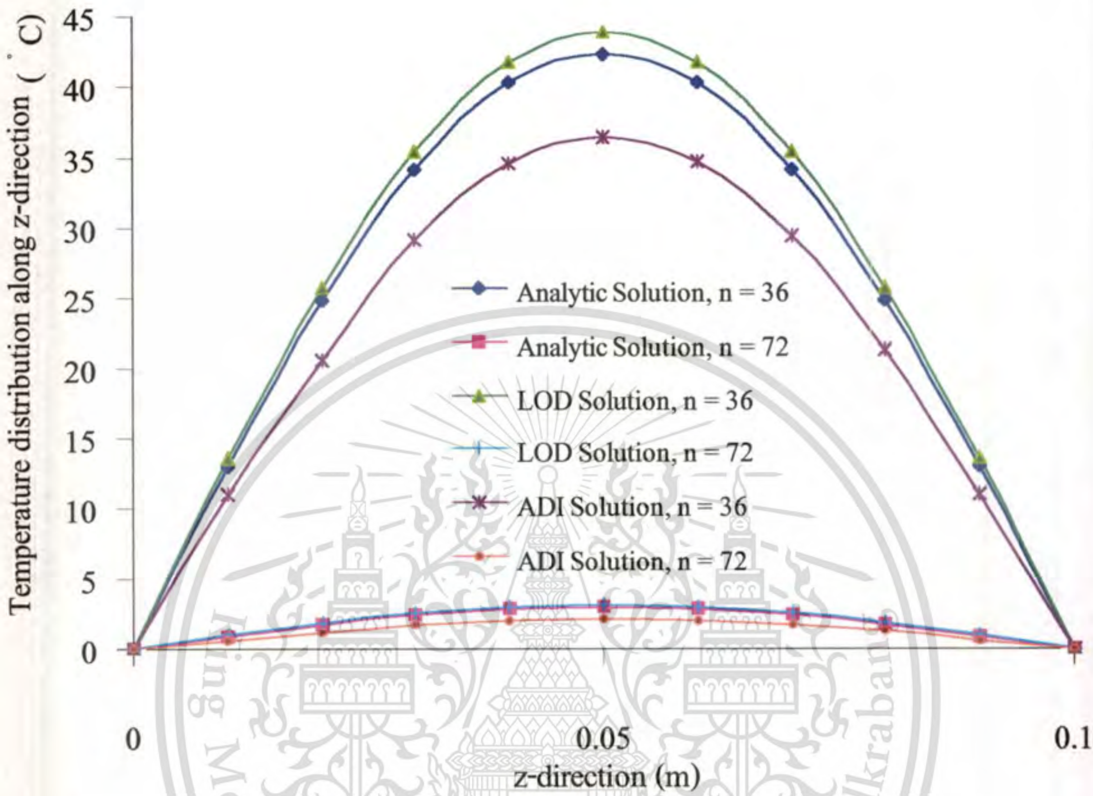

Figure 5.5 Temperature decay along z-direction when $s = 1/2$.

Figure 5.5 presents values of analytic solution, $u(0.1, 0.1, z, t)$ and numerical solution $U(0.1, 0.1, z, n\Delta t)$ when $z = 0, 0.01, 0.02, \ldots, 0.1\,m$. Let $\Delta x = \Delta y = \Delta z = 0.01\,m$, $\Delta t = 49.41541563306090\,s$. The graph is symmetry and it is in bell shape, which is put upside down. It is not surprised that the peak of graphs occurs at $0.05\,m$ in z-direction. Since all six edges of the brick is equal $0^\circ C$. We can observe that the LOD method gives a better approximation than the ADI method.

In order to compare temperature distribution when thermal diffusivity values, α are different. We first consider the clay brick, then a paving brick and a building brick respectively. The experiment carries on by considering temperature distribution when time T is about half of an hour at the point $(0.1, 0.1, 0.05, t)$. Let $\Delta x = \Delta y = \Delta z = 0.01\,m$, $s = 1/5$ in all three kinds of bricks and show values of temperature distribution for all bricks in table 5.8. Here we show the results, which are expressed as the following graphs.

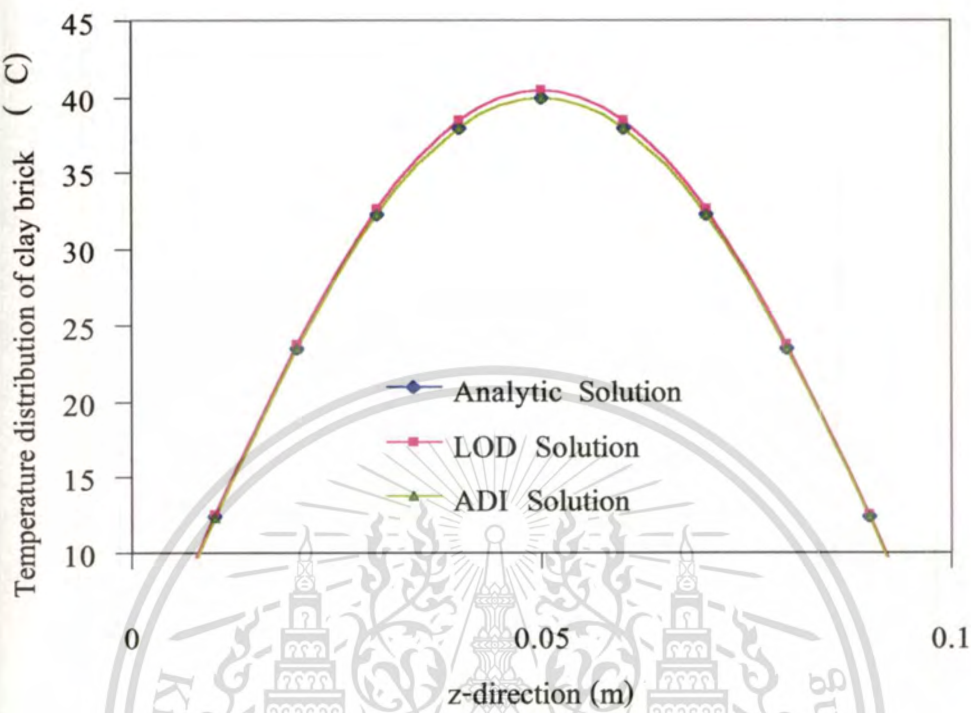

Figure 5.6 Temperature distribution of the clay brick.

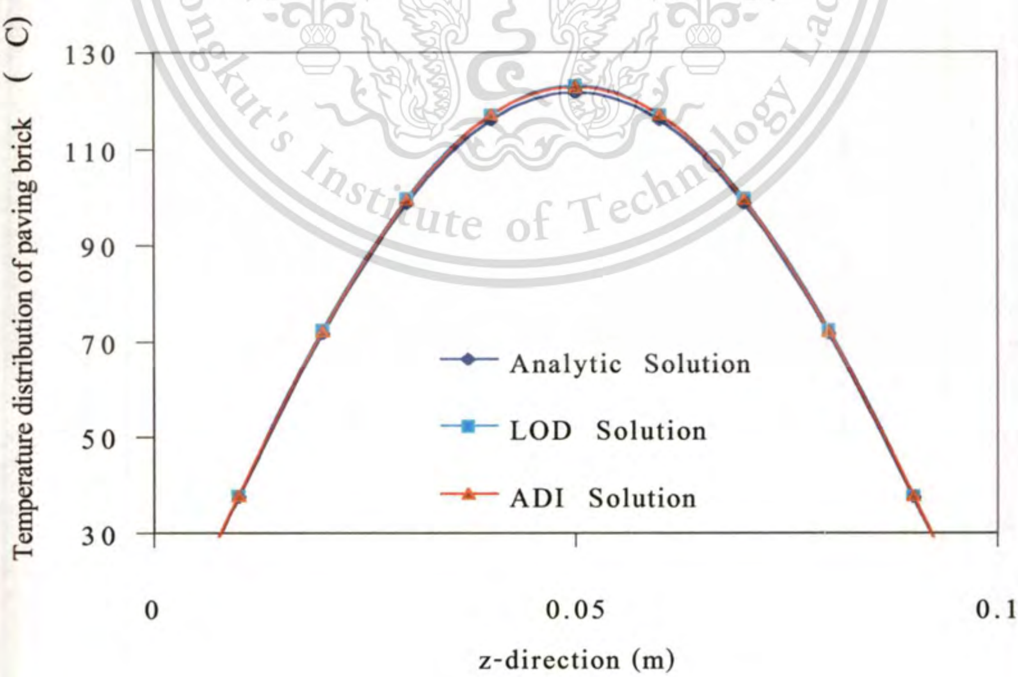

Figure 5.7 Temperature distribution of the paving brick.

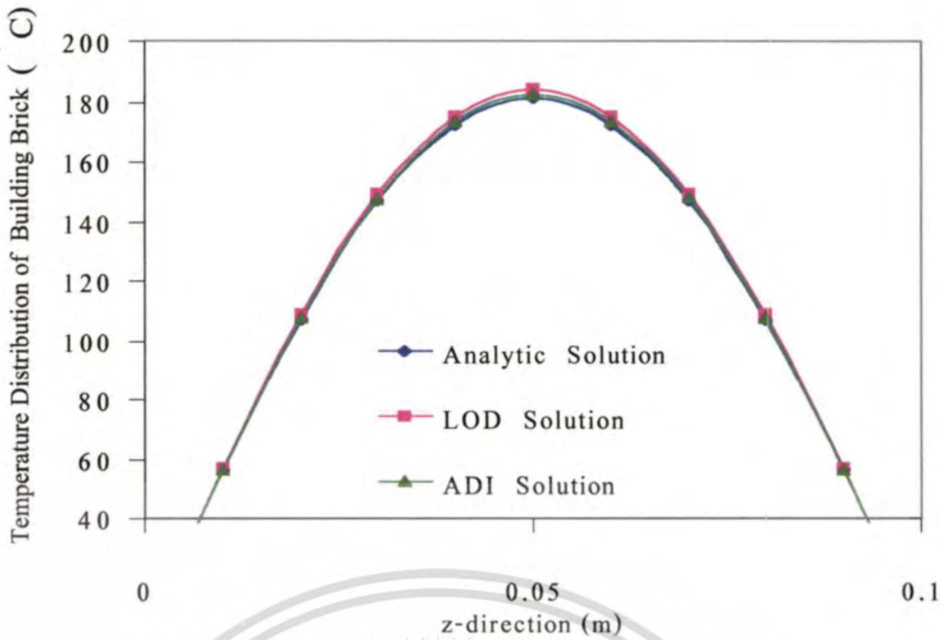

Figure 5.8 Temperature distribution of the building brick.

From Figure 5.6-5.8 we then can make a conclusion that as α is decrease the ability of heat to propagate its thermal energy is also decrease. Hence thermal diffusivity value, α, can be used as an indicator of heat distribution. The building brick propagates its thermal energy slower than other kind of bricks. Therefore this property makes it suitable for use in construction of buildings in cold climates.

Table 5.8 shows temperature distribution of three kinds of bricks at the point $(0.1, 0.1, z, T)$, for the clay brick $\Delta t = 19.7661625322436\ s$ and $T = 1818.4872952966\,4100\ s$, for the building brick $\Delta t = 50.00000000000001\ s$ and $T = 1800.00000000000000\ s$, for the paving brick $\Delta t = 34.78260869565218\ s$ and $T = 1808.69565217391300\ s$.

Table 5.8 Compares temperature distribution in three kinds of bricks when $s = 1/5$.

z (m)	Temperature of the Clay Brick at Grid Point $(0.1, 0.1, z, 92\Delta t)$			Temperature of the Building Brick at Grid Point $(0.1, 0.1, z, 36\Delta t)$			Temperature of the Paving Brick at Grid Point $(0.1, 0.1, z, 52\Delta t)$		
	Analytic	LOD	ADI	Analytic	LOD	ADI	Analytic	LOD	ADI
0	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000
0.01	12.33443453627536	12.48495209973736	12.31146374777462	56.22826535817722	57.16727619720331	56.53055474987412	37.64188860857810	38.06848588061536	37.82044560186994
0.02	23.46148484596236	23.75130157815477	23.44636097229842	106.83176924890000	108.66619877087290	107.51780505151990	71.59264846342066	72.41715962711859	71.96819798527045
0.03	32.29195704469688	32.69238580013121	32.28421876180119	146.83589168885400	149.38254060726640	147.86184801101460	98.52780522090100	99.66945718384457	99.09393212564609
0.04	37.96146603171685	38.43295848786287	37.96369720090406	172.42057643910600	175.42251876963670	173.66360187663480	115.81589938088800	117.16191219393680	116.51627235003270
0.05	39.91504501684302	40.41103195302075	39.92365152874366	181.21525977242300	184.37333086959250	182.54627886167440	121.77183322708400	123.18840021209270	122.52616365128700
0.06	37.96146603171685	38.43295848786287	37.97123526581054	172.42057643910600	175.42251876963670	173.69535286802680	115.81589938088800	117.16191219393680	116.53777317221900
0.07	32.29195704469688	32.69238580013121	32.29821613415653	146.83589168885400	149.38254060726640	147.91639329678830	98.52780522090100	99.66945718384457	99.13582920166859
0.08	23.46148484596236	23.75130157815477	23.46201271842268	106.83176924890000	108.66619877087290	107.60626344452620	71.59264846342067	72.41715962711859	72.02164861543916
0.09	12.33443453627536	12.48495209973736	12.33193062670095	56.22826535817722	57.16727619720331	56.61709305869038	37.64188860857812	38.06848588061536	37.85645835992330
0.1	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000	0.00000000000000

In order to compare the absolute of percentage errors of the numerical methods for all three kinds of bricks, using data in table 5.8 to obtain

Table 5.9 Compares the error in three kinds of bricks using data in table 5.8.

z (m)	Clay Brick		Building Brick		Paving Brick	
	|*percentage error*| of LOD method	|*percentage error*| of ADI method	|*percentage error*| of LOD method	|*percentage error*| of ADI method	|*percentage error*| of ADI method	|*percentage error*| of ADI method
0.01	1.20559183775455	0.18658048280320	1.64256704445196	0.53473629090395	1.12060477891107	0.47211763492023
0.02	1.22021410590386	0.06450414067158	1.68813259571255	0.63806715761279	1.13855772298086	0.52182704633879
0.03	1.22483797261663	0.02396924315493	1.70478350954525	0.69386142264648	1.14543812638384	0.57130330041528
0.04	1.22679198973171	0.00587711248301	1.71126395378739	0.71576624237693	1.14884845069852	0.60109455530869
0.05	1.22735528445386	0.02155742666587	1.71286762693636	0.72914063083148	1.14991913408227	0.61564844742046
0.06	1.22679198973171	0.02572798600125	1.71126395378739	0.73391510358333	1.14884845069852	0.61943331477960
0.07	1.22483797261663	0.01937905621058	1.70478350954525	0.73048131032125	1.14543812638384	0.61332414896203
0.08	1.22021410590386	0.00224990271149	1.68813259571255	0.71974824776392	1.13855772298084	0.59565444594186
0.09	1.20559183775455	0.02030427878817	1.64256704445196	0.68676733386876	1.12060477891102	0.56679827073400

From the preceding table for all three kinds of bricks, the ADI gives a smaller error than the LOD method.

Example 5.3 Next we will show an example of diffusion effect in other kind of brick. The problem presents mathematical modelling of an insulating firebrick (IFB) which were burnt until the temperature of brick is $900^{\circ}C$. Its thermal diffusivity is $7.955 \times 10^{-6}\ m^2/s$ [9]. We then take it on a grid when the surrounding temperature inside the room is $30^{\circ}C$.

Coolant, 30°C

Figure 5.9 $0.2 \times 0.1 \times 0.05\ m^3$ insulating firebrick.

For simplicity, it is assumed that the heat transfer coefficient between the brick surface and the coolant is very large $(h \to \infty)$. The mathematical modelling is

$$u_t = 7.955 \times 10^{6} (u_{xx} + u_{yy} + u_{zz}),\ 0 < x < 0.2, 0 < y < 0.1, 0 < z < 0.05, 0 < t \le T \quad (5.12)$$

subject to initial condition which is expressed as

$$u(x, y, z, 0) = 900, \qquad 0 \le x \le 0.2,\ 0 \le y \le 0.1,\ 0 \le z \le 0.05 \quad (5.13)$$

and boundary conditions are

$$u(x, y, z, t) = 30, \qquad \text{for all side edges} \quad (5.14)$$

For simplicity, we let $u(x,y,z,t)=u_0(x,y,z,t)+30$ when $u_0(x,y,z,t)$ is the solution of the original problem with homogeneous boundary conditions and its initial condition $u_0(x,y,z,0) = 870\,^\circ C$. Thus $u(x,y,z,t)$ can be expressed as

$$u(x,y,z,t)=\frac{8}{0.2\times 0.1\times 0.05}$$
$$\times\sum_{p=1}^{\infty}\sum_{q=1}^{\infty}\sum_{r=1}^{\infty}\left\{\int_0^{0.2}\left\langle\int_0^{0.1}\left[\int_0^{0.05}u_0(x,y,z,0)\,sin\left(\frac{r\pi z}{0.05}\right)dz\right]sin\left(\frac{q\pi y}{0.1}\right)dy\right\rangle sin\left(\frac{p\pi x}{0.2}\right)dx\right\}$$
$$\times sin\left(\frac{p\pi x}{0.2}\right)sin\left(\frac{q\pi y}{0.1}\right)sin\left(\frac{r\pi z}{0.05}\right)exp\left[-\alpha\pi^2 t\left(\frac{p^2}{(0.2)^2}+\frac{q^2}{(0.1)^2}+\frac{r^2}{(0.05)^2}\right)\right]+30 \qquad (5.15)$$

When $\alpha = 7.955\times 10^{-6}$.

We notice that $\lim_{t\to\infty}u(x,y,z,t)=30$. In order to present this behavior, we consider the value at the point $(0.03,0.03,z,n\Delta t)$ when $\Delta t = 6.28535512256443\,s$, $n = 50$ and $s = 1/2$ in the table 5.10 and let $\Delta t = 2.09511837418814\,s$, $n = 90$ and $s = 1/6$ in the table 5.11. In both tables we let $\Delta x = \Delta y = \Delta z = 0.01\,m$.

Table 5.10 Temperature distribution of the insulation firebrick when $s = 1/2$.

z (m)	Analytic Solution	LOD Solution		ADI Solution	
		$U(0.03,0.03,z,t)$	$\|percentage\ error\|$	$U(0.03,0.03,z,t)$	$\|percentage\ error\|$
0.00	30.0000000000000	30.0000000000000	0.0000000000000	30.0000000000000	0.0000000000000
0.01	30.00092245213359	30.00023339947634	0.00229677156877	25.54804014105378	14.84248465421147
0.02	30.00149255890514	30.00048807584744	0.00334811028395	20.47807934485005	31.74313143040052
0.03	30.00149255890514	30.00049882530433	0.00331228054358	19.65215679022499	34.49606964840231
0.04	30.00092245213359	30.00029361834579	0.00209604817586	25.60297118420390	14.65938680701106
0.05	30.0000000000000	30.0000000000000	0.0000000000000	30.0000000000000	0.0000000000000

Table 5.11 Temperature distribution of the insulation firebrick when $s = 1/6$.

z (m)	Analytic Solution	LOD Solution		ADI Solution	
		$U(0.03,0.03,z,t)$	$\|percentage\ error\|$	$U(0.03,0.03,z,t)$	$\|percentage\ error\|$
0.00	30.0000000000000	30.0000000000000	0.0000000000000	30.0000000000000	0.0000000000000
0.01	30.16944372161788	30.00000165051650	0.56163472109355	30.16901967502223	0.00140554993179
0.02	30.27416570075800	30.09467756142866	0.59287559268676	30.27347957895343	0.00226636073592
0.03	30.27416570075800	30.13254693548381	0.46778750791684	30.27347957895343	0.00226636073592
0.04	30.16944372161788	30.09088913855774	0.26037796316362	30.16901967502223	0.00140554993179
0.05	30.0000000000000	30.0000000000000	0.0000000000000	30.0000000000000	0.0000000000000

The tables show symmetry values of the analytic solutions, $u(0.03, 0.03, z, t)$ in z-direction. This is not surprising, since all boundary conditions equal 30. We obtain the results that the LOD method gives a better approximation than the ADI method when $s = 1/2$, furthermore the ADI solutions are less than 30 which is not satisfied $\lim_{t \to \infty} u(x, y, z, t) = 30$. However the ADI method gives a better approximation than the LOD method when $s = 1/6$.

From what we discussed in example 5.2, thermal diffusivity, α, plays a role as an indicator of heat distribution. When we compared α of bricks in example 5.2 and IFB in this example, α of IFB is highest when compare with other kinds of brick, so we can predict that its ability of heat distribution will be better than the other kinds of bricks. Furthermore, when we consider α in physical sense, it is a ratio of k, thermal conductivity $(cal/m\,s\,C)$ per multiple of ρ, density (kg/m^3), with c_p, specific heat $(cal/kg\,C)$: ($\alpha = k/\rho\, c_p$). We automatically obtain that if α is a high value (k is a high value or/and $\rho\, c_p$ is a small value) the object can propagate heat by conduction more than saving energy or heat distributes the energy out of the object rapidly. For the IFB, its thermal conductivity is $0.0417\,(cal/m\,s\,C)$, density is $650\ (kg/m^3)$ and heat capacity is $8.0640\ (cal/kg\,C)$. Since its density is a small value this causes its thermal diffusivity to be a high value. The typical applications of the IFB for applications are a low temperature kiln (since its temperature use limit is about $900^\circ C$). For this kind of application we need a special kind of brick, IFB, sine it can propagate heat rapidly so the heat of this brick will not exceed its heat storage.

Example 5.4 We discussed a diffusion problem with homogeneous boundary conditions in example 5.2 and a diffusion problem with nonhomogeneous boundary conditions when all boundary conditions are equal in example 5.3. Next we will show example in diffusion effects when nonhomogeneous boundary conditions are not equal. The work carries on by presenting mathematical problem of a stainless steel box.

This edge is mounted by hot surface, $100^\circ C$

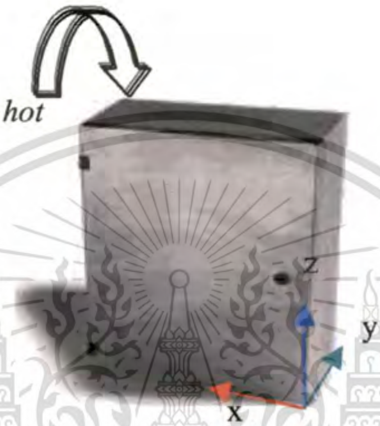

Figure 5.10 $0.3\times 0.2\times 0.5\,m^3$ stainless steel box, which its thermal diffusivity is $3.649\times 10^{-6}\,m^2/s$ [10].

Initially, a box is at a uniform temperature of $100^\circ C$ (at time $t = 0$). Then the box is mounted on a hot surface $100^\circ C$, when the surrounding temperature is denoted by $T_\infty = 27^\circ C$. Let the heat transfer coefficient between the box surface and the surrounding temperature is very large $(h \to \infty)$. The mathematical problem is

$$u_t = 3.649\times 10^{-6}\left(u_{xx}+u_{yy}+u_{zz}\right), 0<x<0.3, 0<y<0.2, 0<z<0.5, 0<t\le T \quad (5.16)$$

subject to initial condition which is expressed as

$$u(x,y,z,0)=100,\quad 0\le x\le 0.3,\ 0\le y\le 0.2,\ 0\le z\le 0.5 \quad (5.17)$$

and boundary conditions are

$u(x,y,C,t)=100,$ on the edge $z=0.5$ (5.18)

$u(x,y,z,t)=27,$ on other five edges. (5.19)

It is difficult to find $u(x,y,z,t)$ by using the technique in chapter 3. Since besides finding u_∞ by add u_1 through u_6. WE need to solve $u_0(x,y,z,t)$ which is difficult because of the function $u_0(x,y,z,0) = 100 - u_\infty(x,y,z)$. In order to avoid this task we let $u_\infty(x,y,z) = \theta(x,y,z) + T_\infty$. In the purpose of finding $\theta(x,y,z)$ we then substituting $\theta(x,y,z)=u_\infty(x,y,z)-T_\infty$ into equations (5.16)-(5.19) to obtain

$$\theta_{xx}+\theta_{yy}+\theta_{zz}=0, \quad 0\le x\le 0.3, 0\le y\le 0.2, 0\le z\le 0.5 \tag{5.20}$$

subject to boundary conditions

$\theta(x,y,C)=73,$ on the edge $z=0.5$ (5.21)

$\theta(x,y,z)=0,$ on other five edges. (5.22)

From chapter 3 by separation of variables method we obtain $\theta(x,y,z)$ which is expressed as

$$\theta(x,y,z)=\frac{200}{3}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^{0.3}\left[\int_0^{0.2}73\,sin\left(\frac{n\pi y}{0.2}\right)dy\right]sin\left(\frac{m\pi x}{0.3}\right)dx}{sinh\left(0.5\pi\sqrt{\left(\frac{m}{0.3}\right)^2+\left(\frac{n}{0.2}\right)^2}\right)}\right\} \tag{5.23}$$

$$\times\, sin\left(\frac{m\pi x}{0.3}\right)sin\left(\frac{n\pi y}{0.2}\right)sinh\left(\pi\sqrt{\left(\frac{m}{0.3}\right)^2+\left(\frac{n}{0.2}\right)^2}\,z\right).$$

From $u(x,y,z,t)=u_0(x,y,z,t)+u_\infty(x,y,z)$ and $u_\infty(x,y,z)=\theta(x,y,z)+T_\infty$ we then obtain $u(x,y,z,t)=u_0(x,y,z,t)+\theta(x,y,z)+27$, which can expressed as

$$u(x,y,z,t) = \frac{800}{3}\sum_{p=1}^{\infty}\sum_{q=1}^{\infty}\sum_{r=1}^{\infty}\left\{\int_0^{0.3}\left\langle\int_0^{0.2}\left[\int_0^{0.5} u_0(x,y,z,0)\sin\left(\frac{r\pi z}{0.5}\right)dz\right]\sin\left(\frac{q\pi y}{0.2}\right)dy\right\rangle\sin\left(\frac{p\pi x}{0.3}\right)dx\right\}$$

$$\times\sin\left(\frac{p\pi x}{0.3}\right)\sin\left(\frac{q\pi y}{0.2}\right)\sin\left(\frac{r\pi z}{0.5}\right)\exp\left[-3.649\times10^{-6}\pi^2\left(\frac{p^2}{(0.3)^2}+\frac{q^2}{(0.2)^2}+\frac{r^2}{(0.5)^2}\right)t\right]+$$

$$\frac{200}{3}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left\{\frac{\int_0^{0.3}\left[\int_0^{0.2}73\sin\left(\frac{n\pi y}{0.2}\right)dy\right]\sin\left(\frac{m\pi x}{0.3}\right)dx}{\sinh\left(0.5\pi\sqrt{\left(\frac{m}{0.3}\right)^2+\left(\frac{n}{0.2}\right)^2}\right)}\right\}\sin\left(\frac{m\pi x}{0.3}\right)\sin\left(\frac{n\pi y}{0.2}\right)\sinh\left(\pi\sqrt{\left(\frac{m}{0.3}\right)^2+\left(\frac{n}{0.2}\right)^2}\,z\right)$$

$$+27. \tag{5.24}$$

when $u_0(x,y,z,0) = 73-\theta(x,y,z)$. Though we used this technique to find the solution, which is expressed in (5.24). It still quite complicated to find the solution, need computer program. To compare analytic solutions with numerical solutions, let $\Delta x=\Delta y=\Delta z=0.02\,m$, $\Delta t = 36.5396912396\,0903\ s$ for $s=1/3$ and for $s=1/4$ we obtain $\Delta t = 27.4047684297\,0677\ s$. The result shows in table 5.12-5.13.

Table 5.12 Temperature distribution of the stainless steel box at the point $(0.06, 0.06, z, 30\Delta t)$, using $s = 1/3$.

z (m)	Analytic Solution	LOD Solution	ADI Solution
0.02	29.43541840844241	29.50994772884720	26.71666049196591
0.04	31.75295482959679	31.89725103439875	27.75545230609763
0.06	33.85191612543116	34.05473662290049	29.67419595158131
0.08	35.66159788876389	35.90828510473261	31.79505150294970
0.10	37.14764851187400	37.42201122713243	33.41207463734823
0.12	38.31113302851820	38.59713814261775	34.68953714750978
0.14	39.18167021966178	39.46436992438210	35.63985037539236
0.16	39.80729654514131	40.07287871913121	36.31196921855338
0.18	40.24395270826155	40.47907375890643	36.76448925897734
0.20	40.54683677787824	40.73761980388274	37.05383307208017

Table 5.13 Temperature distribution of the stainless steel box at the point $(0.06, 0.06, z, 30\Delta t)$, using $s = 1/4$.

z (m)	Analytic Solution	LOD Solution	ADI Solution
0.02	31.09343034365165	31.21221259850601	29.20810025919441
0.04	34.92458682580948	35.15519756520413	32.40261389069304
0.06	38.28099438338364	38.60133156880246	35.91901770994107
0.08	41.03390983418130	41.41645451719038	38.87154516189499
0.10	43.14867262717019	43.56574652776546	41.09488725765771
0.12	44.67171768657886	45.09947423787112	42.43064538549579
0.14	45.70264037375149	46.12251780508861	43.81154109714510
0.16	46.36270468094061	46.76046921799351	44.52678991894489
0.18	46.76919514907618	47.13244817522414	44.94245841741817
0.20	47.02019903153988	47.33538235928614	45.16626577082022

Using data in table 5.12-5.13 to plot graphs, which are showed in the figure 5.11 and 5.12 respectively.

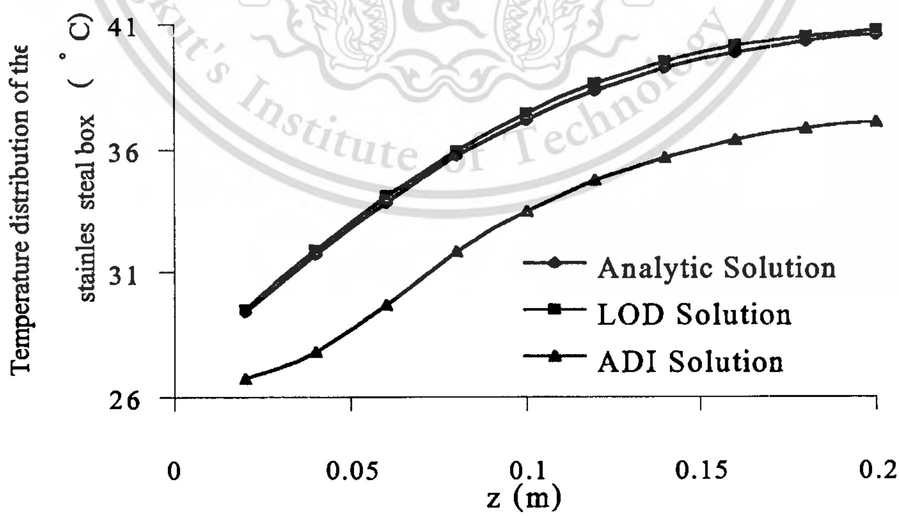

Figure 5.11 Temperature distribution of the stainless steel box using $s = 1/3$.

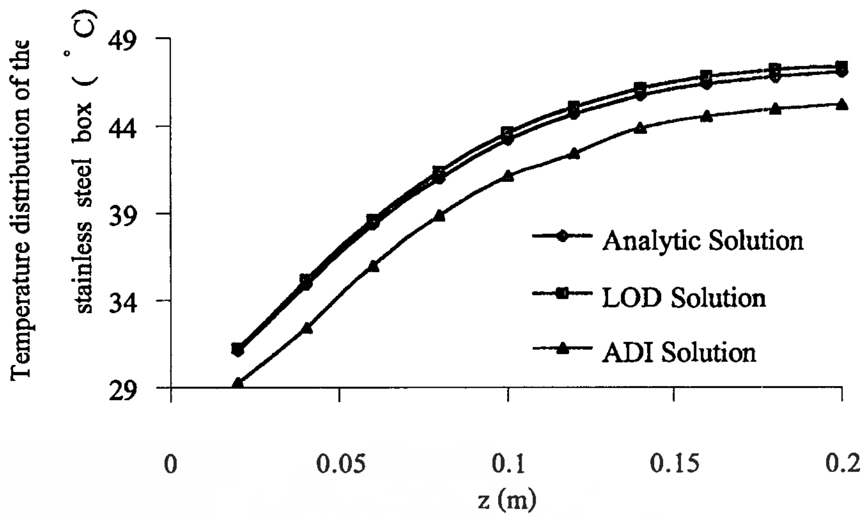

Figure 5.12 Temperature distribution of the stainless steel box using $s = 1/4$.

Consider the above graphs we observe that LOD method gives a better approximation than the ADI method. In both figures as z increases, resulting in the temperature of the stainless steel box increase, since the box is mounted by a hot surface at $z = 0.5\,m$. The LOD method gives a better approximation than the ADI method in both cases of s. However the ADI method when $s = 1/4$ gives a better approximation than $s = 1/3$.

Table 5.14-5.15 present temperature distribution of the stainless steel box at the point $(0.06, y, 0.06, 30\Delta t)$, using $s = 1/3$ in table 5.14 and $s = 1/4$ in table 5.15.

Table 5.14 Temperature distribution of the stainless steel box at the point $(0.06, y, 0.06, 30\Delta t)$, using $s = 1/3$.

y (m)	Analytic Solution	LOD Method		ADI Method	
		$U(0.06, y, 0.06, 30\Delta t)$	$\|percentage\ error\|$	$U(0.06, y, 0.06, 30\Delta t)$	$\|percentage\ error\|$
0.02	29.61819526137832	29.70155332480942	0.28144207537114	26.17353735050870	11.63020866217802
0.04	31.97919903835662	32.12896224581526	0.46831444176889	27.18615730469559	14.98799806684382
0.06	33.85191612543116	34.05473662290049	0.59914037574069	29.67419595158131	12.34116307735782
0.08	35.05367545198700	35.29028672241010	0.67499703632274	30.93917311232764	11.73772018656072
0.10	35.46764879868312	35.71586886592409	0.69984923063234	31.39273894308619	11.48908933525988
0.12	35.05367545198700	35.29028672241010	0.67499703632274	30.93917311232765	11.73772018656069
0.14	33.85191612543116	34.05473662290049	0.59914037574069	29.67419595158131	12.34116307735782
0.16	31.97919903835662	32.12896224581526	0.46831444176889	27.18615730469559	14.98799806684382
0.18	29.61819526137832	29.70155332480942	0.28144207537114	26.17353735050870	11.63020866217802

This table shows a better approximation of the LOD method when compare with the ADI method when $s = 1/3$. The temperature distribution is symmetry this is not surprising because of the boundary condition at $y = 0$ and $y = 0.2$ equal $27\ ^{\circ}C$.

Table 5.15 Temperature distribution of the stainless steel box at the point $(0.06, y, 0.06, 30\Delta t)$, using $s = 1/4$.

y (m)	Analytic Solution	LOD Method		ADI Method	
		$U(0.06, y, 0.06, 30\Delta t)$	$\lvert percentage\ error \rvert$	$U(0.06, y, 0.06, 30\Delta t)$	$\lvert percentage\ error \rvert$
0.02	31.31799109020998	33.64286021235603	7.42342992387147	28.99852413038264	7.40618053420548
0.04	35.20553010081430	36.40217897261064	3.39903665239417	32.54512493890164	7.55678200070940
0.06	38.28099438338364	40.20067354474333	5.01470557983455	35.91901770994107	6.17010271412337
0.08	40.24938854554883	43.15500966962733	7.21904413725518	37.95668766434965	5.69623779154958
0.10	40.92634047961306	44.24333529517835	8.10479211357196	38.64767052373360	5.56773444479980
0.12	40.24938854554883	43.15500966962733	7.21904413725518	37.86409817652728	5.92627728076466
0.14	38.28099438338364	40.20067354474333	5.01470557983455	35.82599069756397	6.41311367524273
0.16	35.20553010081430	36.40217897261064	3.39903665239417	32.36032925823803	8.08168726455410
0.18	31.31799109020998	33.64286021235603	7.42342992387147	28.85415147057711	7.86717006380101

Consider the above table, the LOD method gives a better approximation than the ADI method at some points. However when compare the errors of LOD solutions in table 5.14 with table 5.15, we then can make a conclusion that the LOD method when $s = 1/3$ gives a better approximation than $s = 1/4$ in this example.

CHAPTER 6

CONCLUSION AND SUGGESTIONS

6.1 Conclusion

In this section we will give a conclusion of the advantages and disadvantages of the numerical methods and the analytic method, which are summarized as

6.1.1 The LOD method

6.1.1.1 Advantages

1) It is easier to program when compared with the ADI method.

2) The method gives an accurate approximation. The MDEs which are expressed in equations (4.19)-(4.21) show that the order of the truncation errors (i.e. the first term in right hand side of equations (4.19)-(4.21), $E_x \propto (\Delta x)^4$, $E_y \propto (\Delta y)^4$ and $E_z \propto (\Delta z)^4$) are four. Hence the LOD method has fourth order of accuracy. If we plot a graph of $-log_{10}|E_x|$ against $-log_{10}(\Delta x)$ the graph will give slope four. The theoretical order of accuracy in chapter 4 can be tested by numerical experiment. The function $u(x,y,z,t) = exp(-3\alpha\pi^2 t) sin\pi x\, sin\pi y\, sin\pi z + 100xyz$ in example 5.1 will be used to find the values at grid point $(0.5,0.5,0.5,1)$, where $\alpha = 0.01$ and $\Delta x = \Delta y = \Delta z$.

The table 6.1 shows values of numerical solution by using the LOD method. The values at the grid point $(0.5,0.5,0.5,1)$ will be considered when numbers of grid spaces are 10,20,30,40,50,60 and values of s are $1/2, 1/3, 1/4, 1/5, 1/6$. Table 6.2 presents errors of LOD solutions when compared with the exact solution, $u(0.5,0.5,0.5,1) = 13.24372187941077\ ^\circ C$. We then present values of $-log_{10}(\Delta x)$ and $-log_{10}|error|$ in table 6.3 by using data in table 6.2 when $error = u - U$, u denotes an exact solution and U denotes a numerical solution.

Table 6.1 The numerical solution of the LOD method, $U(0.5,0.5,0.5,1)$, in different numbers of grid spatial separation.

Number of Grid Spacing	$U(0.5,0.5,0.5,1)$ when $s=1/2$	$U(0.5,0.5,0.5,1)$ when $s=1/3$	$U(0.5,0.5,0.5,1)$ when $s=1/4$	$U(0.5,0.5,0.5,1)$ when $s=1/5$	$U(0.5,0.5,0.5,1)$ when $s=1/6$
10	13.24374624418926	13.24372628967231	13.24372421923123	13.24372554793814	13.24372753752586
20	13.24372337982020	13.24372213605401	13.24372198903400	13.24372205735846	13.24372217413729
30	13.24372217451369	13.24372192905047	13.24372189921759	13.24372191217501	13.24372193717197
40	13.24372197265650	13.24372189501278	13.24372188544070	13.24372188930717	13.24372189817792
50	13.24372191758159	13.24372188578489	13.24372188184013	13.24372188335636	13.24372188743890
60	13.24372189781301	13.24372188248101	13.24372188057331	13.24372188128745	13.24372188350495

Table 6.2 Errors of the numerical solutions in table 6.1.

Grid spacing	Error when $s=1/2$	Error when $s=1/3$	Error when $s=1/4$	Error when $s=1/5$	Error when $s=1/6$
10	$0.2436477848988\times10^{-4}$	$0.4410261539078\times10^{-5}$	$0.23398204600511\times10^{-5}$	$0.3668527369882\times10^{-5}$	$0.56581150893464\times10^{-5}$
20	$0.0150040942870\times10^{-4}$	$0.0256643239993\times10^{-5}$	$0.01096232296049\times10^{-5}$	$0.0177947688584\times10^{-5}$	$0.02947265187458\times10^{-5}$
30	$0.0029510291987\times10^{-4}$	$0.0049639698573\times10^{-5}$	$0.00198068192958\times10^{-5}$	$0.0032764239321\times10^{-5}$	$0.00577611984909\times10^{-5}$
40	$0.0009324572936\times10^{-4}$	$0.0015602008574\times10^{-5}$	$0.00060299285565\times10^{-5}$	$0.0009896400143\times10^{-5}$	$0.00187671496121\times10^{-5}$
50	$0.0003817081939\times10^{-4}$	$0.0006374119010\times10^{-5}$	$0.00024293598244\times10^{-5}$	$0.0003945588744\times10^{-5}$	$0.00080281292725\times10^{-5}$
60	$0.0001840223973\times10^{-4}$	$0.0003070239174\times10^{-5}$	$0.0001162538509\times10^{-5}$	$0.0001876680144\times10^{-5}$	$0.00040941792179\times10^{-5}$

The following table presents values of $-log_{10}(\Delta x)$ and $-log_{10}|E|$, when E denotes an error in table 6.2. In order to find a value of Δx, for example when the number of grid spatial separation equals 10, $\Delta x = 1/10 = 0.1$.

Table 6.3 The values of $-log_{10}(\Delta x)$ and $-log_{10}|E|$ when using data in table 6.2.

$-log_{10}\Delta x$	$-log_{10}\|E\|$ when $s=1/2$	$-log_{10}\|E\|$ when $s=1/3$	$-log_{10}\|E\|$ when $s=1/4$	$-log_{10}\|E\|$ when $s=1/$	$-log_{10}\|E\|$ when $s=1/6$
1.00000000000000	4.61323753261262	5.35553565506491	5.63081746575248	5.43550823642443	5.24732822298724
1.30102999566398	5.82379021536919	6.59067017060979	6.96009740734549	6.74970764880413	6.53058078567420
1.47712125471966	6.53002649337780	7.30417086432296	7.70318526061424	7.48459991048674	7.23836380414036
1.60205999132796	7.03037104968355	7.80681948777099	8.21968783341766	8.00452275307800	7.72660168378386
1.69897000433602	7.41826851716523	8.19557983212799	8.61450815494131	8.40388818397302	8.09538564292714
1.77815125038364	7.73512931589970	8.51282779132872	8.93459265189085	8.72660974083848	8.38783315052802

Consider figure 6.1, when place $\alpha = 0.01$, $s=1/3$ and $s=1/6$ in equation (4.19)-(4.21) we obtain

$$E_x \approx -\frac{1}{54000}\frac{\partial^6 u}{\partial x^6}(\Delta x)^4, \quad E_y \approx -\frac{1}{54000}\frac{\partial^6 u}{\partial y^6}(\Delta y)^4 \quad \text{and} \quad E_z \approx -\frac{1}{54000}\frac{\partial^6 u}{\partial y^6}(\Delta y)^4 \qquad (6.1)$$

in all cases. This results the graph when $s = 1/3$ is almost superimposed the graph when $s = 1/6$.

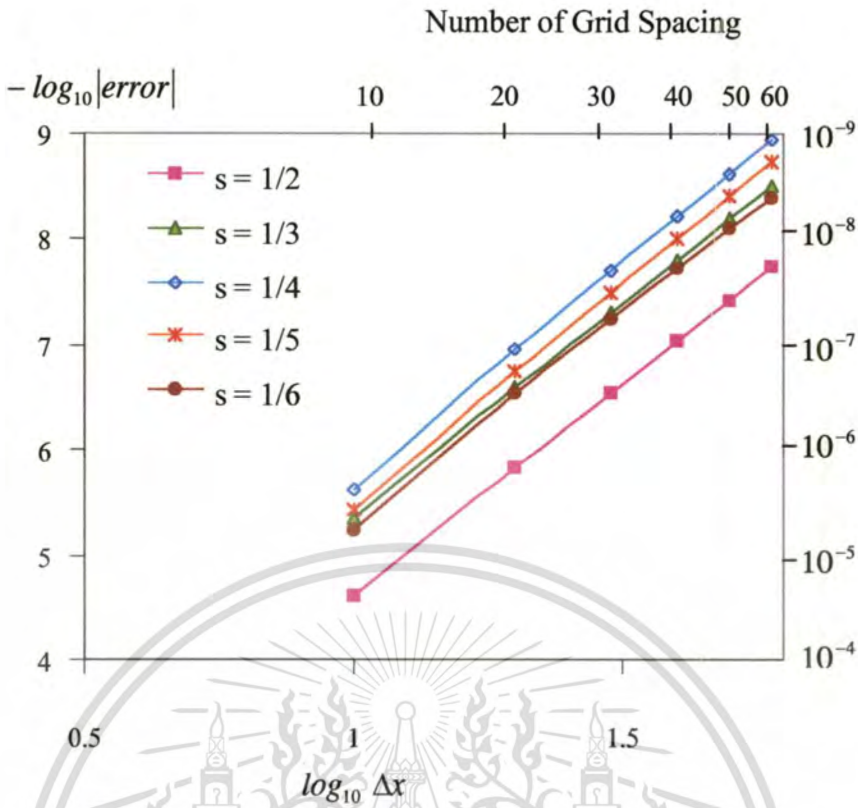

Figure 6.1 The relation between error and spatial grid separation for the LOD method.

Considering the relation between error and spatial grid separation for the LOD method in figure 6.1. For given values of $s = 1/2, 1/3, 1/4, 1/5$ and $1/6$, in all cases the slope of straight lines are about four. This guarantees the theoretical order of accuracy.

6.1.1.2 Disadvantages

1) For $\Delta x, \Delta y, \Delta z$ and Δt must be expressed in terms less than some limit which satisfy stability condition ($0 < s \leq 2/3$). In some cases, Δt must be very small to satisfy stability condition; hence resulting in long computer running times to reach a given interval of T.

2) Supplementary equations (4.5)-(4.6), (4.8)-(4.9) and (4.11)-(4.12) must be used to find the values at grid points adjacent to the boundaries, $x = 0, A, y = 0, B$ and $z = 0, C$ respectively. Hence boundary treatment must be considered.

6.1.2 The ADI method

6.1.2.1 Advantages

1) Simultaneous finite difference equations occur in the method, which can be expressed in a tridiagonal matrix. Using the Thomas algorithm can solve the matrix, which is easier than using other algorithm. This results in a faster program requiring smaller storage space as compared with the general matrix.

2) In example 5.2, which is a homogeneaous boundary conditions problem, and example 5.3, which is an inhomogeneous boundary conditions problem (all its boundary condition are equal $30^{\circ}C$), the ADI method gives a better approximation than the LOD method when we use $0 < s \leq 1/4$.

6.1.2.2 Disadvantages

1) The method is only unconditionally stable in two-dimensional problems in comparison to three-dimensional problems in which it is conditional stable method. The ADI method is stable when $0 < s \leq 1/4$, this results in the stability range of s to be smaller than LOD method.

2) It is more complicated to set up and program, since we need to solve simultaneous equations in matrix form at each time step.

3) In three-dimensional problems, the ADI method is less accurate if the problems have inhomogenous boundary conditions (when all boundary conditions are not equal, see example 5.4).

6.1.3 Analytic method (Separation of variables method)

6.1.3.1 Advantage

1) It has certain form of solution.

2) No round-off error though computer program is used to compute the solution.

6.1.3.2 Disadvantage

1) The solution is in multiple series form hence it still requires a computer program to find the solution.

2) For a problem, which has more than one inhomogeneous condition, a special technique is used to divide the original problem into problems before applying separation of variables method. This technique can only be used when initial and boundary conditions are a piecewise continuous function. The technique and method only works for time independent boundary conditions.

6.2 Suggestions

1. For diffusion problems subject to time dependent boundary conditions, using the numerical methods is easier than using analytical method. Since separation of variables method can not be used to solve this kind of problem, other methods and techniques will be used, Laplace transform, etc.

2. We also can apply numerical methods for diffusion problem with other kind of boundary conditions such as Neumann or Robin boundary conditions.

3. In other applications, the temperature distribution of the samples may be used to utilize the practical work such as the suitable temperature in brick kiln from different district, determining how long food remains cool an hour after we opened a refrigerator, heat sensor for a black box when quickly searching the exact location of an aircraft accident, etc. Considering the cockpit voice recorder (a kind of black box) which is showed in the following figure, held by the robotic arm of the remotely piloted vehicle that retrieved it.

Figure 6.2 The cockpit voice recorder from a downed airplane.

The recovered black box still in good shape so we can then apply the efficiency LOD method to study its temperature distribution.

4. For higher dimensional diffusion problems, the LOD method is a highly accurate and efficient method, which is easy to apply and use to solve the problem.

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APENDDIX A

In this section, we give basic definitions and theorems.

Definition A.1 Let M be any set. A metric for M is a function ρ with domain $M \times M$ and range contained in $[0, \infty)$ such that

1. $\rho(x,x) = 0,$ $\qquad (x \in M)$
2. $\rho(x,y) > 0,$ $\qquad (x, y \in M, x \neq y)$
3. $\rho(x,y) = \rho(y,x),$ $\qquad (x, y \in M)$
4. $\rho(x,y) \leq \rho(x,z) + \rho(z,y)$ $\qquad (x, y, z \in M).$

If ρ is a metric for M, the ordered pair $\langle M, \rho \rangle$ is called a *metric space*.

Definition A.2 Let $\langle M, \rho \rangle$ be a metric space and let $\{S_n\}_{n=1}^{\infty}$ be a sequence of points in M. We say that $\{S_n\}_{n=1}^{\infty}$ is a Cauchy sequence if given $\varepsilon > 0$, there exists $N \in I$ such that

$$\rho(S_m, S_n) < \varepsilon \ , \qquad (m, n) \geq N .$$

Let X be a vector space over a scalar field (the real numbers R or the complex numbers C) on which we have defined a norm $\|\cdot\|$; i.e.; for every $x \in X$, $\|x\|$ is a nonnegative real number satisfying the following properties

1. $\|x\| = 0$ if and only if $x = 0$
2. $\|\alpha x\| = |\alpha| \cdot \|x\|$ for all scalar α
3. $\|x + y\| \leq \|x\| + \|y\|$.

The norm induces a distant function $d(x, y) = \|x - y\|$ so that X is a metric, called a normed vector space. If the normed vector space X is a complete metric space (i.e. all Cauchy sequence converge), then we shall call X, a *Banach space*.

Definition A.3 Let $\langle M, \rho \rangle$ be a metric space. If $a \in M$ and $x > 0$, then $B[a; r]$ is defined to be the set of all points in M where distance to a is less than r that is

$$B[a; r] = \{x \in M \,/\, \rho(x, a)\} < r .$$

Definition A.4 Let M be a metric space. We say that the subset G of M is an *open subset* of M (or, more simply, that G is open) if for every $x \in G$, there exist a number $r > 0$ such that the entire open ball $B[x; r]$ is contained in G.

Theorem A.1 Let $\langle M, \rho \rangle$ be a metric space and let A be a subset of M. Then if A has either one of the following properties, it has the other

1. It is impossible to find nonempty subsets A_1, A_2 of M such that $A = A_1 \cup A_2$, $\overline{A_1} \cap A_2 = \phi$, $A_1 \cap \overline{A_2} = \phi$. (Here $\overline{A_i}$ means the closure of A_i in $\langle M, \rho \rangle$).

2. When $\langle A, \rho \rangle$ is itself regarded as a metric space, then there is no set except A and ϕ which is both open and closed in $\langle A, \rho \rangle$.

Definition A.5 Let $\langle M; \rho \rangle$ be a metric space and let A be a subset of M. If A has either (and hence both) of the properties 1 and 2 of theorem 1, we say that A is *connected.*

Definition A.6 Let $\langle M, \rho \rangle$ be a metric space. We say that the subset A of M is *bounded* if there exists a positive number L such that

$$\rho(x, y) \leq L, \quad (x, y \in A).$$

Definition A.7 Let E be a subset of the metric space M. A point $x \in M$ is called a *limit point* of E if there is a sequence $\{x_n\}_{n=1}^{\infty}$ of points of E which converges to x. The set $\overline{E}$ of all limit point E is called the *closure* of E.

Definition A.8 Let $\sum_{n=1}^{\infty} a_n$ be a series of real numbers

1. If $\sum_{n=1}^{\infty} |a_n|$ converges, we say that $\sum_{n=1}^{\infty} a_n$ *converges absolutely.*
2. If $\sum_{n=1}^{\infty} a_n$ converges but $\sum_{n=1}^{\infty} |a_n|$ diverges, we say that $\sum_{n=1}^{\infty} a_n$ *converges conditionally.*

Definition A.9 A problem is *well posed* if a solution exists, unique and depends continuous on its data.

Definition A.10 If there exists a subdivision $\sigma = \{a = a_0 < a_1 < \cdots \; a_{n-1} < a_n = b\}$ of $[a, b]$ such that f is continuous on each of the open subintervals $(a_{\nu-1}, a_\nu)$ when $(\nu = 1,2,\ldots,n)$. The function f is called a *piecewise continuous function*.

Principle of Superposition : If u_1 and u_2 satisfy a linear homogeneous equation, then an arbitrary linear combination of them, $c_1u_1 + c_2u_2$, also satisfies the same linear homogeneous equation.

Considering, the kernel $K(s,t)$, could be expanded in a series

$$K(s,t) = \sum_{i=1}^{\infty} \frac{\varphi_i(s)\varphi_i(t)}{\lambda_i} \tag{A.1}$$

which would converge uniformly in each variable, then it would follow that every function $g(s)$ of the form

$$g(s) = \int K(s,t)h(t)dt \tag{A.2}$$

where $h(t)$ is any piecewise continuous function, could be expanded in the series

$$g(s) = \sum_{i=1}^{\infty} g_i \varphi_i(s) \tag{A.3}$$

when $g_i = (g, \varphi_i) = \dfrac{(h, \varphi_i)}{\lambda_i}$.

Theorem A.2 (Fundamental Expansion)[15] Every continuous functions $g(s)$ which, as in (A.2), is an integral transform with symmetric kernel $K(s,t)$ of a piecewise continuous function $h(t)$, can be expanded in a series in the eigenfunctions of $K(s,t)$; this series converges uniformly and absolutely.

APPENDIX B

B.1 Von Neumann Stability

The most widely used procedure for determining the stability (or instability) of finite difference approximation is called *von Neumann stability* [12-14]. In essence, it introduces errors as represented by a finite Fourier series and then considers the growth (or decay) of these errors as x increase. The procedure applies only to linear, constant coefficient problem. Because of the linearity, each Fourier component can be treated separately and superposition used to add all other components.

For simplicity, consider any finite difference approximation in which $u_{r,s}$ is a scalar quantity. Now we introduce a decomposition of the error at grid points on a given x level

$$U(y) = \sum_{p}^{P} \Delta_p e^{i\beta_p y} \tag{B.1}$$

where p is equal to the number of grid points on the x line, $|\beta_p|$ is the frequency of the error, and i is the complex number $\sqrt{-1}$. Because of linearity we need only consider one of these p terms and thus only need $e^{i\beta_p y}$ (where β_p is real). Hence we can write the solution of the FDM in separate form as

$$U(x,y) \approx e^{\gamma x} e^{i\beta y} \tag{B.2}$$

where $\gamma = \gamma(\beta)$ is, in general, complex. Note that the solution at $x = 0$ equals the error introduced at $x = 0$. We see from (B.2) that in order for the original error not to grow as x increases, we need

$$\left| e^{\gamma x} \right| \leq 1 \tag{B.3}$$

for all γ. Alternatively, we may write this condition for stability as

$$\left| e^{\gamma h} \right| \leq 1 \tag{B.4}$$

which is call von Neumann condition. For convenient, one defines $G \equiv e^{\gamma h} \equiv$ the *amplification factor* and thus the stability constraint (B.4) becomes

$$|G| \leq 1. \tag{B.5}$$

B.2 Stability of the LOD Method

In this section, the stability of the LOD method by using von Neumann stability will be presented. In 1986, B.J. Noye and K.J. Hayman publised a journal entitled "An Accurate Five-Point Explicit Finite Difference Method for Solving the One-Dimensional Linear Diffusion Equation" [5]. In this journal, Noye and Hayman presented stability range of (4.25). In order to show the stability range of (4.25), we first consider the value of $\beta_1 = m\pi$ when $m \in I$, if $\Delta x = h \in I$ we then obtain $\cos\beta_1 h = \pm 1$. Consider the case $\cos\beta_1 h = 1$, equation (4.25) reduces to $G = 1$, so (4.26) is satisfied. If $\cos\beta_1 h = -1$, equation (4.25) becomes

$$G = 1 - \frac{s_x}{3}(16 - 24s_x) \tag{B.6}$$

from which (4.26) requires that

$$0 < s_x \leq 2/3. \tag{B.7}$$

For $\Delta x \notin I$, we find that the extremum of the function $\cos\beta_1 h$ in (4.25) occurs at

$$\cos\beta_1 h = \frac{6s_x - 4}{6s_x - 1} \tag{B.8}$$

which when substitute into (4.25) gives

$$G = \frac{3s_x - 1}{6s_x + 1} \tag{B.9}$$

and this satisfies the condition (4.26) for all positive values of s_x, combining all the above results leads to the conclusion that the FDE is stable over the interval $(0, 2/3]$.

APPENDIX C

Here, we will demonstrate the work on finding $u_0(x, y, z, t)$ that satisfies equations (3.56)-(3.58), by using separation of variables method, defining

$$u_0(x, y, z, t)=\psi(x, y, z)T(t). \tag{C.1}$$

Substituting equation (C.1) into equation (3.56), yields

$$\frac{T'(t)}{T(t)}=\frac{\alpha}{\psi(x, y, z)}(\psi_{xx}+\psi_{yy}+\psi_{zz})=-\mu \tag{C.2}$$

hence we obtain

$$T'+\mu T = 0 \tag{C.3}$$

$$\alpha(\psi_{xx}+\psi_{yy}+\psi_{zz})+\mu\psi = 0 \tag{C.4}$$

in which its boundary conditions are $\psi(0, y, z)=\psi(A, y, z)=\psi(x,0, z)=\psi(x, B, z)=$ $\psi(x, y,0)=\psi(x, y, C)=0$.

Using separation of variable method again for problem (C.4), and letting

$$\psi(x, y, z)= X(x)Y(y)Z(z) \tag{C.5}$$

insert this equation into equation (C.4), we have

$$\frac{X''}{X}=-\frac{Y''}{Y}-\frac{Z''}{Z}-\frac{\mu}{\alpha}=-\lambda^2 \tag{C.6}$$

then

$$X'' + \lambda^2 X = 0 \tag{C.7}$$

and

$$-\frac{Y''}{Y} - \frac{Z''}{Z} = \frac{\mu}{\alpha} - \lambda^2 \tag{C.8}$$

Seeking orthogonality in the two homogeneous directions, we set the y-dependent term of equation (C.8) equal to $-\beta^2$ and the z-dependent term to $-\gamma^2$, to obtain

$$Y'' + \beta^2 Y = 0 \tag{C.9}$$

$$Z'' + \gamma^2 Z = 0 \tag{C.10}$$

for any values at the separation constants $-\lambda^2$, $-\beta^2$ and $-\gamma^2$

$$\mu = \alpha\left(\lambda^2 + \beta^2 + \gamma^2\right) \tag{C.11}$$

thus we can then express (C.3) as

$$T' + \alpha\left(\lambda^2 + \beta^2 + \gamma^2\right)T = 0\,. \tag{C.12}$$

Solving the above ordinary differential equations (C.7), (C.9)-(C.10) and (C.12), by substituting the solution into the equation (C.1) yields

$$u_0(x, y, z, t) = (A_1\, sin(\lambda x) + A_2\, cos(\lambda x))\,(A_3\, sin(\beta\, y) + A_4\, cos(\beta\, y))$$
$$(A_5\, sin(\gamma\, z) + A_6\, cos(\gamma\, z))\, exp\left\{-\alpha\left(\lambda^2 + \beta^2 + \gamma^2\right)t\right\}. \tag{C.13}$$

To evaluate the constants A_1 to A_6 , λ , β and γ, we will make use of the conditions (3.57) as well as the orthogonality property of the sine functions. One immediately notices that boundary condition (3.57) when $x = y = z = 0$, yields

$$A_2 = A_4 = A_6 = 0. \qquad (C.14)$$

Next, applying other boundary conditions, yields

$$\lambda_p = \frac{p\pi}{A}, \qquad p = 1,2,3\ldots \qquad (C.15)$$

$$\beta_q = \frac{q\pi}{B}, \qquad q = 1,2,3\ldots \qquad (C.16)$$

$$\gamma_r = \frac{r\pi}{C}, \qquad r = 1,2,3\ldots \qquad (C.17)$$

Combining equations (C.13)-(C.17) we then summarize the expression for the diffusion as follows

$$u_{0,pqr} = A_{pqr}\ sin\left(\frac{p\pi x}{A}\right) sin\left(\frac{q\pi y}{B}\right) sin\left(\frac{r\pi z}{C}\right)\ exp\left(-\alpha\pi^2\left(\frac{p^2}{A^2}+\frac{q^2}{B^2}+\frac{r^2}{C^2}\right)t\right). \qquad (C.18)$$

The constant A_{pqr} was obtained by combining the constants A_1, A_3 and A_5. The subscript p, q, r accounts for all values of $p, (p = 1,2,3,\ldots)$, all values of $q, (q = 1,2,3,\ldots)$ and all values of $r, (r = 1,2,3,\ldots)$ yield solutions for the problem. Based on the above, the general solution for the diffusion is the linear combination

$$u_0 = \sum_{p=1}^{\infty}\sum_{q=1}^{\infty}\sum_{r=1}^{\infty} A_{pqr}\ sin\left(\frac{p\pi x}{A}\right)\times exp\left(\frac{-\alpha\pi^2 p^2 t}{A^2}\right)$$
$$\times sin\left(\frac{q\pi y}{B}\right)\times exp\left(\frac{-\alpha\pi^2 q^2 t}{B^2}\right)\times sin\left(\frac{r\pi z}{C}\right)\times exp\left(\frac{-\alpha\pi^2 r^2 t}{C^2}\right) \qquad (C.19)$$

where the exponential term was conveniently split into three parts. We notice that the quantity $\sum_{p=1}^{\infty} A_{pqr}\, sin\left(\frac{p\pi x}{A}\right) exp\left(\frac{-\alpha\pi^2 p^2 t}{A^2}\right)$ depends only on q and r when specific values have been assigned on the index p, defining

$$G_{qr}(x,t) = \sum_{p=1}^{\infty} A_{pqr}\, sin\left(\frac{p\pi x}{A}\right) exp\left(\frac{-\alpha\pi^2 p^2 t}{A^2}\right). \tag{C.20}$$

Combining equation (C.19) and (C.20) yields

$$u_0(x,y,z,t) = \sum_{q=1}^{\infty}\sum_{r=1}^{\infty} G_{qr}(x,t)\left\{ sin\left(\frac{q\pi y}{B}\right) exp\left(\frac{-\alpha\pi^2 q^2 t}{B^2}\right)\right\} \times \left\{ sin\left(\frac{r\pi z}{C}\right) exp\left(\frac{-\alpha\pi^2 r^2 t}{C^2}\right)\right\}. \tag{C.21}$$

Similarly, the quantity $\sum_{q=1}^{\infty} G_{qr}(x,t)\, sin\left(\frac{q\pi y}{B}\right) exp\left(\frac{-\alpha\pi^2 q^2 t}{B^2}\right)$ depends only on r (after the summation is carried out) we can then define

$$G_r(x,y,t) = \sum_{q=1}^{\infty} G_{qr}(x,t)\, sin\left(\frac{q\pi y}{B}\right) exp\left(\frac{-\alpha\pi^2 q^2 t}{B^2}\right). \tag{C.22}$$

Combining equation (C.19) and (C.22) yields

$$u_0(x,y,z,t) = \sum_{r=1}^{\infty} G_r(x,y,t)\, sin\left(\frac{r\pi z}{C}\right) exp\left(\frac{-\alpha\pi^2 r^2 t}{C^2}\right). \tag{C.23}$$

Next, we apply the initial condition (3.58)

$$u_0(x,y,z,0) = F(x,y,z) - u_\infty(x,y,z) = \sum_{r=1}^{\infty} G_r(x,y,0)\, sin\left(\frac{r\pi z}{C}\right). \tag{C.24}$$

Utilizing the orthogonality property of the sine function in equation (C.24), we obtain

$$G_r(x,y,0) \;=\; \frac{2}{C}\int_0^C \left(F(x,y,z)-u_\infty(x,y,z)\right)sin\left(\frac{r\pi\, z}{C}\right)\,dz\,. \tag{C.25}$$

From (C.22) we have

$$G_r(x,y,0) = \sum_{q=1}^{\infty} G_{qr}(x,0)\,sin\left(\frac{q\pi y}{B}\right)$$
$$= \frac{2}{C}\int_0^C \{F(x,y,z)-u_\infty(x,y,z)\}\,sin\left(\frac{r\pi z}{C}\right)\,dz\,. \tag{C.26}$$

Utilizing the orthogonality property of the *sine* function in equation (C.26), to obtain

$$G_{qr}(x,0) = \frac{4}{BC}\int_0^B\left[\int_0^C \{F(x,y,z)-u_\infty(x,y,z)\}\,sin\left(\frac{r\pi z}{C}\right)\,dz\right]sin\left(\frac{q\pi y}{B}\right)\,dy\,. \tag{C.27}$$

Combining equation (C.20) and (C.27) and applying the orthogonality property of the sine function yields the final expression for A_{pqr}

$$A_{pqr} = \frac{8}{ABC}\int_0^A\left\langle\int_0^B\left[\int_0^C \{F(x,y,z)-u_\infty(x,y,z)\}\,sin\left(\frac{r\pi z}{C}\right)\,dz\right]sin\left(\frac{q\pi y}{B}\right)dy\right\rangle sin\left(\frac{p\pi x}{A}\right)dx. \tag{C.28}$$

Substituting equation (C.28) into equation (C.19) results in the diffusion

$$u_0(x,y,z,t) = \frac{8}{ABC}\sum_{p=1}^{\infty}\sum_{q=1}^{\infty}\sum_{r=1}^{\infty}\left\{\int_0^A\left\langle\int_0^B\left[\int_0^C u_0(x,y,z,0)\,sin\left(\frac{r\pi z}{C}\right)dz\right]sin\left(\frac{q\pi y}{B}\right)dy\right\rangle sin\left(\frac{p\pi x}{A}\right)\,dx\right\}$$
$$\times\, sin\left(\frac{p\pi x}{A}\right)sin\left(\frac{q\pi y}{B}\right)sin\left(\frac{r\pi z}{C}\right)exp\left[-\alpha\pi^2\left(\frac{p^2}{A^2}+\frac{q^2}{B^2}+\frac{r^2}{C^2}\right)t\right]. \tag{C.29}$$

Considering (C.25) when initial temperature $u(x,y,z,0)$ is a constant and the diffusion problem has homogeneous boundary conditions, we obtain

$$G_r(x,y,0) = \frac{2}{C}H\int_0^C sin\left(\frac{r\pi z}{C}\right) dz = \frac{2H}{Cr\pi}(1 - cos\, r\pi)$$

$$= \begin{cases} 0, & r \text{ are even} \\ \dfrac{16H}{qrBC\pi^2}, & r \text{ are odd} \end{cases} \tag{C.30}$$

when $H = u(x, y, z, 0)$. Since $cos\, r\pi = (-1)^r$ which is equal 1 when r is an even and -1 for r is an odd, to obtain (C.30) as

$$G_r(x,y,0) = \frac{2H}{Cr\pi}\left(1-(-1)^r\right). \tag{C.31}$$

In the same manner, as the preceding procedure, to obtain $G_{qr}(x,0)$ in (C.27) which is expressed as

$$G_r(x,y,0) = \frac{4H}{BCqr\pi^2}\left(1-(-1)^q\right)\left(1-(-1)^r\right)$$

$$= \begin{cases} 0, & q \text{ or } r \text{ are even} \\ \dfrac{16H}{qrBC\pi^2}, & p \text{ and } r \text{ are odd} \end{cases} \tag{C.32}$$

and A_{pqr} in (C.28) as

$$A_{pqr} = \frac{8H}{ABCpqr\pi^3}\left(1-(-1)^p\right)\left(1-(-1)^q\right)\left(1-(-1)^r\right)$$

$$= \begin{cases} 0, & p \text{ or } q \text{ or } r \text{ are even} \\ \dfrac{64H}{pqrABC\pi^3}, & p \text{ and } q \text{ and } r \text{ are odd} \end{cases} \tag{C.33}$$

hence we can manipulate (C.29) as

$$u_0(x,y,z,t) = \sum_{p=1}^{\infty}\sum_{q=1}^{\infty}\sum_{r=1}^{\infty} A_{pqr}\, sin\left(\frac{p\pi x}{A}\right) sin\left(\frac{q\pi y}{B}\right) sin\left(\frac{r\pi z}{C}\right) exp\left[-\alpha\pi^2\left(\frac{p^2}{A^2}+\frac{q^2}{B^2}+\frac{r^2}{C^2}\right)t\right] \tag{C.34}$$

since A_{pqr} equals 0 when p,q or r is an even, and A_{pqr} equals $\frac{64H}{ABCpqr\pi^3}$ when p,q and r are odds. Thus

$$u_0(x,y,z,t)=\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\sum_{r=0}^{\infty}A_{(2p+1)(2q+1)(2r+1)}\, sin\left(\frac{(2p+1)\pi x}{A}\right)sin\left(\frac{(2q+1)\pi y}{B}\right)sin\left(\frac{(2r+1)\pi z}{C}\right)$$
$$\times exp\left[-\alpha\pi^2\left(\frac{(2p+1)^2}{A^2}+\frac{(2q+1)^2}{B^2}+\frac{(2r+1)^2}{C^2}\right)t\right] \qquad \text{(C.35)}$$

when $A_{(2p+1)(2q+1)(2r+1)} = \dfrac{64H}{(2p+1)(2q+1)(2r+1)ABC\pi^3}$. The above computation and manipulation of $u_0(x,y,z,t)$ demonstrates that only odd terms are desired in (C.35). Hence, for diffusion problems in which all boundary conditions are zero, it requires a shorter time in running a computer program as compared to other kinds of boundary conditions (constant boundary conditions etc.). It shows that for computing $u_0(x,y,z,t)$ only odd terms of summation are used in (C.35).

APPENDIX D

D.1 Thomas Algorithm

We start this appendix by introducing a popular algorithm for solving a tridiagonal matrix, it is known as the *Thomas algorithm*. Consider the matrix equation, which can be expressed as

$$Tx = b \tag{D.1}$$

where T is a tridiagonal matrix. Augmenting T with b and writing in expanded form, we obtain

$$\left[\begin{array}{ccccccccc|c} a_{11} & a_{12} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & b_1 \\ a_{21} & a_{22} & a_{23} & 0 & 0 & \cdots & 0 & 0 & 0 & b_2 \\ 0 & a_{32} & a_{33} & a_{34} & 0 & \cdots & 0 & 0 & 0 & b_3 \\ 0 & 0 & a_{43} & a_{44} & a_{45} & \cdots & 0 & 0 & 0 & b_4 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} & b_{n-1} \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & a_{n,n-1} & a_{n,n} & b_n \end{array}\right]. \tag{D.2}$$

For simplicity, the tridiagonal matrix T will be stored as the three singly subscripted column vectors l, d and u. The elements $d_1, d_2, \ldots, d_n$ correspond to the major diagonal elements a_{ii} of the full matrix T. The elements $l_2, l_3, \ldots, l_n$ correspond to the elements below the major diagonal of T are elements $a_{i,i-1}$ of the full T matrix. The elements $u_1, u_2, \ldots, u_{n-1}$ correspond to the elements above the major diagonal of T are $a_{i,i+1}$ elements in the full T matrix. The elements l_1 and u_n do not exist.

Equation (D.1), when expressed in terms of the l, d and u column vectors, becomes

$$\begin{bmatrix} d_1 & u_1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ l_2 & d_2 & u_2 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & l_3 & d_3 & u_3 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & l_4 & d_4 & u_4 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & l_{n-1} & d_{n-1} & u_{n-1} \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & l_n & d_n \end{bmatrix} [x_i] = [b_i]. \tag{D.3}$$

Augmenting the T matrix by the b vector and performing the row reduction operations yields

$$\left[\begin{array}{ccccccccc|c} d_1 & u_1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & b_1 \\ l_2 & d_2 & u_2 & 0 & 0 & \cdots & 0 & 0 & 0 & b_2 \\ 0 & l_3 & d_3 & u_3 & 0 & \cdots & 0 & 0 & 0 & b_3 \\ 0 & 0 & l_4 & d_4 & u_4 & \cdots & 0 & 0 & 0 & b_4 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & l_{n-1} & d_{n-1} & u_{n-1} & b_{n-1} \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & l_n & d_n & b_n \end{array}\right] R_2 - \frac{l_2}{d_1} R_1 . \tag{D.4}$$

This procedure is repeated until l_n has been eliminated from row n.

The first row of T is unchanged. All the elements of l are reduced to zero exactly, without calculation. The row elimination multipliers, (l_i / d'_{i-1}), can be stored in place of the elements of l. Since the elements above the elements of u are all zero, name of the elements of u are changed, so they are not recalculated. Consequently, the only terms that need to be recalculated in the T matrix are the elements of d. The elements of the b vector must be recalculated, corresponding to the row operations indicated in equation (D.4). The upper triangularized T matrix and the transformed b vector become

$$\left[\begin{array}{ccccccccc|c} d_1 & u_1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & b_1 \\ (l_2/d_1) & d_2' & u_2 & 0 & 0 & \cdots & 0 & 0 & 0 & b_2' \\ 0 & (l_3/d_2') & d_3' & u_3 & 0 & \cdots & 0 & 0 & 0 & b_3' \\ 0 & 0 & (l_4/d_3') & d_4' & u_4 & \cdots & 0 & 0 & 0 & b_4' \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & (l_{n-1}/d_{n-2}') & d_{n-1}' & u_{n-1} & b_{n-1}' \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & (l_n/d_{n-1}') & d_n' & b_n' \end{array}\right] \quad \text{(D.5)}$$

The row reduction equations are

$$d_i' = d_i - \frac{l_i}{d_{i-1}'} u_{i-1}, \qquad i = 1,2,3,\ldots,n. \qquad \text{(D.6)}$$

The elements of the transformed b vector are computed from

$$b_1' = b_1 \qquad \text{(D.7)}$$

$$b_i' = b_i - \frac{l_i}{d_{i-1}'} b_{i-1}', \qquad i = 1,2,3,\ldots,n. \qquad \text{(D.8)}$$

The computation of the transformed b vector can be done after the reduction of the T matrix by using the elimination multipliers stored in place of the l vector. The solution vector x is obtained by back substitution, then equation (D.5) becomes

$$x_n = \frac{b_n'}{d_n'} \qquad \text{(D.9)}$$

$$x_i = \frac{b_i' - u_i x_{i+1}}{d_i'} \qquad i = 1,2,3,\ldots,n. \qquad \text{(D.10)}$$

Thus the Thomas algorithm, for programming for a digital computer, is summarized as

1. Store the $n \times n$ tridiagonal matrix T in the three $n \times 1$ column vectors l, d and u. The right-hand-side vector b is also an $n \times 1$ column vector.

2. Compute the d_i' terms from the equation

$$d_i' = d_i - \frac{l_i}{d_{i-1}'} u_{i-1}, \qquad i = 1,2,3,\ldots,n \tag{D.11}$$

store the row reduction multipliers (l_i/d_{i-1}') in place of l_i.

3. Compute the b_i' terms from the equations

$$b_1' = b_1 \tag{D.12}$$

$$b_i' = b_i - \frac{l_i}{d_{i-1}'} b_{i-1}', \qquad i = 1,2,3,\ldots,n. \tag{D.13}$$

4. Solve for x_i using back substitution from the equations.

$$x_n = \frac{b_n'}{d_n'} \tag{D.14}$$

$$x_i = \frac{b_i' - u_i x_{i+1}}{d_i'} \qquad i = n-1, n-2, \ldots, 1. \tag{D.15}$$

Next, we apply the above algorithm to write the ADI method program for solving a problem in example 5.1 (Chapter 5). We then show the LOD method program to find numerical solutions in Appendix D.3. In all examples, we let $\Delta x = \Delta y = \Delta z$.

D.2 The ADI Method Program for Solving Example 5.2

```
%The ADI method program
a = 1;                                   % α, Thermal diffusivity (m^2/s)
s = 1/2;                                 % Grid Fourier Number
dx = 1/10;                               % Δx, Gridspacing
dt = (s*dx*dx)/(a);                      % Δt, Time step size
I = (1/(dx))-1; J = (1/(dx))-1; K = (1/dx)-1;
M = I*J*K;
N = 20;
t = 0:dt:N*dt;
x = 0:dx:1; y = 0:dx:1; z = 0:dx:1;
```

```
%----------------------- Assign initial value-------------------
for n = 1
 for i = 1:I+2
  for  j = 1:J+2
    for k = 1:K+2
          U(n,i,j,k) = sin(x(i)*pi)*sin(y(j)*pi)*sin(z(k)*pi) +(100*x(i)*y(j)*z(k));   %Initial value
     end
   end
  end
end
%----------------------- Finding Matrix d , l and u -------------
for i = 1:M
   d(i)=-4*(1+(3*s));                                      %Diagonal element
end
for i = 1:M-1
  if mod(i,K) = = 0
   uz(i) = 0;
  else uz(i) = ((6*s)-1);                                   %Matrix u  in z-direction
  end
   lz(i+1) = uz(i);                                         %Matrix l  in z-direction
end
for i = 1:M-1
  if mod(i,J) = = 0
            uy(i) = 0;
  else uy(i) = ((6*s)-1);                                   %Matrix u  in y-direction
  end
   ly(i+1) = uy(i);                                         %Matrix l  in y-direction
end
for i = 1:M-1
  if mod(i,I) = = 0
   ux(i) = 0;
  else ux(i) = ((6*s)-1);                                    %Matrix u  in x-direction
  end
   lx(i+1) = ux(i);                                          %Matrix l  in x-direction
end
```

```
%------------------------ Assign boundary values----------------
for n = 2:N
   for i = 1
     for j = 1:J+2
       for k = 1:K+2
              U(n,i,j,k) = 0;                              %Boundary value at x = 0
       end
    end
end
 for i = I+2
    for j = 1:J+2
       for k = 1:K+2
              U(n,i,j,k) = 100*y(j)*z(k);                  %Boundary value at x = A
       end
    end
 end
 for i = 1:I+2
     for j = 1
       for k = 1:K+2
               U(n,i,j,k) = 0;                             %Boundary value at y = 0
       end
    end
 end
for i = 1:I+2
    for j = J+2
      for k = 1:K+2
               U(n,i,j,k) = 100*x(i)*z(k);                 %Boundary value at y = B
     end
  end
end
for i = 1:I+2
    for j = 1:J+2
      for k = 1
               U(n,i,j,k) = 0;                             %Boundary value at z = 0
     end
    end
```

```
    end
    for i=1:I+2
        for j=1:J+2
            for k=K+2
                    U(n,i,j,k) = 100*x(i)*y(j);            %Boundary value at z = C
            end
        end
    end
end
%------------------------- Using eq1 to finding U(2,i,j,k)-------------
for n = 1
    for i = 2:I+1
        for j = 2:J+1
            for k = 2:K+1
                    f(n,i,j,k) = (-s*(U(n,i-1,j,k-1)+U(n,i-1,j,k+1)+U(n,i+1,j,k-1)+U(n,i+1,j,k+1)))...
                    -((4*s)*(U(n,i-1,j,k)+U(n,i+1,j,k)))...
                    -(s*(U(n,i,j-1,k-1)+U(n,i,j-1,k+1)+U(n,i,j+1,k-1)+U(n,i,j+1,k+1)))...
                    -((4*s)*(U(n,i,j-1,k)+U(n,i,j+1,k)))...
                    +(((2*s)+(2*s)-1)*(U(n,i,j,k-1)+(4*U(n,i,j,k))+U(n,i,j,k+1)));
            end
        end
end

if lz(i) <  uz(i)
  f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j,k-1));
  elseif lz(i) = = uz(i)
  f(n,i,j,k) = f(n,i,j,k)+((4*(1+(3*s)))*U(n+1,i,j,k));
  else
  f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j,k+1));
  end
m = 1;
for i = 2:I+1
    for j = 2:J+1
        for k = 2:K+1
                b(m) = f(n,i,j,k);                     %Assign matrix b in (D.1)
              m = m+1;
```

```
            end
        end
    end
    clear f;
    d1(1) = d(1);                                          %Computing matrix d_i', b_i'
    b1(1) = b(1);
    for i = 2:M
        d1(i) = (d(i)-((lz(i)*uz(i-1))/d1(i-1)));
        b1(i) = b(i)-((lz(i)*b1(i-1))/d1(i-1));
    end
        x(M) = b1(M)/d1(M);
    for i = M-1:-1:1
        x(i) = (b1(i)-(uz(i)*x(i+1)))/d1(i);
    end
    m = 1;
    for i = 2:I+1
        for j = 2:J+1
            for k = 2:K+1
                    U(n+1,i,j,k) = x(m);                   %Assign U(2,i,j,k)
                  m = m+1;
            end
        end
      end
     end %(end of n=1)
     %- - - - - - - - - - - - - - - - - - - - - - - Using eq2 to finding U(3,i,j,k)- - - - - - - - - - - - - - -
     for n = 2
       for i = 2:I+1
         for j = 2:J+1
             for k = 2:K+1
                     f(n,i,j,k) = -(s*(U(n,i-1,j-1,k) + U(n,i-1,j+1,k)+U(n,i+1,j-1,k)+U(n,i+1,j+1,k)))...
                               -((4*s)*(U(n,i-1,j,k)+U(n,i+1,j,k)))...
                                -(s*(U(n,i,j-1,k-1)+U(n,i,j-1,k+1)+U(n,i,j+1,k-1)+U(n,i,j+1,k+1)))...
                                -((4*s)*(U(n,i,j,k-1)+U(n,i,j,k+1)))...
                                +((((2*s)+(2*s)-1)*(U(n,i,j-1,k)+(4*U(n,i,j,k))+U(n,i,j+1,k))));
            end
          end
```

```
  end
 if ly(i) <  uy(i)
   f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j-1,k));
   elseif ly(i) = = uy(i)
   f(n,i,j,k) = f(n,i,j,k)+((4*(1+(3*s)))*U(n+1,i,j,k));
   else
   f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j+1,k));
   end
  m = 1;
for i = 2:I+1
    for k = 2:K+1
       for j = 2:J+1
                    b(m) = f(n,i,j,k);
                    m = m+1;
       end
    end
end
clear f;
b1(1) = b(1);
for i = 2:M
   b1(i) = b(i)-((ly(i)*b1(i-1))/d1(i-1));
end
   x(M) = b1(M)/d1(M);
for i = M-1:-1:1
   x(i) = (b1(i)-(uy(i)*x(i+1)))/d1(i);
end
m = 1;
for i = 2:I+1
     for k = 2:K+1
         for j = 2:J+1
                    U(n+1,i,j,k) = x(m);                    %Assign U(3,i,j,k)
                    m=m+1;
         end
     end
  end
end%(end of n=2)
```

```
%---------------------Using eq3 to finding U(4,i,j,k)--------------
for n = 3
 for i = 2:I+1
     for j = 2:J+1
         for k = 2:K+1
                   f(n,i,j,k) = -s*(U(n,i-1,j-1,k)+U(n,i-1,j+1,k)+U(n,i+1,j-1,k)+U(n,i+1,j+1,k))...
                           -(4*s)*(U(n,i,j-1,k)+U(n,i,j+1,k))...
                           -s*(U(n,i-1,j,k-1)+U(n,i-1,j,k+1)+U(n,i+1,j,k-1)+U(n,i+1,j,k+1))...
                           -(4*s)*(U(n,i,j,k-1)+U(n,i,j,k+1))...
                           +(((2*s)+(2*s)-1)*(U(n,i-1,j,k)+(4*U(n,i,j,k))+U(n,i+1,j,k)));
         end
     end
 end
 if lx(i) <  ux(i)
   f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i-1,j,k));
   elseif lx(i) = = ux(i)
   f(n,i,j,k) = f(n,i,j,k)+((4*(1+(3*s)))*U(n+1,i,j,k));
   else
   f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i+1,j,k));
   end
m=1;
for j = 2:J+1
    for k = 2:K+1
       for i = 2:I+1
                   b(m) = f(n,i,j,k);
                   m = m+1;
       end
   end
end
clear f;
b1(1) = b(1);
for i = 2:M
   b1(i) = b(i)-((lx(i)*b1(i-1))/d1(i-1));
end
   x(M) = b1(M)/d1(M);
for i = M-1:-1:1
```

```
    x(i) = (b1(i)-(ux(i)*x(i+1)))/d1(i);
end
 m = 1;
for j = 2:J+1
    for k = 2:K+1
        for i = 2:I+1
                U(n+1,i,j,k) = x(m);                    %Assign U(4,i,j,k)
                m = m+1;
     end
   end
  end
end %(end of n)
%- - - - - - - - - - - - - - - - - - - - - -Finding U(n,i,j,k)when n>4 - - - - - - - - - - - - - - - - - --
for r = 1:3
   q = (3*r)+1;
for n = q
  for i = 2:I+1
    for j = 2:J+1
      for k = 2:K+1
                 f(n,i,j,k) = (-s*(U(n,i-1,j,k-1)+U(n,i-1,j,k+1)+U(n,i+1,j,k-1)+U(n,i+1,j,k+1)))...
                -((4*s)*(U(n,i-1,j,k)+U(n,i+1,j,k)))...
                -(s*(U(n,i,j-1,k-1)+U(n,i,j-1,k+1)+U(n,i,j+1,k-1)+U(n,i,j+1,k+1)))...
                -((4*s)*(U(n,i,j-1,k)+U(n,i,j+1,k)))...
                +(((2*s)+(2*s)-1)*(U(n,i,j,k-1)+(4*U(n,i,j,k))+U(n,i,j,k+1)));
      end
    end
 end
if lz(i)< uz(i)
   f(n,i,j,k)=f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j,k-1));
   elseif lz(i)==uz(i)
   f(n,i,j,k)=f(n,i,j,k)+((4*(1+(3*s)))*U(n+1,i,j,k));
   else
   f(n,i,j,k)=f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j,k+1));
   end
m=1;
for i=2:I+1
```

```
    for j=2:J+1
      for k=2:K+1
          b(m)=f(n,i,j,k);
           m=m+1;
        end
    end
end
 clear f;
 d1(1)=d(1);b1(1)=b(1);
 for i = 2:M
      d1(i) = (d(i)-((lz(i)*uz(i-1))/d1(i-1)));
      b1(i) = b(i)-((lz(i)*b1(i-1))/d1(i-1));
end
    x(M) = b1(M)/d1(M);
for i = M-1:-1:1
      x(i) = (b1(i)-(uz(i)*x(i+1)))/d1(i);
end
m = 1;
for i = 2:I+1
    for j = 2:J+1
       for k = 2:K+1
                    U(n+1,i,j,k) = x(m);
                 m = m+1;
       end
    end
 end
end %(end of n)
%- - - -- - - Using formula in equation 2 to compute U(n,i,j,k) in the next time step- - -
for n = q+1
    for i = 2:I+1
       for j = 2:J+1
         for k = 2:K+1
                    f(n,i,j,k) = -(s*(U(n,i-1,j-1,k) + U(n,i-1,j+1,k)+U(n,i+1,j-1,k)+U(n,i+1,j+1,k)))...
                                   -((4*s)*(U(n,i-1,j,k)+U(n,i+1,j,k)))...
                                   -(s*(U(n,i,j-1,k-1)+U(n,i,j-1,k+1)+U(n,i,j+1,k-1)+U(n,i,j+1,k+1)))...
                                   -((4*s)*(U(n,i,j,k-1)+U(n,i,j,k+1)))...
```

```
                                    +((((2*s)+(2*s)-1)*(U(n,i,j-1,k)+(4*U(n,i,j,k))+U(n,i,j+1,k))));
        end
      end
    end
  if ly(i)< uy(i)
    f(n,i,j,k)= f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j-1,k));
    elseif ly(i)==uy(i)
    f(n,i,j,k)= f(n,i,j,k)+((4*(1+(3*s)))*U(n+1,i,j,k));
    else
    f(n,i,j,k)= f(n,i,j,k)-(((6*s)-1)*U(n+1,i,j+1,k));
    end
m = 1;
for i = 2:I+1
      for k = 2:K+1
            for j = 2:J+1
     b(m) = f(n,i,j,k);
                        m = m+1;
            end
      end
end
clear f;
b1(1) = b(1);
for i =  2:M
    b1(i) = b(i)-((ly(i)*b1(i-1))/d1(i-1));
end
    x(M) = b1(M)/d1(M);
for i = M-1:-1:1
    x(i) = (b1(i)-(uy(i)*x(i+1)))/d1(i);
end


m = 1;
for i = 2:I+1
    for k = 2:K+1
        for j = 2:J+1
                        U(n+1,i,j,k) = x(m);
                        m = m+1;
```

```
      end
    end
  end
end %(for n)
%- - - - - - -Using formula in equation 3 to compute U(n,i,j,k) in the next time step - - - - - - - -
for n = q+2
   for i = 2:I+1
      for j = 2:J+1
         for k = 2:K+1
                  f(n,i,j,k) = -s*(U(n,i-1,j-1,k)+U(n,i-1,j+1,k)+U(n,i+1,j-1,k)+U(n,i+1,j+1,k))...
                           -(4*s)*(U(n,i,j-1,k)+U(n,i,j+1,k))...
                           -s*(U(n,i-1,j,k-1)+U(n,i-1,j,k+1)+U(n,i+1,j,k-1)+U(n,i+1,j,k+1))...
                           -(4*s)*(U(n,i,j,k-1)+U(n,i,j,k+1))...
                           +(((2*s)+(2*s)-1)*(U(n,i-1,j,k)+(4*U(n,i,j,k))+U(n,i+1,j,k)));
        end
      end
  end
 if lx(i)< ux(i)
   f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i-1,j,k));
   elseif lx(i) = = ux(i)
   f(n,i,j,k) = f(n,i,j,k)+((4*(1+(3*s)))*U(n+1,i,j,k));
   else
   f(n,i,j,k) = f(n,i,j,k)-(((6*s)-1)*U(n+1,i+1,j,k));
   end
m = 1;
for j = 2:J+1
   for k = 2:K+1
       for i = 2:I+1
                  b(m) = f(n,i,j,k);
                   m = m+1;
       end
    end
end
clear f;
b1(1) = b(1);
for i = 2:M
```

```
    b1(i) = b(i)-((lx(i)*b1(i-1))/d1(i-1));
end
    x(M) = b1(M)/d1(M);
for i = M-1:-1:1
    x(i) = (b1(i)-(ux(i)*x(i+1)))/d1(i);
end
 m = 1;
for j = 2:J+1
     for k = 2:K+1
          for i = 2:I+1
                    U(n+1,i,j,k) = x(m);
                    m = m+1;
          end
        end
      end
   end %(end of  "for n")
end %(end of  "for r")
```

D.3 LOD Method Program for Solving Example 5.1

```
%The LOD method program
a=1;
s=1/2;
dx=0.1;
dt=(s*dx*dx)/a;
X = 1;Y = 1;Z = 1;
I = (X/dx)+1;J = (Y/dx)+1;K= (Z/dx)+1;N = 20;
x = 0:dx:X; y = 0:dx:Y; z = 0:dx:Z;
D1 = ((s*((6*s)-1))/12);
D2 = (((2*s)*(2-(3*s)))/3);
D3 = ((2-(5*s)+(6*s*s))/2);
E1 = ((8*(2+(3*s)))/((6*s)+1));
E2 = ((6*(2+(5*s)+(6*s*s)))/(s*((6*s)+1)));
E3 = (12/(s*((6*s)+1)));
F1 = (((6*s)+1)/(8*(2+(3*s))));
F2 = ((3*(2+(5*s)+(6*s*s)))/(s*((12*s)+8)));
F3 = (3/(s*((6*s)+4)));
```

```
%- - -- - - - - - - - - - - - - - - - - - - - - - initial and boundary conditions- - - - - - - - - - - - - - - - - - -
for n=1
 for i=1:I
   for j=1:J
     for k=1:K
       u(n,i,j,k) = (sin(pi*x(i))*sin(pi*y(j))*sin(pi*z(k)))+100*x(i)*y(j)*z(k);%initial value
     end
   end
 end
end
for n = 2:N
   for i = 1
     for j = 1:J
       for k = 1:K
                  u(n,i,j,k) = 0;                          %Boundary value at x = 0
       end
   end
end
 for i = I
    for j = 1:J
       for k = 1:K
                  u(n,i,j,k) = 100*y(j)*z(k);              %Boundary value at x = A
       end
    end
 end
 for i = 1:I
     for j = 1
       for k = 1:K
                   u(n,i,j,k) = 0;                         %Boundary value at y = 0
       end
    end
 end
 for i = 1:I
    for j = J
      for k = 1:K
```

```
                    u(n,i,j,k) = 100*x(i)*z(k);                 %Boundary value at y = B
        end
      end
    end
    for i = 1:I
      for j = 1:J
        for k = 1
                    u(n,i,j,k) = 0;                             %Boundary value at z = 0
        end
      end
    end
    for i=1:I
      for j=1:J
        for k=K
                    u(n,i,j,k) = 100*x(i)*y(j);                 %Boundary value at z = C
        end
      end
    end
end
%- - - - - - - - - - - - - - - - - - - - - - - - -x-direction- - - - - - - - - - - - - - - - - - - - - -
 for n = 2:N
  for i = 3:I-2
   for j = 1:J
    for k = 1:K
       w(n,i,j,k) = D1*(u(n-1,i-2,j,k)+u(n-1,i+2,j,k))+D2*(u(n-1,i-1,j,k)+u(n-1,i+1,j,k))...
                    +D3*u(n-1,i,j,k);
    end
   end
  end
  for i = 2
    for j = 1:J
      for k = 1:K
      w(n,i,j,k) = E1*(w(n,i+1,j,k)+w(n,i+3,j,k))-E2*w(n,i+2,j,k)-w(n,i+4,j,k)+E3*u(n-1,i+2,j,k);
      end
    end
  end
```

```
for i = I-1
  for j = 1:J
    for k = 1:K
   w(n,i,j,k) = E1*(w(n,i-1,j,k)+w(n,i-3,j,k))-E2*w(n,i-2,j,k)-w(n,i-4,j,k)+E3*u(n-1,i-2,j,k);
    end
  end
 end
%-------------------------------------------------y-direction--------------------------------
for i= 2:I-1
   for j = 3:J-2
     for k = 1:K
    v(n,i,j,k) = D1*(w(n,i,j-2,k)+w(n,i,j+2,k))+D2*(w(n,i,j-1,k)+w(n,i,j+1,k))+D3*w(n,i,j,k);
    end
  end
   for j = 2
       for k = 1:K
         v(n,i,j,k)=E1*(v(n,i,j+1,k)+v(n,i,j+3,k))-E2*v(n,i,j+2,k)-v(n,i,j+4,k)+E3*w(n,i,j+2,k);
     end
   end
   for j = J-1
       for k = 1:K
         v(n,i,j,k) = E1*(v(n,i,j-1,k)+v(n,i,j-3,k))-E2*v(n,i,j-2,k)-v(n,i,j-4,k)+E3*w(n,i,j-2,k);
       end
 end
%-------------------------------------------------z-direction--------------------------------
   for j = 2:J-1
       for k = 3:K-2
         u(n,i,j,k)=D1*(v(n,i,j,k-2)+v(n,i,j,k+2))+D2*(v(n,i,j,k-1)+v(n,i,j,k+1))+D3*v(n,i,j,k);
      end
       for k=2
         u(n,i,j,k)=F1*(u(n,i,j,k-1)+u(n,i,j,k+3))+F2*u(n,i,j,k+1)-u(n,i,j,k+2)-F3*v(n,i,j,k+1);
      end
        for k=K-1
          u(n,i,j,k)=F1*(u(n,i,j,k+1)+u(n,i,j,k-3))+F2*u(n,i,j,k-1)-u(n,i,j,k-2)-F3*v(n,i,j,k-1);
       end
      end
  end
end %(end of 'for n')
```

AUTHOR BIOGRAPHY

Author	:	Tiwaporn Pinlaor
Date of Birth	:	April 23, 1976
Bachelor Degree	:	B.Ed. Science-Mathematics
Institution	:	Faculty of Education, Mahasarakarm University, Mahasarakarm, Thailand.
Year of Graduation	:	1997