Approximate Solution of Thermal Expulsion of Fluid from a Long Slender Heated Pipe

by

Kanwal Shahzadi

Centre for Advanced Mathematics and Physics

National University of Sciences and Technology

Islamabad, Pakistan

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Supervised by

Dr. Azad Akhter Siddiqui

Centre for Advanced Mathematics and Physics
National University of Sciences and Technology
Islamabad, Pakistan

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Dedicated to

My Loving Parents

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Abstract

Most of the fundamental problems in science and engineering, when formulated mathematically give rise to non-linear partial differential equations. Thermal expulsion of fluid from a long slender heated tube is one of them. The direct search for the exact solution of the thermal expulsion equation is usually a hard task. Therefore, finding the techniques that give the approximate solution of this problem needs special attention. There are different ways to find approximate solution of a non-linear partial differential equation (PDE), but one of them is to reduce it from a non-linear PDE to an ordinary differential equation (ODE) by similarity transformation. Then by finding the solution of the reduced ODE, one may get the solution of non-linear PDE. Unfortunately, most often the similarity transformations reduce the non-linear PDEs to non-linear ODEs that is again difficult to solve. So, the idea is to find the numerical solution of this reduced ODE and then approximate it by a function. Then by applying the inverse similarity transformations to the approximated function, one may get the approximate solution of the non-linear PDE in the form of a function. Another way to find the approximate solution of non-linear PDE is to apply the direct numerical techniques. In this Thesis, we will use both approximation techniques to find the solution of non-linear thermal expulsion PDE, and then compare both solutions and analyze the errors.

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Symbols

c_p Specific heat ($Jkg^{-1}K^{-1}$).

c Speed of sound.

D Hydraulic diameter of helium filled part of the conductor.

f Fanning friction.

F Frictional forces per unit mass (Ng^{-1}).

p Pressure (Pa).

$\dot{q}$ Heating rate per unit mass of helium (Wg^{-1}).

t Time (sec).

T Temperature (K).

u Specific internal energy (Jkg^{-1}).

v Flow velocity ($msec^{-1}$).

x Distance (m).

β Volume coefficient of thermal expansion.

ρ Density (kgm^{-3}).

τ Specific Volume (ρ^{-1}).

Chapter 1

Introduction

One of the important and subtle features of mathematics is the great difference between linearity and non-linearity. One always tries to linearize, whenever possible because linear problems are easier to solve. Unfortunately, the mathematical modeling of most physical processes in fields like diffusion and fluid mechanics are not linear, so we have to learn how to deal with these non-linear problems. Similarly, in PDEs the distinction between the linear and non-linear equations is extremely important. Linear PDEs can be solved easily by using techniques such as separation of variable, superposition, Fourier series, Laplace transform and Fourier transform, etc. But non-linear PDEs are difficult to solve analytically. Non-linear PDEs have always remained the center of great attention, because of their vast range of applications in science and engineering. Therefore, special attention should be given in seeking the solutions of these non-linear PDEs.

A powerful general technique for analyzing non-linear PDE is given by Lie symmetry method also called similarity method [1, 2, 3]. About a hundred years ago, an Austrian physicist Boltzman was the first who used the algebraic symmetries to study diffusion equation. Boltzman did not mention explicitly the transformation groups or the symmetries that he used. After this, in 1950s, American mathematician Garrett Brikhoff reviewed Boltzman's procedure of algebraic symmetry

of diffusion equation and then generalized this procedure to other PDEs including non-linear ones. He showed, that the solution of the PDE can be found easily by merely solving related reduced ODE [4].
By applying the similarity method, the non-linear PDEs is reduced in to an ODEs. The solution of this reduced ODE leads us to solution of the given non-linear PDE. But the difficulty is increased, when the resulting ODE is also non-linear and is not integrable in term of elementary functions. Thus, we implement numerical approach to find the solution of the reduced ODE. But the numerical solution of the reduced ODE cannot be easily utilized to get the approximate solution of the PDE. Thus, we approximate the numerical solution of the ODE in the form of a function to get the approximate solution of non-linear PDE. We, then compare this approximate solution with the numerical solution of the PDE and analyze the errors.

The main contribution of this thesis is to solve a non-linear heat equation known as thermal expulsion problem. The application of this problem is in cable-in conduit superconductors which uses Helium as a fluid. The warm helium is treated as a perfect gas having uniform pressure and temperature and its temperature is presumed as a function of time. Whereas, the cold helium is treated as dense fluid and when it is heated by conductors then it causes its temperature to rise. When the pressure of in cable-in-conduit conductor rises then the helium is expelled from its ends of the conductor. The hazard that one faces is that the pressure rise can damage the structure of the conductor. In addition to this, the rapid expulsion of the helium from the conductor back into the refrigeration system may also cause damage. To overcome these problems, we should know the rate of efflux of helium for the first few seconds, because after this the refrigeration system is protected by the valves that control the flow [5].

The mathematical formulation of this problem enables to obtain an equation in the form of non-linear PDE. By solving that equation, we get an expression that shows explicitly the dependence of expulsion velocity on various parameters of conductor. For this, we should know some basic definitions of heat transfer in fluid. The rest of the chapter includes the basic definitions of heat and the mathematical formulation of thermal expulsion problem.

1.1 Basics of Heat

Temperature plays an important role in the theory of heat transfer. It is a measure of hotness or coldness of a body with units of Kelvin, Fahrenheit, etc. In thermodynamical point of view, it is an intensive property, i.e., it does not depend upon the amount of a material within the substance. Heat is basically a form of energy (usually called heat energy) that is transferred from one substance to another substance by thermal interactions. Its SI unit is Joule ($1J = 1Nm$). Both heat and temperature are closely related to each other. As a general statement, when heat energy of a system rises its temperature also rises.
Heat transfer is a phenomenon which concerns to the conversion or exchange of energy and heat between two physical systems. When a fluid is heated then energy enters into the fluid. Due to this energy, the kinetic energy of molecules increases. This is the way through which the heat transfer takes place in the fluid and results in increase of the temperature of the fluid.

Specific heat

It is the amount of heat required to raise the temperature of unit mass of a substance by one degree celsius.

$$Q \propto m\Delta T,$$

or

$$Q = c_p m \Delta T, \tag{1.1}$$

where Q is heat, m is mass and ΔT is change in temperature. In Eq. (1.1) c_p is the constant of proportionality and is known as specific heat. Its unit is $Jkg^{-1}K^{-1}$.

Kinetic and potential energies are macroscopic forms of energy of a substance but there are also some microscopic forms of energies which are caused by rotations, vibrations, translations and interactions among the molecules of a substance. These microscopic forms of energies are collectively called the internal energy (U). Specific internal energy, u, is defined as an internal energy U per unit mass m, defined as

$$u = \frac{U}{m}.$$

Volume Coefficient of Thermal Expansion

When the temperature of a substance changes then the energy stored in the intermolecular bonds of atoms changes. When the stored energy increases, the length of molecular bonds also increases. This change in volume with temperature is called volume coefficient of thermal expansion.

First Law of Thermodynamics

We can increase the energy of a system by doing work on it or by heating it. In general, the change in the internal energy of a closed system is given by

$$\Delta U = Q + W. \tag{1.2}$$

The quantity ΔU represents the change in the energy of a system due to heating ($Q > 0$) or cooling ($Q < 0$) and W is the work done on the system. Eq. (1.2) expresses the law of conservation of energy and also known as the first law of thermodynamics [7].

Fanning Friction Factor

Fanning friction factor is used to calculate the pressure loss due to friction in a pipe. It depends upon the roughness of pipe and the level of turbulence in the liquid flow and is given as

$$F = \frac{2fv^2}{D}, \tag{1.3}$$

where f represents the frictional forces, v is the velocity, and D is the diameter of the pipe.

Fluid Flow

There are three states of matter: Solids, liquids and gases. Gases and liquids have flow property but solids do not have this property. On the basis of flow property gases and liquids are called fluids. In general, fluid flow is classified into two types on the basis of velocity of the fluid. These include *laminar flow* and *turbulent flow.* In laminar flow different streamlines run parallel to one another and do not cross. Fluid moving with very low velocity possess laminar flow. Fluid in which different streamlines start crossing one another and fluid flow remains no longer steady is called turbulent flow.

1.2 Mathematical Formulation of Thermal Expulsion Problem

Fluid motion is governed by equation of continuity and the Bernoulli equation. For flow in heated pipe, the momentum equation is an additional equation.

Continuity Equation

The equation of continuity is the mathematical form of the law of conservation of mass. The rate at which mass enters into the systems is equal to the rate at which it leaves the system. Mathematical form of continuity equation is written as

$$\frac{\partial \rho}{\partial t} + div(\rho \mathbf{v}) = 0, \tag{1.4}$$

where ρ is the density and $\mathbf{v}$ is the velocity of the fluid in x, y and z directions. For incompressible fluids the density is constant and equation reduces into $div\mathbf{v}$=0 and

$$\frac{\partial v}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial v}{\partial z} = 0 \tag{1.5}$$

Bernoulli's Equation

Bernoulli equation is a direct consequence of law of conservation of energy. The law of conservation of energy states that any change in the energy of the fluid within the control volume is equal to the net thermal energy transferred into the control volume plus the rate of work done by external forces.

$$\rho \frac{d}{dt}\left(u + \frac{v^2}{2}\right) = -\frac{\partial}{\partial x}(pv) + \rho \dot{q}, \quad \text{where } \dot{q} = \frac{dq}{dm}, \tag{1.6}$$

In Eq. (1.6) $\dot{q}$ represents heating rate per unit mass and ρ is the density of fluid. The energy of the fluid is the sum of absolute thermodynamics internal energy per unit mass u, and the kinetic energy per unit mass $\frac{1}{2}v^2$.

Momentum Equation

The law of conservation of momentum is given by the momentum equation. It states that the rate of change of momentum in the control volume must be equal to net momentum flux plus any external forces.

$$\rho \frac{dv}{dt} = -\frac{\partial p}{\partial x} - \rho F, \tag{1.7}$$

where F is fanning friction. The frictional forces appear only in momentum equation, but not in energy equation because the work done by frictional forces is not removed by the fluid but it is returned to it as heat.

If we multiply Eq. (1.7) by v and then subtract it from Eq. (1.6), we get

$$\frac{du}{dt} + \frac{p}{\rho}\frac{\partial v}{\partial x} = \dot{q} + Fv. \tag{1.8}$$

The mathematical equation of second law of thermodynamics is

$$Tds = du + pd\tau, \tag{1.9}$$

where $\tau = 1/\rho$. Dividing Eq. (1.9) by dt and using Eq. (1.4), we have

$$T\frac{ds}{dt} = \frac{du}{dt} + \frac{p}{\rho}\frac{\partial v}{\partial x}. \tag{1.10}$$

From Eqs. (1.8) and (1.10), we get

$$T\frac{ds}{dt} = \dot{q} + Fv. \tag{1.11}$$

From the thermodynamics identity [6]

$$d\rho = \frac{dp}{c^2} - \frac{\beta\rho}{c_p}Tds, \tag{1.12}$$

or

$$\frac{1}{\rho}\frac{d\rho}{dt} = \frac{1}{c^2\rho}\frac{dp}{dt} - \frac{\beta}{c_p}T\frac{ds}{dt}, \tag{1.13}$$

from Eq. (1.11), we have

$$\frac{1}{\rho}\frac{d\rho}{dt} = \frac{1}{c^2\rho}\frac{dp}{dt} - \frac{\beta}{c_p}\left(\dot{q} + Fv\right). \tag{1.14}$$

where c_p is specific heat, c is speed of sound, and β is the volume coefficient of thermal expansion. The term Fv in Eq. (1.14) represents Entropy. Using Eq. (1.4) in Eq. (1.14), we get

$$\frac{\partial v}{\partial x} + \frac{1}{\rho c^2}\frac{\partial \rho}{\partial t} = \frac{\beta}{c_p}\left(\dot{q} + Fv\right). \tag{1.15}$$

At $t = 0$, initially when pressure rise is zero, imagine $\dot{q}$ is nonzero. At this stage, when v has not risen too much, we have

$$\dot{q} >> Fv,$$

or (using Eq. (1.3))

$$v^3 << \frac{\dot{q}D}{2f}.$$

When this condition is fulfilled, Eq. (1.15) becomes as

$$\frac{\partial v}{\partial x} + \frac{1}{\rho c^2}\frac{\partial p}{\partial t} = \frac{\beta \dot{q}}{c_p}. \tag{1.16}$$

The main assumption of this work is that the frictional forces largely dominate the inertial forces in long, narrow tube. Due to these frictional forces the left hand side of Eq. (1.7) is far less than the term on the right hand side. In other words, the pressure gradient expends itself in overcoming friction, not in accelerating the fluid [5]. Hence, set $dv/dt = 0$, in left hand side of Eq. (1.7)

$$\frac{\partial p}{\partial x} = -\rho F, \tag{1.17}$$

or

$$\frac{\partial p}{\partial x} = \frac{-2\rho f v^2}{D}. \tag{1.18}$$

When $\dot{q} = 0$, Eq. (1.16) takes the form

$$\frac{\partial v}{\partial x} + \frac{1}{\rho c^2}\frac{\partial p}{\partial t} = 0, \tag{1.19}$$

In special units, we take $\rho = c = D/4f = 1$. So the above Eqs. (1.18) and (1.19) become

$$\frac{\partial v}{\partial x} + \frac{\partial p}{\partial t} = 0, \tag{1.20}$$

and

$$\frac{\partial p}{\partial x} + \frac{v^2}{2} = 0. \tag{1.21}$$

Taking partial derivative of Eqs. (1.20) and (1.21) with respect to x and t respectively, and comparing both equations, we get

$$\frac{\partial^2 v}{\partial x^2} = v\frac{\partial v}{\partial t}. \tag{1.22}$$

Since the pressure rise p is zero at $x = 0$ at the open end of the pipe so, from Eq. (1.16) the boundary condition become as

$$\left(\frac{\partial v}{\partial x}\right)_{x=0} = \frac{\beta \dot{q}}{c_p}, \tag{1.23}$$

and

$$v(x, 0) = 0, \quad v(\infty, t) = 0.$$

In dimensionless variables $V = v/c$, $X = -\beta\dot{q}x/cc_p$, $T = D\beta^2\dot{q}^2t/4fcc_p^2$, Eqs. (1.22) and (1.23), take the form

$$\frac{\partial^2 V}{\partial X^2} = V\frac{\partial V}{\partial T}, \tag{1.24}$$

and the initial and the boundary conditions of Eq. (1.24) becomes

$$\left(\frac{\partial V}{\partial X}\right)_{X=0} = -1, \tag{1.25}$$

$$V(X, 0) = 0, \quad V(\infty, T) = 0.$$

In Chapter 2 a brief review of the numerical methods for PDEs is presented. Chapter 3 illustrates the approach that we used to obtain the approximate solution of the non-linear thermal expulsion equation. In addition, last chapter of this thesis includes the comparative analysis of the approximate and numerical solutions of thermal expulsion problem.

Chapter 2

Numerical Methods for Partial Differential Equations

Mathematical formulation of most of the physical and engineering problems are governed by PDEs, whose analytical solutions are difficult to find. In such cases, we may have to content with an approximate solution. There are different techniques to find the approximate solution of PDEs, but numerical techniques are most commonly used. The basic concept of numerical scheme is based on approximation of partial derivatives by algebraic expressions. These algebraic expressions are then solved numerically. This chapter is devoted to study different numerical techniques, such as finite difference and finite volume methods. In this this thesis we have used only finite difference to solve our problem. However, some light is also shed on finite element and spectral methods.

2.1 Finite Difference Method (FDM)

Finite difference method is a simple and commonly used technique to solve PDEs, generally having regular domain. In this method, we place a rectangular grid on the given regular domain consisting of vertical lines which are **h** units apart and horizontal lines which are **k** units apart. Next, we write the difference equation at each grid point [8]. These difference equations are then approximated by the

Taylor series expansion. The Taylor series expansion at $u(x+\Delta x,t)$ is given as

$$u(x+\Delta x,t)=u+\Delta x\frac{\partial u}{\partial x}+\frac{(\Delta x)^2}{2!}\frac{\partial^2 x}{\partial x^2}+\frac{(\Delta x)^3}{3!}\frac{\partial u^3}{\partial x^3}+...$$

Ignoring all the terms involving $(\Delta x)^2$ and all its higher powers

$$u(x+\Delta x,t)=u+\Delta x\frac{\partial u}{\partial x}+O(\Delta x)^2. \tag{2.1}$$

Similarly, the Taylor series for $u(x,t+\Delta t)$ is given as

$$u(x,t+\Delta t)=u+\Delta t\frac{\partial u}{\partial t}+\frac{(\Delta t)^2}{2!}\frac{\partial^2 u}{\partial t^2}+\frac{(\Delta t)^3}{3!}\frac{\partial u^3}{\partial t^3}+...,$$

or

$$u(x,t+\Delta t)=u+\Delta t\frac{\partial u}{\partial t}+O(\Delta t)^2. \tag{2.2}$$

Solving Eqs. (2.1) and (2.2) for $\partial u/\partial x$ and $\partial u/\partial t$ respectively, we get forward difference equations

$$\frac{\partial u}{\partial x}=\frac{u(x+\Delta x,t)-u(x,t)}{\Delta x}+O(\Delta x),$$

and

$$\frac{\partial u}{\partial t}=\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t}+O(\Delta t).$$

Similarly, the Taylor series expansion for $u(x-\Delta x,t)$ and $u(x,t+\Delta t)$ can be written as

$$u(x-\Delta x,t)=u-\Delta x\frac{\partial u}{\partial x}+\frac{(\Delta x)^2}{2!}\frac{\partial^2 x}{\partial x^2}-\frac{(\Delta x)^3}{3!}\frac{\partial u^3}{\partial x^3}+...$$

and

$$u(x,t-\Delta t)=u-\Delta t\frac{\partial u}{\partial t}+\frac{(\Delta t)^2}{2!}\frac{\partial^2 u}{\partial t^2}-\frac{(\Delta t)^3}{3!}\frac{\partial u^3}{\partial t^3}+....$$

or

$$u(x-\Delta x,t)=u-\Delta x\frac{\partial u}{\partial x}+O(\Delta x)^2, \tag{2.3}$$

and

$$u(x, t - \Delta t) = u - \Delta t \frac{\partial u}{\partial t} + O(\Delta t)^2. \tag{2.4}$$

From Eqs. (2.3) and (2.4), we get the backward difference equations for $\partial u/\partial x$ and $\partial u/\partial t$ as following

$$\frac{\partial u}{\partial x} = \frac{u(x,t) - u(x - \Delta x, t)}{\Delta x} + O(\Delta x),$$

and

$$\frac{\partial u}{\partial t} = \frac{u(x,t) - u(x, t - \Delta t)}{\Delta t} + O(\Delta t).$$

Central difference equation, for $\frac{\partial u}{\partial x}$, can be obtain by adding Eqs. (2.1) and (2.3)

$$\frac{\partial u}{\partial x} = \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{2\Delta x} + O(\Delta x^2).$$

For $\partial u/\partial t$, the central difference equation is obtained by subtracting Eqs. (2.2) and (2.4)

$$\frac{\partial u}{\partial t} = \frac{u(x, t + \Delta t) - u(x, t - \Delta t)}{2\Delta t} + O(\Delta t^2).$$

Similarly, central difference equations for $\partial^2 u/\partial x^2$ is obtained as

$$\frac{\partial^2 u}{\partial x^2} = \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{(\Delta x)^2} + O(\Delta x^2).$$

For $\partial^2 u/\partial t^2$, we have

$$\frac{\partial^2 u}{\partial t^2} = \frac{u(x, t + \Delta t) - u(x, t - \Delta t)}{(\Delta t)^2} + O(\Delta t^2).$$

We shall use the following notations

$$u(x \pm \Delta x, t) = u_{i\pm1,j},$$

$$u(x, t \pm \Delta t) = u_{i,j\pm1},$$

$$\Delta x = h,$$

$$\Delta t = k.$$

So, the expression for forward difference takes the form

$$\frac{\partial u}{\partial x} = \frac{u_{i+1,j} - u_{i,j}}{h} + O(h), \tag{2.5}$$

$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{k} + O(k). \tag{2.6}$$

For backward difference, we have

$$\frac{\partial u}{\partial x} = \frac{u_{i,j} - u_{i-1,j}}{h} + O(h), \tag{2.7}$$

$$\frac{\partial u}{\partial t} = \frac{u_{i,j} - u_{i,j-1}}{k} + O(k). \tag{2.8}$$

And the central difference equations are given as

$$\frac{\partial u}{\partial x} = \frac{u_{i+1,j} - u_{i-1,j}}{2h} + O(h), \tag{2.9}$$

$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j-1}}{2k} + O(k), \tag{2.10}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{(u_{i+1,j} + u_{i-1,j} - 2u_{i,j})}{h^2} + O(h^2), \tag{2.11}$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} + O(k^2). \tag{2.12}$$

Most of the concepts associated with the numerical solution of PDEs by FDM can be illustrated and understand by considering a simple diffusion equation in one dimensional (1D) of the form

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < l, \quad t > 0, \tag{2.13}$$

subject to the following initial and boundary conditions

$$u(0,t) = u(l,t) = 0, \quad t > 0,$$

$$u(x,0) = f(x), \quad 0 \leq x \leq l.$$

This is parabolic heat equation in 1D that describes heat flow in a rod or a thin wire. The function $u(x,t)$ is temperature and α is called thermal diffusivity. Following are the three types of schemes that are used in **finite difference method**.

2.1.1 Explicit Finite Difference Scheme

In this scheme, first order forward difference equation for time and second order central difference for space derivative are used. Substituting Eqs. (2.6) and (2.12) in (2.13), we get

$$\frac{u_{i,j+1} - u_{i,j}}{k} = \alpha \frac{(u_{i+1,j} + u_{i-1,j} - 2u_{i,j})}{h^2},$$

or

$$u_{i,j+1} - u_{i,j} = \alpha \frac{k}{h^2}(u_{i+1,j} + u_{i-1,j} - 2u_{i,j}),$$

Substituting $r = \alpha k/h^2$, the final discretizationn of this scheme is as follow

$$u_{i,j+1} = (1 - 2r)u_{i,j} + r(u_{i+1,j} + u_{i-1,j}). \tag{2.14}$$

From boundary conditions, we have

$$u_{0,0} = f(x_0), u_{1,0} = f(x_1), ..., u_{m,0} = f(x_m).$$

For each $i = 1, 2, ..., m$ and $j = 1$, we get the following equations

$$\begin{aligned}
u_{0,1} &= 0, \\
u_{1,1} &= (1-2r)u_{1,0} + r(u_{2,0} + u_{0,0}), \\
u_{2,1} &= (1-2r)u_{2,0} + r(u_{3,0} + u_{1,0}), \\
&\vdots \qquad\qquad\qquad\qquad \vdots \\
u_{m-1,1} &= (1-2r)u_{m-1,0} + r(u_{m,0} + u_{m-2,0}), \\
u_{m,1} &= 0.
\end{aligned}$$

The values of $u_{i,1}$ are used to find the values of $u_{i,2}$. These equations generate a tridiagonal form of matrix of order $(m-1) \times (m-1)$ as follow

$$A = \begin{bmatrix} (1-2r) & r & 0 & \cdots & 0 \\ r & (1-2r) & r & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & r \\ 0 & \cdots & 0 & r & (1-2r) \end{bmatrix}$$

where, $r = \alpha k/h^2$,

$$u^{(0)} = (f(x_1), f(x_2), ..., f(x_{m-1}))^t,$$

and

$$u^{(j)} = (u_{1,j}, u_{2,j}, ..., u_{(m-1),j}), \qquad \text{for each } j = 1, 2, ..., \tag{2.15}$$

$$u^{(j)} = Au^{(j-1)}, \qquad \text{for each } j = 1, 2, ...,$$

This is known as an explicit method called **Forward Time Central Space (FTCS)**.

Stability Analysis

In general, different types of error occur in FDM. Two of them are very important, one is round off error and other is truncation error. These errors are caused by rounding-off error or by application of particular numerical scheme. If the error introduced in numerical scheme is not controlled, then the method is unstable. Understanding and controlling these errors is very essential for successful solution of the PDE. It is done by the stability analysis which provides limitations on step size that are needed for stable solution. A numerical scheme is stable, if the error at each step does not increase with time when the computations are carried out for next steps. Now, we find the stability conditions for explicit forward difference scheme. The Vonn Nuemman stability analysis is commonly used method for determining the stability requirements for finite difference scheme [10]. It is based upon the Fourier series of the form

$$u_{i,j} = e^{\iota\beta x}\xi^{t}. \tag{2.16}$$

Putting Eq. (2.16) in Eq. (2.14), we get the following expression

$$e^{\iota\beta x}\xi^{t+1} = e^{\iota\beta x}\xi^{t} + r(e^{\iota\beta(x+1)}\xi^{t} - 2e^{\iota\beta x}\xi^{t} + e^{\iota\beta(x-1)}\xi^{t}),$$

or

$$e^{\iota\beta x}\xi^{t+1} = e^{\iota\beta x}\xi^{t}(1 + r(e^{\iota\beta} - 2 + e^{-\iota\beta})).$$

After simplification, we get

$$\xi = 1 + r(e^{\iota\beta} + e^{-\iota\beta} - 2). \tag{2.17}$$

From the trigonometric identity

$$\sin^{2}\frac{(\beta)}{2} = -\frac{(e^{\beta} + e^{-\iota\beta} - 2)}{4}, \tag{2.18}$$

and using Eq. (2.18) in (2.17), we get

$$\xi = 1 - 4r\sin^{2}\frac{(\beta)}{2}.$$

For stable solution, we require $|\xi| \leq 1$, such that

$$|1 - 4r\sin^2\frac{(\beta)}{2}| \leq 1, \qquad \text{when} \quad r \leq \frac{1}{2}.$$

Thus, we can say that explicit FDM is applicable only when **h** and **k** are selected such that $r \leq \frac{1}{2}$.

Truncation Error

The truncation error is introduced when we replace the infinite Taylor series by a finite number of terms in difference equations. Truncation error is the sum of all remaining terms that we do not include in the formulation of the difference equations. Again considering Eq. (2.14) and applying the Taylor series at $u_{i,j+1}$, $u_{i+1,j}$ and $u_{i-1,j}$, we get

$$(u_{i,j} + ku_t + \frac{k^2}{2!}u_{tt} + \frac{k^3}{3!}u_{ttt} + \frac{k^4}{4!}u_{tttt} + ... - u_{i,j}) = \frac{k}{h^2}(u_{i,j} + hu_x + \frac{h^2}{2!}u_{xx} + \frac{h^3}{3!}u_{xxx}$$
$$+\frac{h^4}{4!}u_{xxxx} + ... - 2u_{i,j} + u_{i,j} - hu_x + \frac{h^2}{2!}u_{xx} - \frac{h^3}{3!}u_{xxx} + \frac{h^4}{4!}u_{xxxx} + ...).$$

After simplification, we obtain

$$k(u_t - u_{xx}) + (\frac{k^2}{2!}u_{tt} + \frac{k^3}{3!}u_{ttt} + \frac{k^4}{4!}u_{tttt} + ...) = \frac{kh^2}{2!}(u_{xxxx} + ...),$$

or

$$\frac{k}{2!}u_{tt} + \frac{k^2}{3!}u_{ttt} + \frac{k^3}{4!}u_{tttt} + ... = \frac{h^2}{2!}u_{xxxx} + ...,$$

or

$$k(\frac{u_{tt}}{2!} + \frac{k}{3!}u_{ttt} + \frac{k^2}{4!}u_{tttt} + ...) = h^2(\frac{u_{xxxx}}{2!} + ...).$$

This shows that the FTCS has truncation error of an $O(k + h^2)$.

The drawback of FTCS scheme is that it is difficult to apply because we have to choose **h** and **k** in such a way that we can attain sufficient accuracy. For example, if we choose $h = 0.1$ then $k \leq 0.005$. To reach the desired value of **t**, we have to perform many number iterations. To overcome this problem, we should look for a method which does not impose any restriction on the choice of $r = h/k^2$, which means we need an unconditional scheme.

2.1.2 Implicit Finite Difference Scheme

In this scheme, backward-difference equation for the time $\partial u/\partial t$ and second order central difference for the space derivative $\partial^2 u/\partial x^2$ are used. This is also called BTCS.

Considering Eq. (2.13) and apply BTCS scheme, we get,

$$\frac{u_{i,j} - u_{i,j-1}}{k} = \alpha \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h^2},$$

or

$$u_{i,j} - u_{i,j-1} = \frac{\alpha k}{h^2}(u_{i+1,j} + u_{i-1,j} - 2u_{i,j}),$$

or

$$u_{i,j-1} = (1+2r)u_{i,j} - ru_{i+1,j} - ru_{i-1,j}, \quad \text{for each } \ i = 1,2,3,...,m-1 \ \text{ and } \ j = 1,2,..., \tag{2.19}$$

And we have $u_{i,0} = f(x_i)$ and $u_{m,j} = u_{0,j} = 0$.

The matrices representation of Eq. (2.28) takes the following form

$$\begin{bmatrix} (1+2r) & -r & 0 & \cdots & 0 \\ -r & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots\ddots & \ddots & -r \\ 0 & \cdots & 0 & -r & (1+2r) \end{bmatrix} \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{m-1,j} \end{bmatrix} = \begin{bmatrix} u_{1,j-1} \\ u_{2,j-1} \\ \vdots \\ u_{m-1,j} \end{bmatrix},$$

or

$$Au^{(j)} = u^{(j-1)}, \quad \text{for each } \ j = 1,2,.... \tag{2.20}$$

This is an **implicit method** called **Backward Time Central Space**.

Stability Analysis

To determine the stability conditions, we again consider the Fourier series of the form $u_{i,j} = e^{\iota\beta x}\xi^t$. Substitute this expression in Eq. (2.14), we have

$$e^{\iota\beta x}\xi^t = e^{\iota\beta x}\xi^{(t-1)} + r(e^{\iota\beta(x+1)}\xi^t + e^{\iota\beta(x-1)}\xi^t - 2e^{\iota\beta x}\xi^t),$$

or

$$e^{\iota\beta x}\xi^t = e^{\iota\beta x}\xi^t(\xi^{-1} + r(e^{\iota\beta} + e^{-\iota\beta} - 2).$$

Using the trigonometric identity given in Eq. (2.18) and after simplifying the above equation, we get

$$\xi^{-1} = 1 + r(e^{\beta} + e^{-\iota\beta} - 2),$$

or

$$\xi = \frac{1}{1 + 4r\sin^2(\frac{\beta}{2})}. \tag{2.21}$$

The value of ξ determine the stability condition. From Eq. (2.21), $0 < |\xi| \leq 1$ for all $r > 0$. This shows that the backward time central space method is unconditionally stable. Similarly the backward difference method has truncation error of an order $k + h^2$. The weakness of this method results from the fact that the truncation error has portion with order k, requiring that time interval should be made much smaller than the spatial interval. It would be clearly desirable to have a scheme with truncation error of $O(k^2 + h^2)$. The first step in this direction is to use a difference equation that has order k^2 instead of k. To overcome this problem Richardson scheme was introduced [9].

2.1.3 Richardson Scheme (CTCS)

In Richardson scheme, partial derivatives, i.e, $\partial u/\partial t$ and $\partial^2 u/\partial x^2$ are replaced by central difference equations. The discretizationn of this scheme is as follow

$$u_{i,j+1} - u_{i,j} = r(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}). \tag{2.22}$$

For stability condition, substitute $u_{i,j} = e^{\iota\beta x}\xi^t$ in Eq. (2.22)

$$\xi^{t+1}e^{\iota\beta x} - \xi^{t-1}e^{\iota\beta x} = r(\xi^{t+1}e^{\iota\beta(x+1)} - 2\xi^t e^{\iota\beta x} + \xi^t e^{\iota\beta(x-1)}).$$

After simplifying, we get

$$\xi^2 + 4r\xi\sin^2\left(\frac{\beta}{2}\right) - 1 = 0. \tag{2.23}$$

Eq. (2.23) is quadratic in ξ. Let ξ_1 and ξ_2 are the roots of this equation. The sum and product of the roots are as follow

$$\xi_1 + \xi_2 = 4\sin^2\left(\frac{\beta}{2}\right),$$

and

$$\xi_1\xi_2 = -1.$$

For stability $|\xi_1| \leq 1$ and $|\xi_2| \leq 1$. From the product of roots, if $|\xi_1| \leq 1$ then $|\xi_2| \geq 1$. Also if $\xi_1 = 1$ and $\xi_2 = -1$ then $\beta = 0$. The above two results show that Richardsons method is unconditionally unstable.

2.1.4 Crank-Nicolson Scheme

A more rewarding method is obtained by averaging the **backward difference method** and the **forward difference method** [9]. The Forward difference method at j^{th} step is given as

$$\frac{u_{i,j+1} - u_{i,j}}{k} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}. \tag{2.24}$$

Similarly, the backward difference method at $(j+1)^{th}$ step is

$$\frac{u_{i,j+1} - u_{i,j}}{k} = \frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{h^2}. \tag{2.25}$$

After averaging Eqs. (2.24) and (2.25), we get the following relation

$$\frac{(u_{i,j+1} - u_{i,j})}{h} = \frac{1}{2}(\frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h^2} + \frac{u_{i+1,j+1} - 2u_{i,j} + u_{i-1,j+1}}{h^2}).$$

After simplifying, the above equation takes the following form

$$(2+2r)u_{i,j+1} - ru_{i+1,j-1} - ru_{i+1,j+1} = (2-2r)u_{i,j} + ru_{i-1,j} + ru_{i-1,j+1}. \quad (2.26)$$

The above discretization results in the system of linear equations. The solution is found by solving this system of equations. The matrix representation of the above discretization is

$$Au^{(j+1)} = Bu^{(j)}, \quad \text{for each} \quad j = 1, 2, 3, ... \quad (2.27)$$

$$\text{where} \quad u^{(j)} = (u_{1,j}, u_{2,j}, ..., u_{m-1})^t,$$

and the matrices A and B are given as

$$A = \begin{bmatrix} (2+2r) & -r & 0 & \cdots & 0 \\ -r & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots\ddots & \ddots & -r \\ 0 & \cdots & 0 & -r & (2+2r) \end{bmatrix},$$

$$B = \begin{bmatrix} (2-2r) & r & 0 & \cdots & 0 \\ r & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots\ddots & \ddots & r \\ 0 & \cdots & 0 & r & (2-2r) \end{bmatrix}.$$

Stability Analysis

Now we find the stability requirements for the Crank-Nicolson scheme. Substituting $u_{i,j} = e^{\iota\beta h}\xi^t$ in the Eq. (2.26), we get

$$\begin{aligned} (2+2r)\xi^{(t+1)}e^{\iota\beta x} - r\xi^t e^{\iota\beta(x+1)} - re^{\iota\beta(x+1)}\xi^{(t+1)} &= (2-2r)\xi^t e^{\iota\beta x} + r\xi^t e^{\iota\beta(x-1)} \\ &+ re^{\iota\beta(x-1)}\xi^{(t+1)}, \end{aligned}$$

or

$$\xi^t e^{\iota\beta x}[((\xi(2+2r) - re^{\iota\beta} - r\xi e^{\iota\beta}] = \xi^t e^{\iota\beta x}[((\xi(2-2r) + re^{-\iota\beta} + r\xi e^{-\iota\beta}],$$

or

$$\xi - 1 = \frac{r}{2}[(e^{\iota\beta} + e^{-\iota\beta} - 2) + \xi(e^{\iota\beta} + e^{-\iota\beta} - 2)].$$

Using the trigonometric identity given in Eq. (2.18), we get

$$\xi = \frac{1 - 2r\sin^2\frac{\beta}{2}}{1 + 2r\sin^2\frac{\beta}{2}}. \tag{2.28}$$

Eq. (2.28) shows that $|\xi| \leq 1$ for all $r \geq 0$. The local truncation error of the Crank-Nicolson is of the order $k^2 + h^2$.

This proves that Crank-Nicolson method is unconditional stable. This is also an Implicit method and best scheme for small steps.

Crack-Nicolson scheme has significant advantages over the FTCS and BTCS because of unconditional stability and order of accuracy respectively . Finite Difference method is difficult to apply on PDEs having the boundary conditions involving derivatives or having irregular boundary shape. Another drawback of FDM is that when applied to engineering fluid problems great care has to be taken in approximation in order to ensure conservative property, especially in discontinuous solutions.

2.2 Finite Volume Method (FVM)

Finite volume methods was introduced in early 1970's [11]. Finite volume method can be easily implemented on structured as well as unstructured grids. In FVM, we do not discretize the differential form of equation, but discretization is applied on integral form. To understand the concepts related to FVM consider the 1D heat equation.

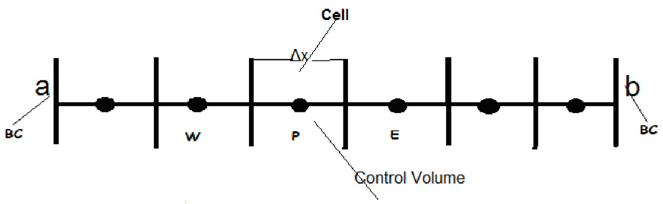
$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\alpha\frac{\partial u}{\partial x}\right), \tag{2.29}$$

subject to the following initial and boundary conditions

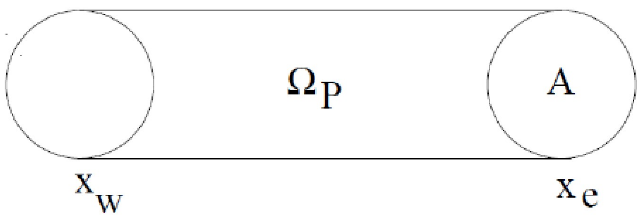
$$u(x,0) = f(x), \qquad x \,\epsilon\, [x_a, x_b],$$

$$u(x_a, t) = u_a(t), \quad u(x_b, t) = u_b(t).$$

In finite volume method divide the whole solution domain in two small cells called control volume.



Applying integral over the control volume, Ω_p, we get



$$\int_{x_w}^{x_e} \frac{\partial u}{\partial t} dx = (\alpha \frac{\partial u}{\partial x})_e - (\alpha \frac{\partial u}{\partial x})_w. \tag{2.30}$$

Next, we define cell average temperature, u_p, in control volume, Ω_p, by integrating $u(x,t)$ over the domain $[x_e, x_w]$ and then divide it by $x_e - x_w = \Delta x_p$ to get the average temperature over the given control volume as

$$u_p = \frac{1}{\Delta x_p} \int_{x_w}^{x_e} \frac{\partial u}{\partial t} dx. \tag{2.31}$$

Using Eq. (2.31) in Eq. (2.30), we get

$$\Delta x_p \frac{du_p}{dt} = \left(\alpha \frac{\partial u}{\partial x} \right)_e - \left(\alpha \frac{\partial u}{\partial x} \right)_w. \tag{2.32}$$

Next, we approximate cell average, u_e, at eastern side as

$$\left(\frac{\partial u}{\partial x} \right)_e \approx \frac{u_e - u_p}{x_e - x_w}. \tag{2.33a}$$

and at western cells, u_w, is given as

$$\left(\frac{\partial u}{\partial x}\right)_w \approx \frac{u_p - u_w}{x_p - x_w}. \tag{2.33b}$$

So the above Eqs. (2.33) now takes the form

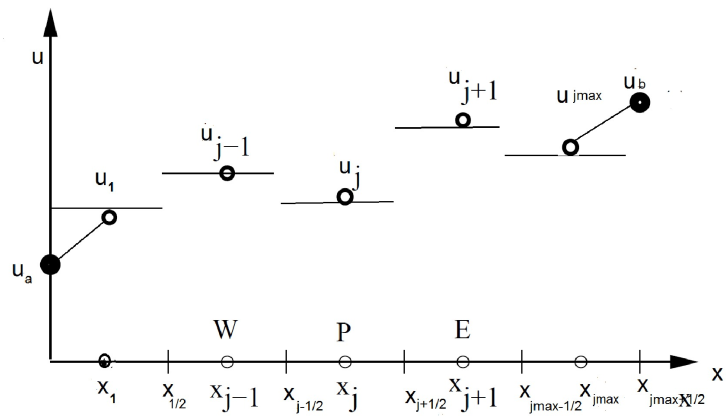
$$\Delta x_p \frac{du_p}{dt} = \alpha \left(\frac{u_e - u_p}{x_e - x_w} - \frac{u_p - u_w}{x_p - x_w} \right). \tag{2.34}$$

At the boundaries, the approximation of $\left(\frac{\partial u}{\partial x}\right)_a$ is given as

$$\left(\frac{\partial u}{\partial x}\right)_a \approx \frac{u_1 - u_a}{x_1 - x_a}. \tag{2.35}$$

Similarly, at the right boundary we have the following approximation for $\left(\frac{\partial u}{\partial x}\right)_b$

$$\left(\frac{\partial u}{\partial x}\right)_b \approx \frac{u_b - u_{jmax}}{x_b - x_{jmax}}. \tag{2.36}$$



We are dividing the interval $[x_a, x_b]$ into N cells $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, for each j=1, 2, 3, ...N. We apply Eq. (2.33) to each cells, except for the first and last ones, to have

$$\Delta x_j \frac{du_j}{dt} = \alpha \left(\frac{u_{j+1} - u_j}{x_{j+1} - x_j} - \frac{u_j - u_{j-1}}{x_j - x_{j-1}} \right), \quad \text{for each } \; j = 2, ..., N-1. \tag{2.37}$$

After simplifying, we have

$$\frac{du_j}{dt} = \frac{\alpha}{\Delta x^2}(u_{j+1} - 2u_j + u_{j-1}), \quad \text{for each } \; j = 2, ..., N-1. \tag{2.38}$$

Approximate slopes at the boundaries are

$$\frac{\partial u}{\partial x}(x_{\frac{i}{2}}, t) \approx \frac{u_1 - a}{\frac{\Delta x}{2}} \approx 2\left(\frac{u_1 - a}{\Delta x}\right), \tag{2.39}$$

and

$$\frac{\partial u}{\partial x}(x_{jmax+\frac{i}{2}}, t) \approx \frac{b - u_{jmax}}{\frac{\Delta x}{2}} \approx 2\left(\frac{b - u_{jmax}}{\Delta x}\right). \tag{2.40}$$

Thus, the final equation at left boundary cell is

$$\frac{du_1}{dt} = \frac{\alpha}{\Delta x^2}[u_2 - u_1 - 2(u_1 - a)]\frac{du_1}{dt} = \frac{\alpha}{\Delta x^2}(u_2 - 3u_1 + 2a). \tag{2.41}$$

At the right boundary cell, we get

$$\frac{du_{jmax}}{dt} = \frac{\alpha}{\Delta x^2}[2(b - u_{jmax}) - (u_{jmax} - u_{jmax-1}) = \frac{\alpha}{\Delta x^2}(2b - 3u_{jmax} + u_{jmax-1}). \tag{2.42}$$

Thus, we get a system of N ordinary differential equations of the form

$$\frac{du}{dt} = R_k(u), \quad k = 1, 2, 3, \ldots, N. \tag{2.43}$$

Where, R_1, R_j and R_N are as follow

$$R_1 = \frac{\alpha}{\Delta x^1}(u_2 - 3u_1 + 2a), \tag{2.44}$$

$$R_j = \frac{\alpha}{\Delta x^2}(u_{j+1} - 2u_j + u_{j-1}), \quad \text{for each} \;\; j = 2, ..., N-1, \tag{2.45}$$

$$R_N = \frac{\alpha}{\Delta x^2}(2b - 3u_{jmax} + u_{jmax-1}). \tag{2.46}$$

The unknown vectors are

$$U = [u_1, u_2, u_3, ..., u_{jmax}]. \tag{2.47}$$

In the next step, we solve the system of ODEs by the following schemes.

Explicit Euler Scheme

In explicit Euler method, we solve du/dt by forward time integration

$$\frac{u^{n+1} - u^n}{\Delta t} = R_k(u^n), \qquad k = 1, 2, 3, \ldots, N,$$

or

$$u^{n+1} = u^n + \Delta t R_k(u^n), \qquad k = 1, 2, 3, \ldots, N,$$

where, $r = \alpha/\Delta x^2$. In this scheme, solution can be found explicitly. This scheme is stable for $0 \leq r \leq \frac{1}{2}$. The truncation error is of the order Δt. The explicit FVM is simple and easy to implement. However, the disadvantage of this scheme is low accuracy and severe stability condition applied to it for convergent solution.

Implicit Euler Scheme

To get rid of stability condition, we solve the system of ODEs by an implicit Euler method

$$\frac{u^{n+1} - u^n}{\Delta t} = R_k(u^{n+1}), \qquad k = 1, 2, 3, \ldots, N,$$

$$u^{n+1} - \Delta t R_k(u^{n+1}) = u^n, \qquad k = 1, 2, 3, \ldots, N. \tag{2.48}$$

Then, the FVM with the implicit Euler method can be expressed as

$$(1 + 3r)u_1^{n+} - ru_2^{n+1} = u_1^n + 2ra, \tag{2.49}$$

$$-ru_{j-1}^{n+1} + (1 + 2r)u_j^{n+1} - ru_{j+1}^{n+1} = u_j^n, \qquad j = 2, ..., N - 1, \tag{2.50}$$

$$-ru_{N-1}^{n+1} + (1 + 3r)u_N^{n+1} = u_N^n + 2rb. \tag{2.51}$$

These N equation can be represented in the matrix form

$$Au^{n+1} = b^n, \tag{2.52}$$

or

$$\begin{bmatrix} (1+3r) & -r & 0 & \cdots & 0 \\ -r & (1+2r) & -r & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & -r & (1+2r) & -r \\ 0 & \cdots & 0 & -r & (1+3r) \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_{N-1}^{n+1} \\ u_N^n \end{bmatrix} = \begin{bmatrix} u_1^n + 2ra \\ u_2^n \\ \vdots \\ u_{N-1}^n \\ u_N^n + 2rb \end{bmatrix}$$

For each time level we solve the linear system of equations. This scheme is unconditionally stable for all $r \geq 0$.

Crank-Nicolson Method

The Crank-Nicolson scheme is also an implicit scheme and is second order in time. In this scheme, we average the forward Euler method at $(n+1)^{th}$ step and backward Euler scheme at n^{th} step as

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}(R_k(u^n) + R_k(u^{n+1}),$$

$$u^{n+1} - \frac{1}{2}\Delta t R_k(u^{n+1}) = u^n + \frac{1}{2}\Delta t R_k(u^n). \tag{2.53}$$

It is unconditionally stable and is second order in time and space. The important feature of FVM is the use of integral form that ensures the conservation of mass, momentum and energy . This feature of FVM makes it quite attractive for those problems for which flux is of importance, such as fluid mechanics, semi conductor device simulation, heat and mass transfer. FVM keeps the local conservativity of numerical fluxes, that is the numerical flux remain conserved from one discretization cell to its neighboring cell.

2.3 Finite Element Method (FEM)

Finite element method was developed in mid of 1950s [12]. FEM is best to handle the problems, whose solution domain are having arbitrary geometry. In this method, we divide the solution domain into elements and this is the fundamental building block in FEM. The finite element discretization allows a variety of elements shapes, for example triangle, quadrilaterals, etc. Each element is formed by the connection of certain number of nodes. The number of nodes employed to form an element depend on the type of element (or interpolating function). In the next step, the unknown function say, is represented within each element by an interpolating polynomial which is continuous along with its derivative to a specified order within the element.

2.4 Spectral Method

Spectral method was developed by Steven Orszag in 1969 [13]. It is used to solve ODEs, PDEs and eigenvalue problems. When applying spectral methods to time-dependent PDEs, the solution is typically written as a sum of basis functions with time-dependent coefficients. After substituting this in the PDE it yields a system of ODEs in the coefficients which can be solved using any numerical method for ODEs. The implementation of this method is normally accomplished either with collocation or a Galerkin method. Spectral methods are computationally less expensive than finite element methods, but become less accurate for problems with complex geometries and discontinuous coefficients.

Chapter 3

Approximate Solution of Thermal Expulsion Problem

The governing mathematical equation of the thermal expulsion problem is the non-linear diffusion equation, that is given as

$$C\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial z^2}, \tag{3.1}$$

where C represents the flow velocity induced in the fluid by heating the tube wall. The initial and the boundary conditions are

$$C(z,0) = 0, \qquad z > 0, \tag{3.2a}$$

$$C_z(0,t) = -b, \qquad t > 0, \tag{3.2b}$$

$$C(\infty,t) = 0, \qquad t > 0, \tag{3.2c}$$

where b is a constant given by

$$b = \frac{\beta \dot{q}}{c_p}. \tag{3.3}$$

Here β is the volume coefficient of thermal expansion (K^{-1}), $\dot{q}$ is the heating rate per unit mass (Wkg^{-1}) and c_p is the specific heat ($Jkg^{-1}K^{-1}$).

The space coordinate z measures the distance into the tube from the open end $z = 0$ [4]. Now we have to find the solution of Eq. (3.1) with given boundary conditions. The analytical solution of non-linear thermal expulsion is too difficult to find. Thus, we find its approximate solution. The procedure that is employed here is as follows. At first, the similarity transformation is used to reduce the PDE to an ODE. The solution of this reduced ODE leads us to the solution of PDE. The difficulty in this procedure is that most often the similarity transformations reduce the non-linear PDE to non-linear ODE, which is again difficult to solve analytically. Thus, we find the numerical solution of this reduced ODE and then approximate it by a function. Finally, we apply inverse similarity transformations to the approximate solution of the reduced ODE, and get the approximate solution of the PDE.

3.1 Similarity Method

Similarity method is a powerful technique for determining transformations that reduces PDEs to ODEs. This method takes advantage of the natural symmetries in a PDE and allows us to define special variables that give rise to reduction. Those equations that model physical phenomenon, inherit symmetries from the underlying system: for example, a physical system that is translation invariant, often produces governing equations that are unchanged under translation coordinates. If Eq. (3.1) is invariant under one parameter stretching groups that are [14]

$$C^* = \epsilon^{\alpha} C, \tag{3.4}$$

$$t^* = \epsilon^{\beta} t, \tag{3.5}$$

$$z^* = \epsilon z, \tag{3.6}$$

where ϵ is the group parameter that labels the individual transformation, α and β are parameters connected by a linear relation

$$M\alpha + N\beta = L, \tag{3.7}$$

where M, N and L are fixed constants determined by the structure of a particular PDE. The characteristic equations of (3.4), (3.5) and (3.6) are

$$\frac{dC}{\alpha C} = \frac{dz}{z} = \frac{dt}{\beta t}. \tag{3.8}$$

By solving these three independent integrals given in Eq. (3.8), we get the following transformations

$$x = \frac{z}{t^{\frac{1}{\beta}}}, \tag{3.9}$$

$$y(x) = \frac{C}{t^{\frac{\alpha}{\beta}}},$$

$$C(z,t) = t^{\frac{\alpha}{\beta}} y(x). \tag{3.10}$$

Taking partial derivatives of Eq. (3.10) w.r.t z and t respectively, we get

$$C_z(z,t) = t^{\frac{\alpha}{\beta}} y'(x) t^{\frac{-1}{\beta}}, \quad \text{where } \frac{dy}{dx} = y'(x), \tag{3.11}$$

and

$$C_t(z,t) = \frac{1}{\beta} t^{\frac{\alpha}{\beta}-1}(\alpha y - xy'). \tag{3.12}$$

Again differentiating Eq. (3.11) w.r.t z, we have

$$C_{zz}(z,t) = t^{\frac{\alpha-2}{\beta}} y''(x). \tag{3.13}$$

Substituting Eqs. (3.12) and (3.13) in Eq. (3.1) and then simplifying, we get

$$t^{\frac{\alpha-\beta+2}{\beta}}(\alpha y^2 - xyy') = \beta y'' \tag{3.14}$$

with condition $t^{\frac{\alpha+2-\beta}{\beta}} = 1$. This implies that $\alpha - \beta = -2$. By initial and boundary conditions of Eqs. (3.2a) - (3.2c) we choose $\alpha = 1$ and $\beta = 3$ in Eq. (3.14). After Substituting α, β in Eqs. (3.10) and (3.9) become

$$C(z,t) = t^{\frac{1}{3}} y(x), \quad x = \frac{z}{t^{\frac{1}{3}}} \tag{3.15}$$

or

$$C(z,t) = t^{\frac{1}{3}} y\left(\frac{z}{\sqrt{3}t^{\frac{1}{3}}}\right). \tag{3.16}$$

In Eq. (3.16) the factor $\sqrt{3}$ is introduced for convenience. Now by using this transformation the Eq. (3.14) take the following form

$$y^2 - xyy' = y'',$$

or

$$y(y - xy') = y''. \tag{3.17}$$

Using the transformation given in Eq. (3.16), the initial and boundary conditions given in Eqs. (3.2a), (3.2b) and (3.2c) become

$$y'(0) = -b, \tag{3.18}$$

and

$$y(\infty) = 0. \tag{3.19}$$

Now these are the initial and boundary conditions of the reduced ODE given in Eq. (3.17).

3.1.1 Numerical Solution of the Reduced ODE

The resulting reduced ODE is non-linear and its analytical solution is difficult to find. Thus, we find numerical solution of the reduced ODE and then approximate it by a function. For the numerical solution of the reduced ODE, we are going to use MATLAB built in function **bvp4c**. We are converting the reduced non-linear ODE in to system of ODES as follow.

Let $y_1 = y$, $y_2 = y'$, then, Eq. (3.17) implies that

$$y_1' = y_2, \tag{3.20}$$

$$y_2' = y'' = y_1(y_1 - xy_2), \tag{3.21}$$

with the boundary conditions

$$y_2(0) = -b\sqrt{3},$$

$$y_1(\infty) = 0.$$

The graph of numerical solution of the reduced ODE is given in Fig. (3.1).

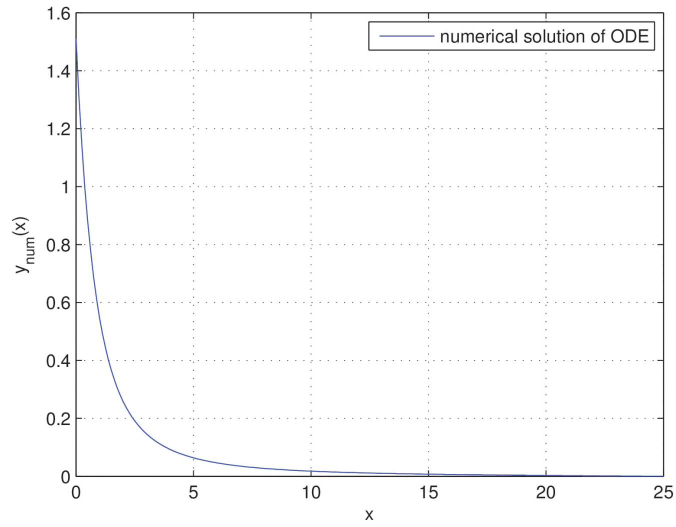


Figure 3.1: **Graph of** y_{num}

3.1.2 Approximation of the Numerical Solution of the Reduced ODE

The numerical solution is not practical in real time problem because the result has long list of points, not an equation, so the idea is to approximate numerical solution of non-linear ODE given in Eq. (3.17) by a function. In this section we review the procedure to obtain the required function as given in [15]. From the curve of numerical solution given in Fig. (3.1), the maximum value of $y(x)$ is 1.5112. The curve is similar to the graph of exponential function of the form

$$y(x) = 1.5112e^{-ax}, \tag{3.22}$$

Differentiating Eq. (3.22) w.r.t x, we get

$$y'(x) = \frac{dy}{dx} = -1.5112ae^{-ax}, \tag{3.23}$$

and from the boundary condition reduced ODE, we get

$$y'(0) = -1.5112a = -\sqrt{3}. \tag{3.24}$$

This gives us the value of a given below

$$a = \frac{\sqrt{3}}{1.5112}. \tag{3.25}$$

Thus, Eq. (3.22) that is the approximation of numerical solution in a form of a function $f(x)$ takes the following form

$$f(x) = 1.5112e^{-\frac{\sqrt{3}}{1.5112}x}. \tag{3.26}$$

The graph of $f(x)$ is shown in Fig. (3.2).

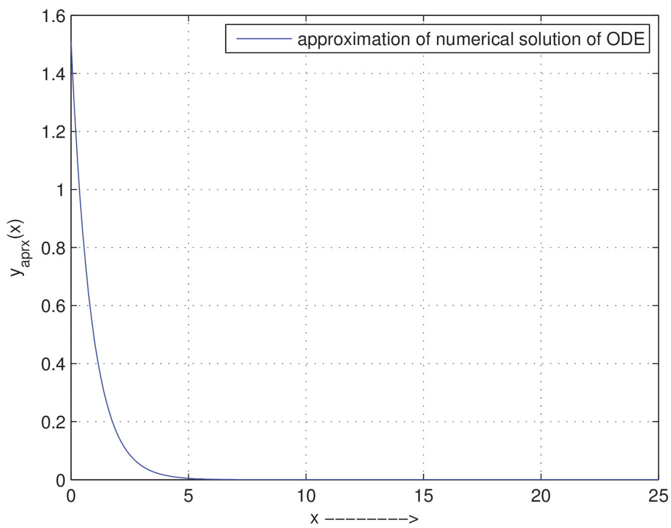


Figure 3.2: **Graph of** $f(x)$

Fig.(3.3) shows the graphs of y_{num} and the function, $f(x)$, that is an approximation of numerical solution of reduced ODE.

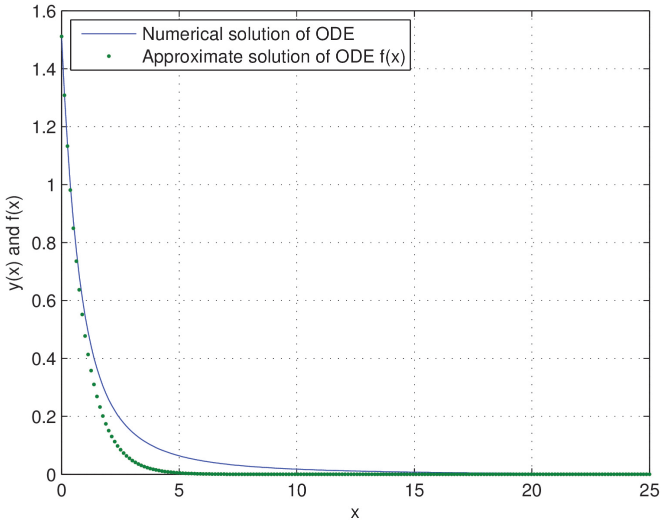


Figure 3.3: **Graph of y_{num} and $f(x)$**

The above Fig. (3.3) shows that there is an error in approximation of numerical solution of reduced ODE. This error is shown by the graph in Fig. (3.4).

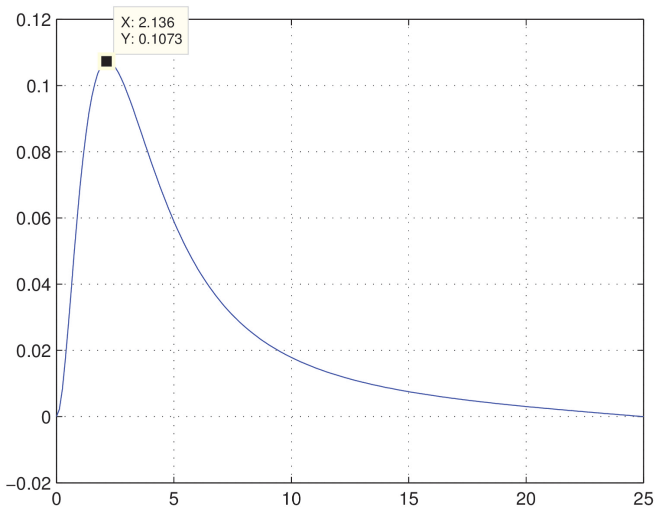


Figure 3.4: **Graph of error between $f(x)$ and $y_{num}(x)$**

From the graph, we can see that the maximum error in approximation of numerical solution is 0.1073. In order to reduce the maximum error we find the function $v(x)$ which approximate the error graph and then add up this to $f(x)$ to get approximate solution which will reduced the error. The graph of this error is similar to the following function

$$v(x) = \alpha x^{\beta} e^{\gamma x}, \tag{3.27}$$

In the function $v(x)$: α, β and γ are unknown constants. In order to find these unknowns take three points on curve i.e. (x_1, v_1), (x_2, v_2) and (x_3, v_3). By substituting these points, we get following three equations

$$v_1 = \alpha x_1^{\beta} e^{\gamma x_1}, \tag{3.28}$$

$$v_2 = \alpha x_2^{\beta} e^{\gamma x_2}, \tag{3.29}$$

$$v_3 = \alpha x_3^{\beta} e^{\gamma x_3}. \tag{3.30}$$

Dividing Eq. (3.28) by Eq. (3.29) and then taking log on both sides

$$\ln\left(\frac{v_1}{v_2}\right) = \beta \ln\left(\frac{x_1}{x_2}\right) + \gamma(x_1 - x_2). \tag{3.31}$$

Similarly, dividing Eq. (3.29) and Eq. (3.30) and then taking log on both sides, we get

$$\ln\left(\frac{v_1}{v_3}\right) = \beta \ln\left(\frac{x_1}{x_3}\right) + \gamma(x_1 - x_3). \tag{3.32}$$

Multiplying Eqs. (3.31) and (3.32) by $(x_1 - x_3)$ and $(x_1 - x_2)$ respectively, we have

$$(x_1 - x_3)\ln\left(\frac{v_1}{v_2}\right) = \beta(x_1 - x_3)\ln\left(\frac{x_1}{x_2}\right) + \gamma(x_1 - x_2)(x_1 - x_3), \tag{3.33}$$

and

$$(x_1 - x_2)\ln\left(\frac{v_1}{v_3}\right) = \beta(x_1 - x_2)\ln\left(\frac{x_1}{x_3}\right) + \gamma(x_1 - x_3)(x_1 - x_2). \tag{3.34}$$

Subtracting Eq. (3.34) from Eq. (3.33), we get

$$(x_1 - x_3)\ln\left(\frac{v_1}{v_2}\right) - (x_1 - x_2)\ln\left(\frac{v_1}{v_3}\right) = \beta((x_1 - x_3)\ln\left(\frac{x_1}{x_2}\right) - (x_1 - x_2)\ln\left(\frac{x_1}{x_3}\right),$$

or

$$\beta = \frac{(x_1 - x_3)\ln(\frac{v_1}{v_2}) - (x_1 - x_2)\ln(\frac{v_1}{v_3})}{(x_1 - x_3)\ln(\frac{x_1}{x_2}) - (x_1 - x_2)\ln(\frac{x_1}{x_3})}. \tag{3.35}$$

Now from Eq. (3.31), we have

$$\gamma = \frac{\ln(\frac{v_1}{v_2}) - \beta\ln(\frac{x_1}{x_2})}{x_1 - x_2}. \tag{3.36}$$

From Eq. (3.28), we get the value of α

$$\alpha = \frac{v_1}{x_1^{\beta} e^{\gamma x_1}} \tag{3.37}$$

Now we take three points on the graph of error curve given in Fig. (3.4) as

$$(0.8794,\ 0.0596),\ (2.1357,\ 0.1073),\ \text{and}\ (7.5377,\ 0.0304).$$

After substituting these points in Eqs. (3.28), (3.29) and (3.30), we get the values of unknowns α, β and γ as

$$\alpha = 0.12009,\ \beta = 1.4836,\ \gamma = -0.57982.$$

Using these values in Eq. (3.27), we have

$$v(x) = 0.12009x^{1.4836}e^{-0.57982x}. \tag{3.38}$$

Fig. (3.5) shows the error graph and its approximation in form of function $v(x)$

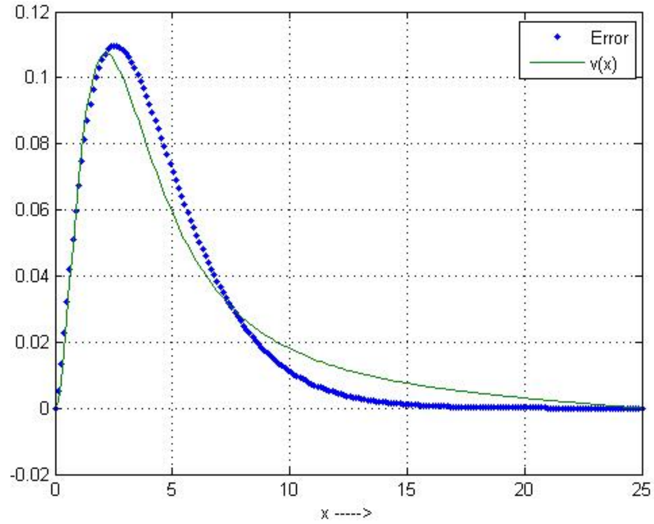


Figure 3.5: **Graph of error and** $v(x)$

Fig. (3.6) shows graph of error between numerical solution and initial approximation $f(x)$ and error between numerical and approximate y_{approx} solutions.

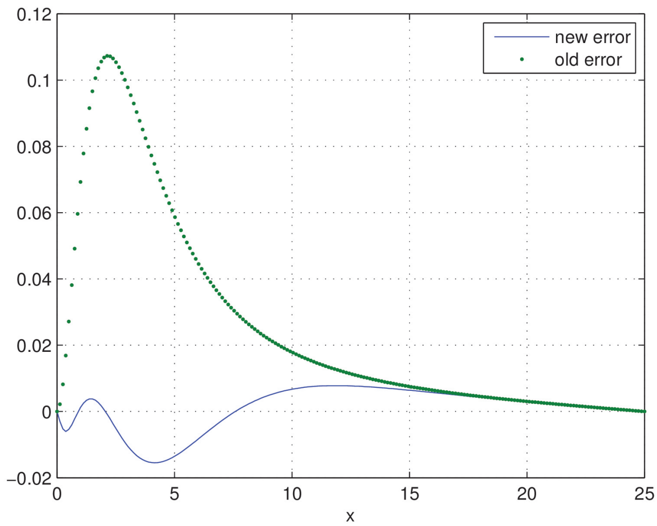


Figure 3.6: **Graph of error between** $f(x)$ **and** $y_{num}(x)$**,** y_{num} **and** y_{apprx}

Now, we can see from the above graph, maximum error is reduced to 0.0148.

The approximate solution is

$$y_{approx}(x) = f(x) + v(x),$$

or

$$y_{approx}(x) = 1.5112e^{-\frac{\sqrt{3}}{1.5112}x} + 0.12009x^{1.4836}e^{-0.57982x}. \qquad (3.39)$$

Fig. (3.7) represents graph of y_{num}, $f(x)$ and y_{approx}.

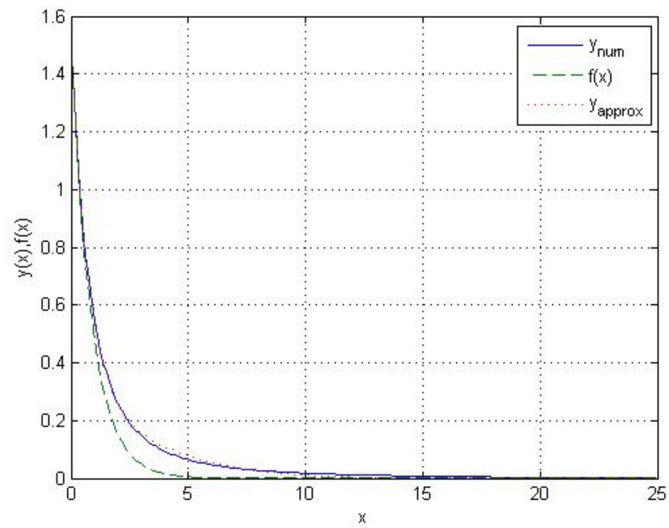


Figure 3.7: **Graph of $f(x)$, y_{num} and y_{approx}**

3.2 Numerical Solution of Thermal Expulsion Equation

There are many other ways to find the approximate solution of thermal expulsion PDE, one of them is the numerical technique. There are different numerical methods, explained in Chapter 2, but the method that we use here is finite difference method. As explained earlier, in this method we approximate the partial derivative by difference equations. First of all, partition the domain using mesh points in space z_0, z_1, ..., z_n, similarly, in time t_0, t_1, ..., t_m, assume uniform partition in both space and time. The distance between two consecutive space points is h and time is k. Suppose

$$C(z_i, t_j) = C_{i,j}. \tag{3.40}$$

Using a backward difference at time t_j and central difference for space z_j, and then substituting difference Eqs. (2.8) and (2.11) in Eq. (**??**), we get the following discretization

$$\frac{C_{i,j}\left(-C_{i,-1+j} + C_{i,j}\right)}{k} - \frac{C_{-1+i,j} - 2C_{i,j} + C_{1+i,j}}{h^2} = 0, \tag{3.41}$$

or

$$\frac{2C_{i,j}}{h^2} - \frac{C_{i-1,j}}{h^2} - \frac{C_{i+1,j}}{h^2} + \frac{C_{i,j}^2}{k} - \frac{C_{i,j-1}C_{i,j}}{k} = 0. \tag{3.42}$$

Taking $h = 0.25$, $k = 0.03125$, Eq. (3.42) becomes

$$-16.C_{-1+i,j} + 32.C_{i,j} - 32.C_{i,-1+j}C_{i,j} + 32.C_{i,j}^2 - 16.C_{1+i,j} = 0. \tag{3.43}$$

The resulting discretization is non-linear equations. For $i = 1, 2, 3, \ldots, 99$ and $j = 1$, we get system of non-linear equations. We obtain the value of $C_{i,j}$ by solving the resulting system of equations. For this we use the Mathematica build in command FindRoot. The 3D plot of numerical solution of non-linear thermal expulsion equation is shown in Fig. (3.8).

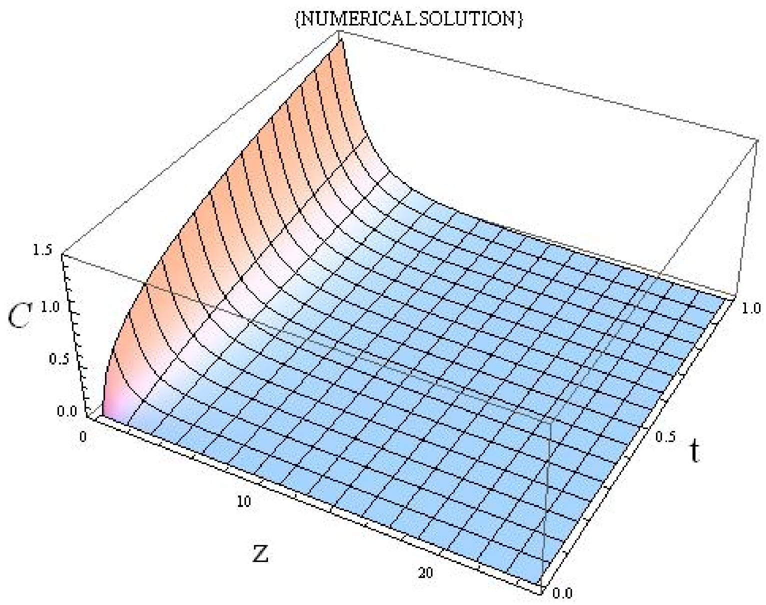


Figure 3.8: **Graph of the** C_{num}

3.3 Closed Form Approximate Solution of Thermal Expulsion Equation

Again considering the similarity transformation given in Eq. (3.10) which is

$$C(z,t) = t^{\frac{1}{3}} y(x), \quad where \quad x = \frac{z}{\sqrt{3} t^{\frac{1}{3}}}. \tag{3.44}$$

Substituting Eq. (3.39) in above equation, we get

$$C(z,t) = t^{\frac{1}{3}} \left(1.5112 e^{\frac{-\sqrt{3}}{1.5112} x} + 0.12009 x^{1.4836} e^{-0.57982 x} \right), \tag{3.45}$$

or

$$C(z,t) = t^{\frac{1}{3}} \left(1.5112 e^{-\frac{z}{1.5112 t^{1/3}}} + 0.12009 \left(\frac{z}{\sqrt{3} t^{1/3}} \right)^{1.4836} e^{-0.57982 \frac{z}{\sqrt{3} t^{1/3}}} \right), \tag{3.46}$$

which is the closed form approximate solution of thermal expulsion problem. The 3D plot of closed form approximate solution of non-linear thermal expulsion equation is shown in Fig. (3.9).

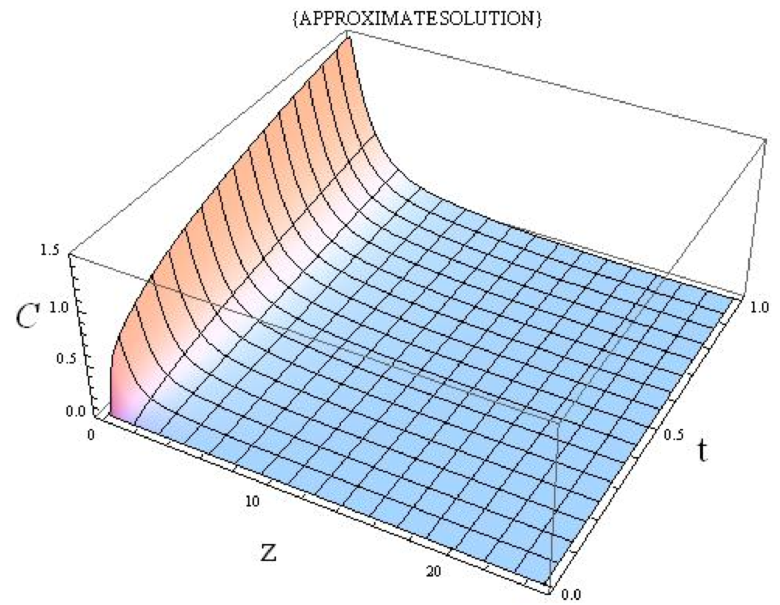


Figure 3.9: **Graph of the close form solution of nonlinear thermal expulsion PDE**

3.4 Comparison Between the Closed Form Approximate and Numerical Solution of Thermal Expulsion Equation

In this step, we compare both closed form and numerical solution of thermal expulsion equation. For this we will keep t constant and discuss the corresponding curve for all the values of z and t. Both are the approximate solutions and are giving almost same results. The behavior of both solutions can be analyzed from the following graphs. At $t = 0.03125$ the approximate and numerical solution of thermal expulsion equation is as

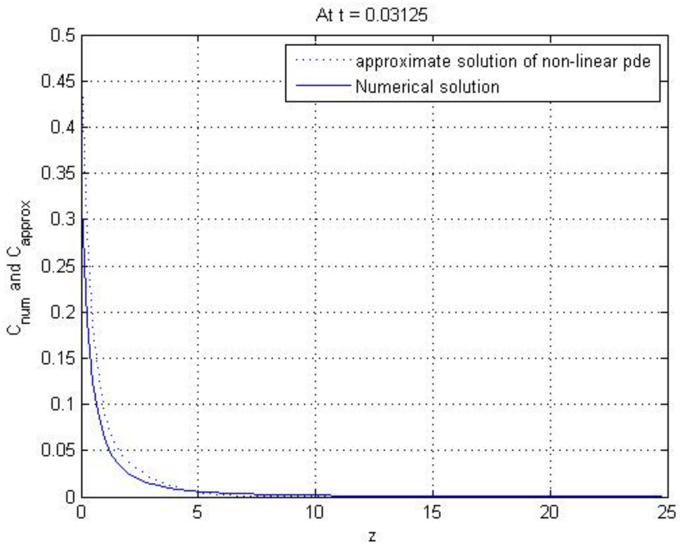


Figure 3.10: **Graph of the C_{num} and C_{approx} at** $t = 0.03125$

At $t = 0.125$ we have the following graph

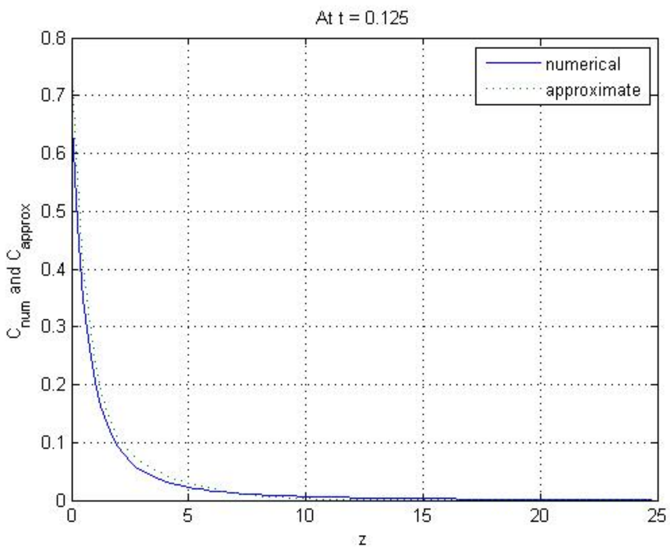


Figure 3.11: **Graph of the C_{num} and C_{approx} at** $t = 0.125$

similarly at $t = 0.21875$

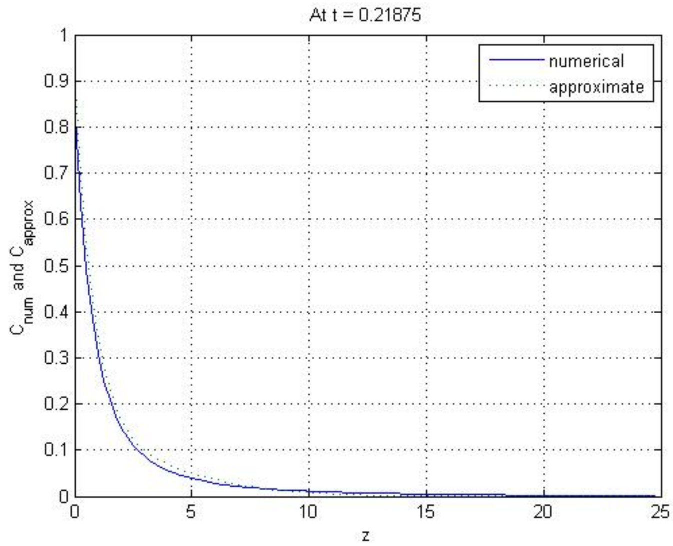


Figure 3.12: **Graph of the C_{num} and C_{approx} at $t = 0.21875$**

At $t = 0.3125$ we have

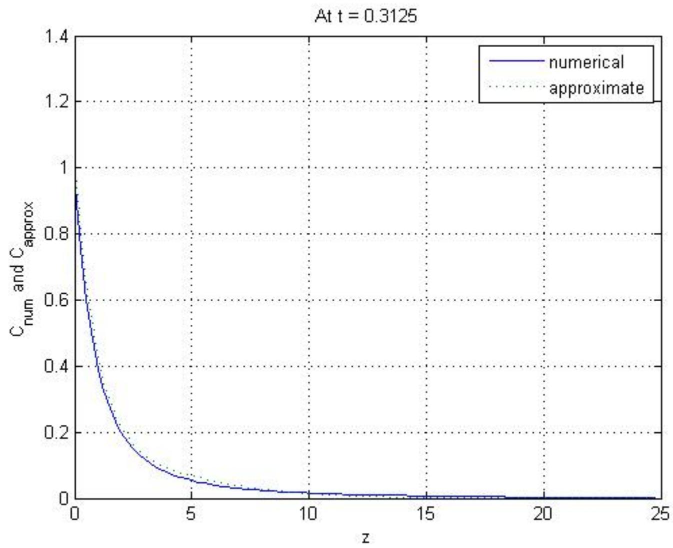


Figure 3.13: **Graph of the C_{num} and C_{approx} at $t = 0.3125$**

The difference between the numerical and approximate solutions of C at $t = 0.03125$ is represented in Fig. (3.14).

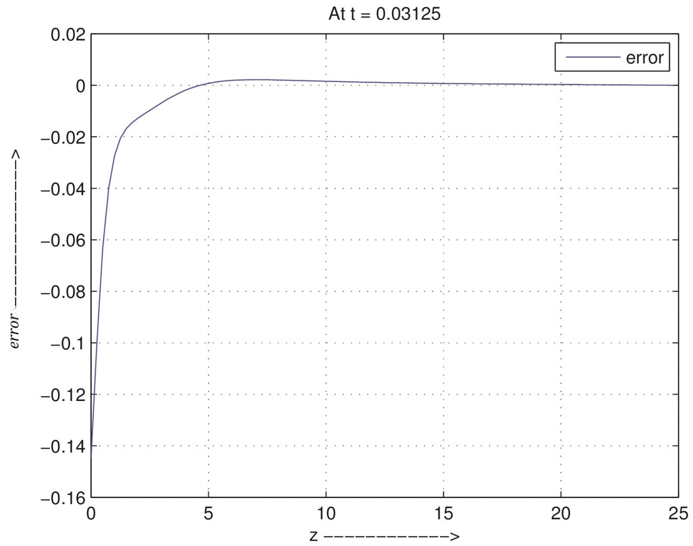


Figure 3.14: **Graph of difference between C_{num} and C_{approx} at $t = 0.03125$**

The absolute maximum difference at $t = 0.03125$ is 0.144918 at $z = 0$, after this, difference decreases and then goes to zero. Similarly the difference at at $t = 0.125$, 0.21875, and 0.3125 are show in Fig. (3.15)

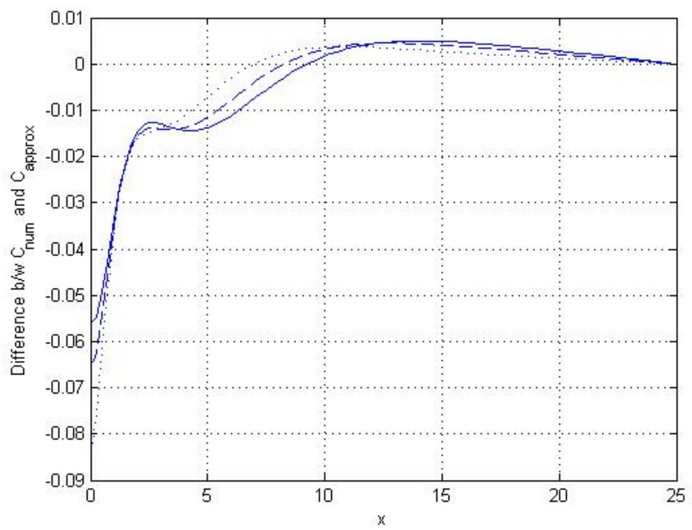


Figure 3.15: **Graph of difference between C_{num} and C_{approx}, dotted line represent the curve at $t = 0.125$, dashed line at $t = 0.21875$ and solid line at $t = 0.3125$**

These graphs clearly show that error at $z = 0$ decreases as we go for larger value of t. The 3D plot of difference is shown in Fig. (3.16).

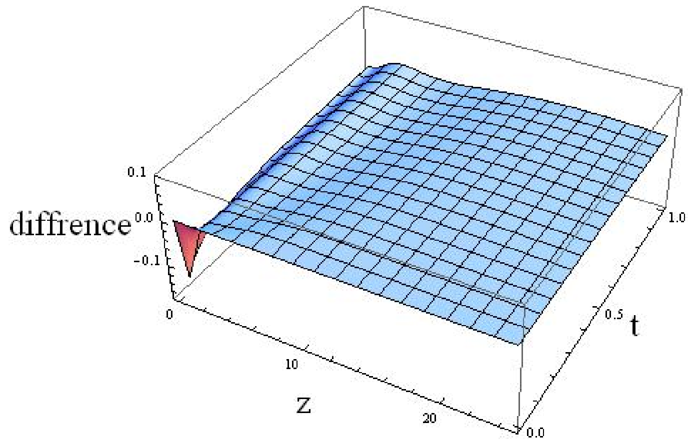


Figure 3.16: **3D plot of difference between C_{num} and C_{approx}**

Note that, the maximum error between the numerical and closed form approximate solution of thermal expulsion equation is at $z = 0$ when $t = 0.03125$, after this when we carry our calculations for larger values of t the error at $z = 0$ is decreases and goes to zero as z is increases.

Chapter 4

Conclusions

In this thesis, we have solved the non-linear thermal expulsion PDE. As the exact solution of this equation was not available, we have found its approximate solution in form of a function. It follows these four steps. First step is to reduce the non-linear thermal expulsion equation to an ODE via similarity variables. Second step involves finding numerical solution of the reduced ODE. In third step, we approximate it by a function and then improve it up to desired level of accuracy to obtain approximate solution of reduced ODE. In fourth step, with the help of this approximate solution of the reduced ODE we find the approximate solution of thermal expulsion PDE by using the similarity variables. Now, the exact solution of the thermal expulsion equation is not available, therefore we find its numerical solution by finite difference method and then made the comparison between both solutions. From the section 3.14 that is the comparison of closed form and approximate solution it is cleared that the closed form approximate solution is satisfactory except at the start when $t = 0$. The approximate solution of thermal expulsion equation obtained in the form of function has more advantages over the numerical solution. Since, it involves parameters and variables of problems, so it require less time for processing and is more applicable in real time applications. As we have observed that there is error between the closed form approximate and numerical solutions of thermal expulsion equation. This error is due to the approximation of numerical solution of reduced ODE. For further work it is required to refine the closed form approximate solution of thermal expulsion equation and also reduce the error at start when $t = 0$. That can be done by refining the approximation of numerical solution of reduced ode. And also solve thermal expulsion equation by other numerical methods like FVM or FEM, etc, then compare both solutions and analyze errors between them.

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Appendix

The MATLAB code that was used to solve reduced non-linear ODE is given below

clc

function thermal_bvp

”%” solution

sol = bvpinit(linspace(0,25), [1 0]);

sol1 = bvp4c(@ode, @bc, sol);

clf reset

x=linspace(0,25,200);

y=deval(sol1,x);

size(y)

$f = 1.5112 * exp(-3^(1/2) * x/1.5112);$

maxerror=max(imabsdiff(f,y(1,:)))

figure(1)

plot(x,y(1,:),x,f,’r’)

diff=y(1,:)-f;

figure(2)

plot(x,diff,’g’)

$g = 0.12009. * x.^1.4836. * exp(-0.57982. * x);$

figure(3)

plot(x,diff,’g’,x,g,’r’)

fn=f+g;

nmaxerror=max(imabsdiff(fn,y(1,:)))

figure(4)

plot(x,y(1,:),x,f,'r',x,fn,'g')

figure(5)

plot(x,maxerror)

"%" Boundary conditions

function res = bc(y0, yinf)

$res = [y0(2) + sqrt(3); yinf(1)];$

end

"%" First Order ODEs

function yprime = ode(x,y)

$yy1 = y(1).^2 - x * y(2) * (y(1));$

yprime = [y(2);yy1];

end

end"

This is the Mathematica code for the numerical solution of thermal expulsion PDE

$C_{\mathrm{zz}} = \left(C_{i+1,j} - 2C_{i,j} + C_{i-1,j}\right)/h^2;$

$C_t = (C_{i,j} - C_{i,j-1})/\,k;$

$C_{i,j}C_t - C_{\mathrm{zz}}{=}{=}0;$

$e = \mathrm{Expand}[\%];$

$v = \mathrm{Table}\left[e/.\left\{C_{i,0} \to 0, C_{-1,j} \to C_{1,j} + 2h, C_{100,j} \to 0\right\}, \{j, 1, 32\}, \{i, 0, 99\}\right];$

$v/.\{h \to 0.25, k \to 0.03125\};$

$\mathrm{sol} = \mathrm{FindRoot}\left[\%, \mathrm{Flatten}\left[\mathrm{Table}\left[\{C_{i,j}, 0\}, \{j, 1, 32\}, \{i, 0, 99\}\right], 1\right]\right];$

Length[sol];

$s = \mathrm{Table}[\mathrm{sol}[[i, 2]], \{i, 1, 3200\}];$

$\mathrm{max} = \mathrm{Max}[s];$

$w = \mathrm{Table}[s[[i]], \{i, 1, 3200\}]$

$x = \text{Flatten}[\text{Table}[\{0.25 * i\}, \{j, 1, 32\}, \{i, 0, 99\}]];$

$q = \text{Flatten}[\text{Table}[\{0.25 * i\}, \{j, 1\}, \{i, 0, 99\}]];$

$\text{Length}[q]$

$t = \text{Flatten}[\text{Table}[\{(j * 0.03125)\}, \{j, 1, 32\}, \{i, 0, 99\}]];$

$z = \text{Table}[\{x[[i]], t[[i]], w[[i]]\}, \{i, 1, 3200\}];$

$\text{int} = \text{Table}[\{q[[i]], 0, 0\}, \{i, 1, 100\}];$

$\text{points} = \text{Join}[\text{int}, z];$

$\text{p1} = \text{ListPlot3D}[\text{points}, \text{AxesLabel} \to \{\text{zspace},$

$\text{ttime}, C\}, \text{PlotLabel} \to \{\text{NUMERICALSOLUTION}\}, \text{PlotRange} \to \{0, 1.5\}]$

$\text{x1} = \text{z1} \,/\, \left(\sqrt{3} * \text{t1}^{1/3}\right) ;$

$\text{tab} = \text{t1}^{1/3} * \left(1.5112 * \text{Exp}[-(\sqrt{3} * \text{x1})/1.5112] + 0.12009 * \text{x1}^{1.4836} * \text{Exp}[-0.57982 * \text{x1}]\right) ;$

$\text{Length}[\text{s2}]$

$\text{w2} = \text{Table}[\text{s2}[[i]], \{i, 1, 3200\}]$

$\text{Length}[\text{w2}];$

$\text{z2} = \text{Table}[\{x[[i]], t[[i]], \text{w2}[[i]]\}, \{i, 1, 3200\}];$

$\text{points2} = \text{Join}[\text{int}, \text{z2}];$

$\text{p2} = \text{ListPlot3D}[\text{points2}, \text{AxesLabel} \to \{\text{zspace},$

$\text{ttime}, C\}, \text{PlotStyle} \to \text{Directive}[\text{Pink}, \text{Specularity}[\text{White}, 40]],$

$\text{PlotLabel} \to \{\text{APPROXIMATESOLUTION}\}, \text{PlotRange} \to \{0, 1.5\}]$

$\text{Show}[\text{p2}, \text{p1}]$

$\text{error} = w - \text{w2Length}[\text{error}];$

$\text{maxerror} = \text{Max}[\text{error}];$

$\text{w3} = \text{Table}[\text{error}[[i]], \{i, 1, 3200\}];$

$\text{z3} = \text{Table}[\{x[[i]], t[[i]], \text{w3}[[i]]\}, \{i, 1, 3200\}];$

$\text{points3} = \text{Join}[\text{int}, \text{z3}];$

$\text{ListPlot3D}[\text{points3}, \text{AxesLabel} \to \{\text{zspace}, \text{ttime},$

$\text{Error}\}, \text{PlotLabel} \to \{\text{ERROR}B/W\text{NUMANDAPRX}\}, \text{PlotRange} \to \{-0.18, 0.1\}]$