NUMERICAL TECHNIQUES FOR A VISCOUS REACTING FLOW IN A TUBE

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CERTIFICATION

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DEDICATION

This work is dedicated to:
My dear mother, Mrs J. Alao,
all less privileged Nigerians, and
my CREATOR, THE ALMIGHTY GOD

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ABSTRACT

A viscous fluid flowing through a cylinder is studied. The flow is reacting and heat is generated through reaction and viscosity.

To ensure that the problem represents a physical problem we discuss the existence and uniqueness of the problem. It is shown that.the solution is unique when the parameters a and d_1 are greater than zero and h-mesh size is such that

$h < 2.0/(|1/a-3a(\frac{1}{2}a)^{\frac{1}{2}}|)$ and $h < 2.0/(|1/d_1-3d_1(\frac{1}{2}d_1)^{\frac{1}{2}}|)$

for Equations (2.27) and (2.33).

The problem has no analytical solution, hence, we investigate the problem using numerical techniques based on Shooting method and Finite difference Scheme. The methods are compared and the best recommended based on a test solution.

Finally, the effects of the parameters a,b, d_1, d_2, d_3 and viscosity on the temperature was discovered. The results show that the temperature of the reacting system increases as the parameters a, d_2 and d_3 increase. On the other hand the parameters b and d_1 have opposite effects on the temperature, that is, the temperature decreases as the two parameters increase. Moreover, our numerical scheme confirmed what is physically expected - the temperature increases as we increase the viscosity of the reactants. Graphs depicting the relationships between, the temperature and the parameter, and that of the temperature and the space variable feature prominently in the thesis.

NOMENCLATURE

Y = Pre-mixed reactants

ρ = Density

c = Specific heat

T = Temperature

μ = Dynamic viscosity

Q = Heat release/unit mass

D = Diffusion coefficient

K = Thermal conductivity

R = Universal gas constant

β = Pre-exponential factor

P = Pressure

U = Velocity Component along Z-axis

t = Time.

Nondimensionalized Variables

$U = \frac{u}{v}$

$y = \frac{Y}{y_0}$

$\theta = \frac{E(T - T_0)}{RT_0^2}$

E = activation energy

$x = r/R$

$\tau = \frac{t\bar{v}}{R}$

$a = \frac{D}{VR}$

$b = \frac{\beta}{R\rho V}$

$d_1 = \frac{k}{\rho GVR}$

$d_2 = \frac{4U\epsilon\mu}{RR_0T_0^2}$

$d_3 = \frac{R\epsilon Q\beta}{UR_0T_0^2}$

$\epsilon = \frac{RT_0}{E}$

Ø = heat release per unit mass.

CHAPTER ONE

1.0 Introduction

The physical situation to be studied in this project deals with viscous reacting fluid flowing in a tube. Of particular interest is the numerical techniques to solve the steady state of the problem. The general problem of the flow through a pipe of uniform, but arbitrary cross-section is considered. The flow may be caused by either an applied pressure gradient or the gravitational factors.

Fluids can be classified into viscous and non-viscous. 'Sleep' palm oil, blood, honey, engine oil and so on, are examples of viscous fluid, while water, is an example of non-viscous fluid. The study of fluid mechanics becomes very important, because of the vital role it plays in engineering, medical and science fields. Whenever light is switched on, energy is drawn from a hydroelectric source that operates by the flow of water through turbines. Also fluid processes are involved in the manufacture of the paper. finally, human existence depends on a very important fluid mechanic process- the flow of blood through our veins and artries. The above are some of the areas where fluid mechanic is relevant.

Almost all viscous are exothermal, that is, they generates heats when flowing through a medium, this reaction may be caused due to friction between the fluid and the medium through which it flows and some other factors. For the purpose of this research, internal fluid flowing through a pipe in which the presence of frictional forces are acting is considered. The analysis of such flows is important in the many situations in which fluid must be transported from one place to another. By no-slip conditions, the layers of the fluid at the wall of the pipe through which it flows, has zero velocity. The fluid velocity increases progressively as we move from the wall to the source of the tube. A velocity distribution in a pipe is built up as shown in Fig. 1. (for more details, see John and Haberman (1983)).

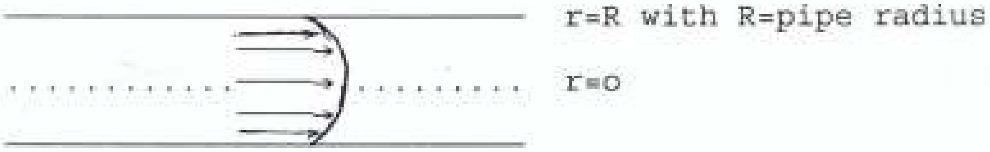


Fig. 1: Velocity distribution in pipe flow.

The velocity distribution in the pipe is a function of the type of flow in the pipe. Type of flow also plays an important part in the determination of the magnitude of the frictional forces acting on the fluid. There are two basic types of flow; Laminar and turbulent flows. The laminar viscous reacting fluid moving steadily through a tube is studied.

In standard texts on fluid flow in pipes, the basic equation describing the structure and motion of viscous reacting flow have been considered for particular situations in order to isolate a number of specific phenomena. In the general case, we need to integrate the basic equation with respect to time and space coordinates. Variables starting with a given temperature at a particular point in time so that a simulation can be provided for the temperature behaviour at subsequent point in time, are assumed.

The equation employed for these early studies was the continuity equation applied to a control volume. Writing the temperature θ in terms of the spherical coordinates $(r, \emptyset, Z)$, we have a parabolic partial differential equation of the form

$$\frac{(1 - \eta^2)\partial\theta}{\partial\eta} = \frac{1}{\eta}\frac{\partial(\eta\partial\theta)}{\partial\eta\ \partial\eta} \tag{1.1}$$

Subject to the conditions

$$\theta(0,\eta) = 1 \tag{1.2}$$

$$\frac{\partial\theta(Z,0)}{\partial Z} = 0 \tag{1.3}$$

and the Dirichlet conditions

$$\theta\ (Z,\ L) = 0 \tag{1.4}$$

(For details, see Campo and Lacoa (1994)).

Various methods of solution have been employed. They include analytical or geometrical and numerical methods.

1.0.1 The specific objectives of this research:

To formulate mathematical equations for a steady viscous reacting fluid flow in a tube.

To provide numerical techniques for solving the problem

To explain the advantages for each techniques

To give the physical meaning of the numerical results.

1.0.2 The research methodology:

The formulation of the problem is based on the theory of combinations and Navier-strokes equations for viscous fluids.

In this work, two numerical methods; Finite difference and Shooting methods are used to approximate the steady cases of the Boundary-Value Problems. These methods are compared and the best recommended based on test solution.

In chapter two, the mathematical equations of the problem is formulated. This is based on momentum, species and energy equations.

Finally, some of the programming tools- algorithms, flowcharts and program are used to implement the methods imployed.

1.0.3 Organisation of work

In chapter three, we establish the techniques for solving equations in chapter two.

Chapter four deals with the computer implementations and results. Here, the computer programs used to implement the methods described in chapter three are examined

Finally, chapter five deals with the analysis of the results gotten from chapter four and their physical implications. Also, the method are compared and the best is recommended.

1.1 Review of Literature

In the existing literature, Campo and Lacoa (1994) examined the meanbulk and wall-temperature distribution of hot fluids flowing inside horizontal tube and rejecting heat by natural convection to an external fluid. The mathematical formulation of this problem is a parabolic, partial differential equation together with a temperature-dependent, non-linear boundary conditions of the third kind. They critically examined the thermal responses of this kind of in-tube flows using two different mathematical models -

(a) a complete two-dimensional differential model.

(b) a largely simplified one-dimensional lumped model.

They assumed that the change in temperature does affect the thermophysical properties of the fluid. They used the finite volume method of Patanka (1980) for the numerical calculations of the temperatures field of the moving fluid. The velocity distribution of Szymaski (1985) for the start up flow in circular pipes has been verified experimentally by Letecher and Leutheusser (1991).

Shonet, Cess and Roidt (1962) examined the problem of unsteady viscous fluid flow in the entrance region. Jayaraman, et. al. (1986) equally studied the problem of entry flow into a circular tube of slowly varying cross-section.

In another development, Ayeni, Akinrelere and Amao (1985) sought for conditions under which the weakening can keep the temperature in the thermal boundary layer bounded for all time when the viscosity varies with temperature. To achieve this, they assumed that:

i. the material is incompressible

ii. the body forces are negligible

iii. there is no slip at the boundary

iv. the radius of the curvature of the surface is large compared with the lubricant thickness.

v. the velocity and temperature fields are given by

$$\underline{V} = \{u(y',t'),\ 0\},\ T\ (y',t') \qquad (1.5)$$

respectively.

vi. the boundary conditions are $u(0,t') = \Omega R = u$, $u(h,t') = 0$ $t' > o$ or alternatively

$$\frac{\mu du}{dy'} = \frac{\mu\beta}{\sqrt{t}}\ ,\ u(h,t') = 0\ ,\ \text{at } y'=0$$

$$t' > 0 \qquad (1.6$$

and $T(0,t') = T(h,t') = T_o,\ t' > 0$ (1.7)

where

R = radius of the Shaft

Ω = angular velocity

h = Lubricant thickness

β = positive constant

t' = the time

vii. the initial conditions are

$$u(y',0) = 0,\ T(y',0) = T_o \qquad (1.8)$$

viii. the viscosity μ is given by

$$\mu = \mu_o e^{-q\alpha(T-T_o)}\ ,\quad T_o > 0$$

or $\mu = \mu, e^{ql/T}$ (1.9)

where μ_o, μ_1 are characteristic viscosities and q_o, q_1, are constants.

ix. the relationship between the stress τ^1 and μ is given by

$$\tau^1 + \alpha\,\tau^{13} = \frac{\mu\partial u}{\partial y'} \tag{1.10}$$

They used Winter (1977) technique which showed that the relative difference between the expressions in equation (1.9) and equation (1.10) is less than 0.25%, if $T - T_o = 10k$ and $q_o = 10^{-2}$ per k, where k is thermal conductivity and $q_o = E/R$, such that,

E = the activation energy

R = the universal gas constant.

x. Thermal conductivity, k and the specific heat, c depend on temperature. They considered $k = K_o e^{q_2(T-T_o)}$

$$c = C_o e^{q_3(T-T_o)}$$

where K_o = characteristic thermal conductivity

C_o = a thermal specific heat

and q_2, q_3 are constants.

They considered the energy and momentum equations in the form

$$\frac{\rho\partial u}{\partial t'} = \frac{\partial\tau'}{\partial y'} - \frac{\partial P'}{\partial x'} \tag{1.12}$$

$$\frac{\rho c\partial T}{\partial t'} = \frac{\partial(k\partial T)}{\partial y} + \frac{\tau'\partial u}{\partial y'} \tag{1.13}$$

where ρ = lubricant density

P^1 = pressure

They used asymptotic techniques to estimate the temperature rise.

In his contribution, Ayeni (1982) considered a viscous flow through a cylinder whose motion was unsteady. He used asymptotic techniques to determine the criteria for thermal runaway. Also, Okoya and Ayeni (1994) studied reacting flows. The fluid is not viscous. From the existing literature, it can be seen that this work is new because all the previous investigations on fluid flows are either viscous or reacting flow. Non combines the two characteristics together, but this work combines the characteristics of Ayeni (1982), and Okoya and Ayeni (1994), because the fluid flow is viscous and at the same time reacting. The viscosity depends on temperature and the form of dependence is new. The resulting flow can be steady or unsteady and the equations are non-linear. Such class of equations hardly have analytical solution. Hence, we focus on using numerical techniques for a steady state of a viscous reacting flow in a tube.

Chuen-Yen Chow (1982) observed that the theoretical structure of a Shock in the presence of viscosity and conductivity was first thoroughly investigated by Becker(1922). Various numerical methods were developed for computing unsteady, one-dimensional shock profiles.

S.B. Angenent and M. Fila (1996) considered the method of sub and upper solutions of interior gradient blow-up in a similar parabolic equation.

Finally, discussions on many of these numerical methods can be found in Richlunyer and Morton (1967), J. Buckmaster(1996) and Roache (1972).

CHAPTER TWO

MATHEMATICAL EQUATIONS

We consider a viscous fluid flowing through a pipe. The fluid is not just an ordinary fluid, it reacts as it flows. Moreover, we assume that the flow is exothermal. That is, heat is generated as it flows. The co-ordinates are (r,θ,z). See Fig. (2) below.

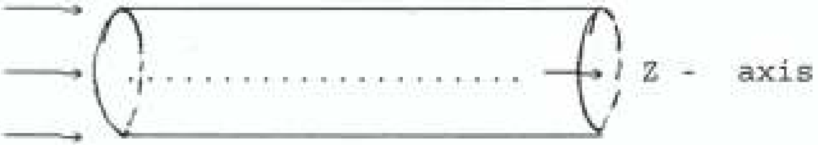


Figure 2: flow in a pipe

Flow of fluids in a pipe is governed by continuity equation. According to Round and Garg (1986), for a control volume, the continuity equation implies a balance between the masses entering and leaving per unit time and the change of density.

This equation was derived on the basis of the conservation of mass which states that fluid can neither be created nor destroyed. That is fluid is not created in the tube. Hence

Mass going in (m) = Mass inside + mass out

Let the tube be parallel to the x-axis along which $\frac{\partial u}{dx} = 0$

See Fig. (3) below.

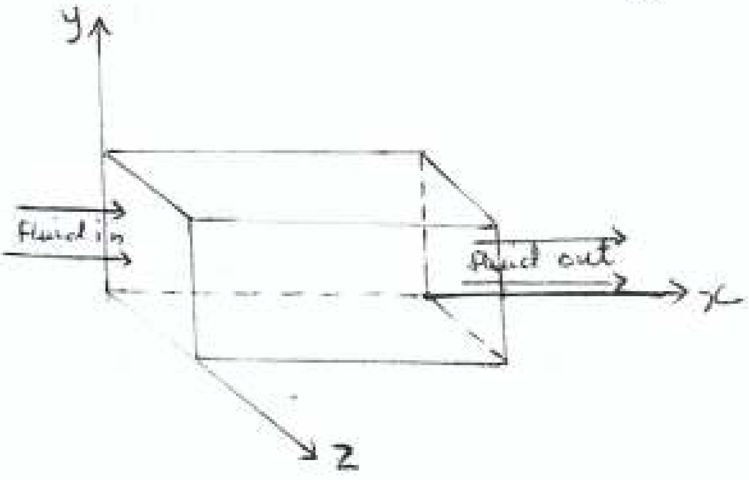


Figure 3: flow through an elemental cuboid

Because of this particular geometry, the flow has only one non-vanishing velocity component U in the axial direction, that is the velocity components are $\underline{q} = (0,0,U(r))$, so that the continuity equation is written in differential form as

$$\frac{\partial\rho}{\partial t} + \nabla(\rho\underline{q}) = 0$$

where $\underline{q}$ is as defined above and $\rho = \rho(x,y,z,t)$ is the density.

We shall now state the momentum, species and energy equations respectively as

$$-\frac{\partial P}{\partial z} + \frac{\mu}{r}\frac{\partial}{\partial r}\frac{(r\partial u)}{\partial r} = 0 \qquad (2.2)$$

$$\frac{\rho\partial y}{\partial t} = \frac{\rho D}{r}\frac{\partial}{\partial r}\frac{(r\partial y)}{\partial r} - \beta y e^{-E/RT} \qquad (2.3)$$

$$\frac{c\rho\partial T}{\partial t} = \frac{k}{r}\frac{(\partial}{\partial r}\frac{(\partial T))}{\partial r} + \mu\frac{(\partial u)^2}{\partial r} + \emptyset\beta e^{-E/RT} \qquad (2.4)$$

where all the relevant terms are as defined in the nomenclature.

Equations (2.2), (2.3) and (2.4) are formed, as a result of adding some parameters to the Navier-Stokes' equation.

Consider equation (2.2)

$$-\frac{\partial P}{\partial z} + \frac{\mu\partial}{r\partial r}\frac{(r\partial u)}{\partial r} = 0 \qquad (2.5)$$

where P is a function of Z alone and

U is a function of r alone.

If we consider $\frac{\partial P}{\partial z}$ = constant, that is, the pressure gradient is constant along the pipe axis. Since equation (2.5) involves only one variable r, it could be written as total differentiation to give

$$\frac{\mu}{r}\frac{d}{dr}\frac{(rdu)}{dr} = \frac{dP}{dz} \tag{2.6}$$

Integrating, we obtain

$$\frac{d(\mu rdu)}{dr} = (r\frac{dP}{dz})\,dr$$

$$\int\frac{d(\mu rdu)}{dr} = \int\frac{(rdP)dr}{dz} + C_1$$

$$\frac{\mu rdu}{dr} = (\tfrac{1}{2}r^2)\frac{dP}{dz} + C_1 \tag{2.7}$$

integrating further, we get

$$\int\mu du = \int\{\tfrac{1}{2}r\left(\frac{dP}{dz}\right) + \frac{c_1}{r}\}dr + c_2$$

$$\mu u = r^2/4\left(\frac{dP}{dz}\right) + c_1\ln r + c_2 \tag{2.8}$$

Let $\frac{dP}{dz} = P'$, Equation (2.8) reduces to

$$u = r^2/4\mu\, P' + C_1\ln r + C_2 \tag{2.9}$$

where, C_1 and C_2 are integrating constants whose values are determined by the boundary conditions. The boundary condition is U = 0 (i.e, no slip condition) and the other condition is the requirement of a finite velocity at r=0 where r = R for finiteness, $C_1 = 0$, this gives rise to equation

$$u = \frac{r^2P'}{4\mu} + C_2 \tag{2.10}$$

$$u'(0) = \frac{2(0)P'}{4\mu} + 0 = 0$$

From Equation (2.10),

$$u(R) = 0$$

$$\therefore \quad 0 = \frac{R^2P'}{4\mu} + C_2$$

hence,

$$C_2 = \frac{-R^2P'}{4\mu}$$

Also equation (2.10) becomes

$$u = \frac{r^2P'}{4\mu} + \frac{(-R^2P')}{4\mu}$$

$$u = \frac{P'(R^2 - r^2)}{4\mu} \qquad (2.11)$$

which is parabolic in shape, with the maximum velocity at the axis.

From initial and boundary-conditions, we have

$u = 0$ at $r=R$, $U(0)$ is finite

$u'(0) = 0$

$T(0,t) = T_o$, $T(R,t) = T_o$, $T'(0,t) = 0$

$Y(0,t) = 0$, $Y(R,t) = Y_o$

Non dimensionalization

Krishnamurthy and Sen (1986) observed that the amount of computation involved in solving a difference equation is usually enormous. They observed that it is advantageous and economical to seek, whenever possible, a common solution for a variety of partial differential equations which can be achieved by expressing all related partial differential equations in terms of dimensionless variables. They concluded that nondimensionalizing is useful not only for the problems that are dimensionally different but also for those that are mere variant of the dimensionally same problem.

Since equations (2.3) and (2.4) are in form of Partial Differential Equation, hence nondimensionalization of these equations becomes necessary. To nondimensionalize these equations we introduce the following nondimensional variables.

$$\text{Let } U = \frac{u}{V}$$

$$\text{for } u = \frac{P'R^2}{4\mu} \quad \text{or} \quad \frac{-1}{4\mu}\frac{(\partial P)}{\partial z}R^2 \qquad (2.12)$$

where μ = constant,

Recall (2.11),

$$u = \frac{-1}{4\mu}\frac{\partial P}{\partial z}(R^2 - r^2) \qquad (2.13)$$

Solution to equation (2.2).

Putting equation (2.12) into equation (2.13), we get

$$U = u(1 - x^2), \text{ where } x = r/R \quad \Big\} \tag{2.14}$$

$$\frac{U}{u} = 1-x^2$$

Let $\dfrac{U}{u} = w$

$$w = 1 - x^2 \quad \Big\} \tag{2.15}$$

Hence, $U = uw$

$$\text{Let, } \theta = \frac{(T - T_o)E}{RT_o^2} \quad \Big\} \tag{2.16}$$

$$\therefore \quad T = \frac{RT_o^2\theta}{E} + T_o$$

$$y = \frac{Y}{Y_o} \quad \Big\} \tag{2.17}$$

$$Y = yY_o$$

and

$$t^* = \frac{R}{v}, \quad \tau = \frac{t}{t^*}$$

$$\tau = \frac{t}{R/v} \quad \Big\} \tag{2.18}$$

$$\tau = \frac{tv}{R}$$

Introducing these nondimensional variables into equations (2.3) and (2.4), we obtain the following.

Equations (2.3) and (2.4) can be written as

$$\rho\left(\frac{\partial Y}{\partial t} + U\frac{\partial Y}{\partial r}\right) = \frac{\rho D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial Y}{\partial r}\right) - \beta Y e^{-E/RT} \tag{2.19}$$

$$\rho c\left(\frac{\partial T}{\partial t} + \frac{U\partial T}{\partial r}\right) - \frac{k}{r}\frac{\partial}{\partial r}\frac{(r\partial T)}{\partial r} + \frac{\mu(\partial u)^2}{\partial r} + Q\beta e^{-\epsilon/RT} \qquad (2.20)$$

respectively.

Putting equations (2.14) to (2.17) into equation (2.20), we obtain

$$\rho\left(\frac{U}{R}\frac{\partial(yY_o)}{\partial\tau} + \frac{(uw)}{R}\frac{\partial(yY_o)}{\partial x}\right) = \frac{\rho D}{Rx}\frac{\partial}{R\partial r}\frac{(R\partial(yY_o))}{R\partial x} - Y_o\beta y e^{-\epsilon/RT}$$

where $\frac{\partial}{\partial t} = \frac{\partial}{\partial\tau}.\frac{\partial\tau}{\partial t} \quad \frac{v}{R}\frac{\partial}{\partial\tau}$ and

$$\frac{\partial}{\partial\tau} = \frac{\partial}{\partial r}.\frac{\partial x}{\partial r} = \frac{1}{R}\frac{\partial}{\partial x} \qquad (2.21)$$

Simplifying equation (2.21), to get

$$\rho\left(\frac{uY_o}{R}\frac{\partial y}{\partial\tau} + \frac{vY_o}{R}\frac{w\partial y}{\partial x}\right) = \frac{\rho DY_o}{R^2x}\frac{\partial}{\partial x}\frac{(x\partial y)}{\partial x} - Y_o\beta y e^{-\epsilon/RT}$$

$$\frac{uY_o}{R}\frac{\partial y}{\partial\tau} + \frac{uY_o(1-x^2)}{R}\frac{\partial y}{\partial x} = \frac{DY_o}{R^2x}\frac{\partial}{\partial x}\frac{(x\partial y)}{\partial x} - \frac{Y_o\beta}{\rho}y e^{-\epsilon/RT} \qquad (2.22)$$

dividing through by uYo and multiplying through by R, to get

$$\frac{\partial y}{\partial\tau} + \frac{(1-x^2)\partial y}{\partial x} = \frac{D}{vRx}\frac{\partial}{\partial x}\frac{(x\partial y)}{\partial x} - \frac{\beta}{R\rho v}y e^{-\epsilon/RT} e^{\theta/1+\epsilon\theta} \qquad (2.23)$$

Let $\epsilon \rightarrow 0$, so that $e^{-\epsilon/RT} e^{\theta/1+\epsilon\theta} \rightarrow 1$

equation (2.23) reduces to

$$\frac{\partial y}{\partial\tau} + \frac{(1-x^2)\partial y}{\partial x} = \frac{a\partial}{x\partial x}\frac{(x\partial y)}{\partial x} - by$$

where $a = \frac{D}{vR}$, and $b = \frac{\beta}{R\rho V}$ (2.24)

Define $t = \tau$

$$\frac{\partial}{\partial\tau} = \frac{\partial}{\partial t}.\frac{\partial t}{\partial\tau} = \frac{\partial}{\partial t} \tag{2.25}$$

Hence, Equation (2.24) can be written as

$$\frac{\partial y}{\partial t} + (1-x^2)\frac{\partial y}{\partial x} = \frac{a\partial}{x\partial x}\left(\frac{x\partial y}{\partial x}\right) - by \tag{2.26}$$

Equation (2.26) is the dimensionless form of Equation (2.19) and is the unsteady case

with Boundary conditions

$y(0,t) = 0$, $y(L,t) = 1$

and initial condition

$y(x,0) = x - 1$

For a steady state flow, $\frac{\partial y}{\partial t} = 0$, equation (2.26) becomes

$$(1-x^2)\frac{\partial y}{\partial x} = \frac{a\partial}{x\partial x}\left(\frac{xdy}{\partial x}\right) - by$$

with Boundary conditions (2.27)

$y(0) = 0$, $y(1) = 1$

Similarly, putting equations (2.16) to (2.18) into equation (2.20), we get

$$\rho c\left\{\frac{u}{R}\frac{\partial}{\partial\tau}\left(\frac{RT_o^2\theta + T_o}{E}\right) + \frac{uw}{R}\frac{\partial}{\partial x}\left(\frac{RT_o^2\theta + T_o}{E}\right)\right\}$$

$$= \frac{kw}{RxR}\frac{\partial}{\partial x}\left\{\frac{Rx}{R}\frac{\partial}{\partial x}\left(\frac{RT_o^2\theta + T_o}{E}\right)\right\} + \frac{\mu}{R}\left\{\frac{\partial}{\partial x}(uw)\right\}^2 + Q\beta e^{-\epsilon/RoT} \tag{2.28}$$

$$\rho c\left(\frac{u}{R}\,\frac{RT_o^2}{E}\,\frac{\partial\theta}{\partial\tau} + v(1-x^2)\frac{RT_o^2}{RE}\,\frac{\partial\theta}{\partial x}\right)$$

$$= \frac{k}{R^2x}\,\frac{\partial}{\partial x}\left(\frac{xRT_o^2}{E}\,\frac{\partial\theta}{\partial x}\right) + \frac{\mu v^2}{R^2}\left(\frac{\partial(1-x^2)}{\partial x}\right)^2 + Q\beta e^{-\epsilon/R_oT}e^{\theta/1+\epsilon\theta}$$

dividing through by ρc

$$\frac{VT_o^2}{E}\,\frac{\partial\theta}{\partial\tau} + \frac{V(1-x^2)T_o^2}{E}\,\frac{\partial\theta}{\partial x}$$

$$= \frac{kT_o^2}{E\rho CRx}\,\frac{\partial}{\partial x}\,\frac{(x\partial\theta)}{\partial x} + 4\mu(v^2/R^2)x^2 + Q\beta e^{-\epsilon/R_oT}e^{\theta/1+\epsilon\theta} \qquad (2.29)$$

Multiply through by $\frac{E}{VT_o^2}$, we get

$$\frac{\partial\theta}{\partial\tau} + (1-x^2)\,\frac{\partial\theta}{\partial x}$$

$$= \frac{k\partial(x\partial\theta)}{\rho CVRx\,\partial x\partial x} + \frac{4\mu vEx^2}{R^2T_o^2} + \frac{Q\beta E}{vT_o^2}\,e^{-\epsilon/R_oT}e^{\theta/1+\epsilon\theta} \qquad (2.30)$$

Let $\epsilon = \frac{R_oT_o}{E}$ and $E \neq 0$, equation (2.30) reduces to

$$\frac{\partial\theta}{\partial\tau} + (1-x^2)\,\frac{\partial\theta}{\partial x} = \frac{d_1}{x}\,\frac{\partial}{\partial x}\,\frac{(x\partial Q)}{\partial x} + d_2x^2 + d_3 \qquad (2.31)$$

where $d_1 = \frac{k}{\rho CVR}$, $d_2 = \frac{4\mu VE}{RR_oT_o^2}$ and $d_3 = \frac{REQ\beta}{VR_oT_o^2}$

Equation (2.31) can be written as

$$\frac{\partial\theta}{\partial t} + (1-x^2)\,\frac{\partial\theta}{\partial x} = \frac{d_1}{x}\,\frac{\partial}{\partial x}\,\frac{(x\partial Q)}{\partial x} + d_2x^2 + d_3 \qquad (2.32)$$

equation (2.32) is the dimensionless form of equation (2.20) and is unsteady.

The Boundary conditions are

$$\theta(0,t) = 0 \ , \ \theta(L,t) = 1$$

The initial condition is

$$\theta(x,0) = x - 1$$

Also for a steady state, $\frac{\partial \theta}{\partial t} = 0$, equation (2.32) becomes

$$(1-x^2)\frac{\partial \theta}{\partial x} = \frac{d_1}{x}\frac{\partial}{\partial x}\left(x\frac{\partial \theta}{\partial x}\right) + d_2x^2 + d_3 \tag{2.33}$$

with Boundary conditions

$$\theta(0) = 0, \ \theta(1) = 1$$

Equations (2.27) and (2.33) now form the basis of our discussion The numerical techniques that solve these equations are discussed in chapter three.

CHAPTER THREE

NUMERICAL METHODS OF SOLUTION

3.1 Removal of Singularity

Different numerical techniques are available to solve Boundary-Value problem of these type of equations (2.27) and (2.33). In this work two different approaches are considered to solve the steady state equations (2.27) and (2.33). These approaches are Finite difference method and shooting method. We shall consider the numerical methods of solutions of equation (2.27) for various values of parameters a and b and equation (2.33) for various values of d_1, d_2 and d_3.

Consider

$$\frac{(1-x^2)\partial y}{\partial x} = \frac{a}{x}\frac{\partial}{\partial x}\frac{(x\partial y)}{\partial x} - by$$

with Boundary values (3.1)

$y(0) = 0, \; y(1) = 1$

Since Equation (3.1) involves only one variable, it can be written as total differentiation, hence equation (3.1) becomes

$$\frac{(1-x^2)dy}{dx} = \frac{a}{x}\frac{d}{dx}\frac{(xdy)}{dx} - by$$

with Boundary values

$$y(0) = 0, \; y(1) = 1 \tag{3.2}$$

Simplifying, we get

$$\frac{d^2y}{dx^2} = \frac{(x - x^3 - a)}{ax}\frac{dy}{dx} + \frac{by}{a}$$

$y(0) = 0, \; y(1) = 1$ (3.3)

and the second equation

$$(1 - x^2)\frac{d\theta}{dx} = \frac{d_1}{x}\frac{d}{dx}\frac{(xd\theta)}{dx} + d_2x^2 + d_3$$

with Boundary conditions.

$$\theta(0) = 0,\ \theta(1) = 1 \qquad (3.4)$$

Simplifying, we obtain

$$\frac{d^2\theta}{dx^2} = \frac{(x - x^3 - d_1)}{d_1x}\frac{d\theta}{dx} - \frac{d_2x^2}{d_1} - \frac{d_3}{d_1}$$

$$\theta(0) = 0\ ,\ \theta(1) = 1 \qquad (3.5)$$

Equations (3.3) and (3.5) can only be solved for all values of x, except zero, because we shall run into problem of singularity at x = 0. In order to avoid this problem, we adapt the method of Hicks and Weize (1962) to remove the singularity with approximation

$$\lim_{x\to 0}\frac{1}{x}\frac{(dy)}{dx} = \frac{(d^2y)}{dx^2}/x = 0 \qquad (3.6)$$

Hence, equation (3.3) becomes

$$\frac{d^2y}{dx^2} = \frac{(x - x^3 - a)}{a}\frac{(d^2y)}{dx^2}/x{=}0 + \frac{by}{a} \qquad (3.7)$$

At x = 0

$$\frac{d^2y}{dx^2} = -\frac{d^2y}{dx^2} + \frac{b(0)}{a}$$

$$\therefore \frac{d^2y}{dx^2/x{=}0} = 0 \qquad (3.8)$$

Putting equation (3.8) into equation (3.7) we obtain

$$\frac{d^2y}{dx^2} = \frac{(x - x^3 - a)\ (0)}{a} + \frac{by}{a}$$

$$\therefore \frac{d^2y}{dx^2} = \frac{b\ y}{a} \qquad (3.9)$$

Similarly, equation (3.5) becomes

$$\frac{d^2\theta}{dx^2} = \frac{(x - x^3 - d_1)}{d1}\frac{(d^2\theta)}{dx^2\ /x=0} - \frac{d_2x^2}{d_1} - \frac{d_3}{d_1} \qquad (3.10)$$

at x = 0

$$\frac{d^2\theta}{dx^2} = - \frac{(d^2\theta)}{dx^2} - \frac{d_3}{d_1}$$

$$\frac{d^2\theta}{dx_2/x=0} = - \frac{d_3}{2d_1} \qquad (3.11)$$

Substituting equation (3.11) into equation (3.10), we get

$$\frac{d^2\theta}{dx^2} = \frac{(x - x^3 - d_1)}{d_1}\frac{(-d_3)}{2d_1} - \frac{d_2x^2}{d_1} - \frac{d_3}{d_1}$$

re-arranging, we obtain

$$\frac{d^2\theta}{dx^2} = - \frac{d_3\ (x-x^3-d_1)}{2d_1^2} - \frac{d_2x^2}{d_1} - \frac{d_3}{d_1} \qquad (3.12)$$

The removal of the singularity of equations (3.3) and (3.5) makes them solvable for all values of x, including neighbourhood of zero.

3.2 Finite difference method

According to Burden and Faires (1993), the differential quotients y' and y'' are approximated by the difference quotients substituting into equations (3.3), (3.9), (3.5) and (3.12). This can be done by partitioning interval (0,1) into n subintervals of length 1/n, such that $x_i = ih$, $i = 0(1)n$. x_i and ih are used interchangeably, x_i is adopted.

$$\text{For } y' = \frac{y_{i+1} - y_{i-1}}{2h} \tag{3.13}$$

and

$$y'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \tag{3.14}$$

Putting these equations into equation (3.3), we obtain

$$\left(2a + \frac{h(x_i - x_i^3 - a)}{x_i}\right)y_{i-1} - (4a + 2h^2 b)y_i + \left(2a - \frac{h(x_i - x_i^3 - a)}{x_i}\right)y_{i+1} = 0 \tag{3.15}$$

Similarly, equation (3.9) becomes

$$y_{i-1} - (2+bh^2)\ y_i + y_{i+1} = 0, \quad i = 1(1)n \tag{3.16}$$

These methods are called Finite difference methods with truncation error of order $0(h^2)$.

Equations (3.15) and (3.16) are tridiagonal, of the form

$$Ay = \underline{b}^* \tag{3.17}$$

For,
$$A = \begin{bmatrix} a_{11} & a_{12} & & & \\ a_{21} & a_{22} & a_{23} & & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & a_{n,n-1} & a_{n,n} \end{bmatrix}$$

where, $a_{ii} = -(4a + 2h^2b)$, for $i = 1(1)n$,

$$a_{i,i+1} = 2a - \frac{h(x_i - x_i^3 - a)}{xi}$$

and

$$a_{i+1,i} = 2a + \frac{h\ (x_i - x_i^3 - a)}{xi}, \text{ for } i,\ldots,n,$$

Also,

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_{n-1} \end{bmatrix}$$

and

$$b^* = \begin{bmatrix} -\left(2a + \frac{h(x_1 - x_1^3 - a)}{x_1}\right) y_0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ -\left(2a - \frac{h(x_n - x_n^3 - a)}{x_n}\right) y_{n+1} \end{bmatrix} \tag{3.18}$$

where $y_0 = y(0) = 0$

$y_N = y(1) = 1$

Also, in solving equation (3.5) for various values of d_1, d_2, and d_3, we make use of the equations (3.13) and (3.14), to obtain

$$d_1\frac{(\theta_{i+1} - 2\theta_i + \theta_{i-1})}{h^2} = \frac{(x_i - x_i^3 - d_1)}{x_i}\cdot\frac{(\theta_{i+1} - \theta_{i-1})}{2h}$$

$$- \frac{d_2 x_i^2}{d_1} - \frac{d_3}{d_1}$$

$$2d_1(\theta_{i+1} - 2\theta_i + \theta_{i-1}) = \frac{(x_i - x_i^3 - d_1)}{x_i}(\theta_{i+1} - \theta_{i-1})$$

$$- 2h^2 d_2 x_i^2 - 2h^2 d_3$$

re-arranging, to obtain

$$(2d_1 + h\,\frac{(x_i - x_i^3 - d_1)}{x_i})\theta_{i-1} - 4d_1\theta_i + (2d_1 - h\frac{(x_i - x_i^3 - d_3)}{x_i})\theta_{i+1}$$

$$= - 2h^2(d_2 x_i^2 - d_3) \qquad (3.19)$$

Similarly, equation (3.12) becomes

$$2d_1\theta_{i+1} - 4d_i\theta_i + 2d_i\theta_{i+1}$$

$$= - h^2 d_3 x^3 + h^2 d_2 x^2 + h^2 d_3 x - h^2 d_3 d_1 \qquad (3.20)$$

Equations (3.19) and (3.20) are tridiagonal and of the form

$\underline{A}\theta = b*$

where,

$$A = \begin{bmatrix} -4d_1 & 2d_1 - h\frac{(x_i - x_i^3 - d_1)}{x_i} & & \\ 2d_1 + h\frac{(x_i - x_i^3 - d_1)}{x_i} & -4d_1 & 2d_1 - h\frac{(x_i - x_i^3 - d_1)}{x_i} & \\ \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots \\ & & 2d_1 - h\frac{(x_i - x_i^3 - d_1)}{x_i} & -4d_1 \end{bmatrix}$$

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \cdot \\ \cdot \\ \cdot \\ \theta_{n-1} \end{bmatrix}$$

and

$$b^* = \begin{bmatrix} -\ 2h^2(d_2x_i^2 + d^3) - (2d_1 + h\frac{(x_i - x_i^3 - d_1)}{x_i}\ \theta_o \\ -\ 2h^2(d_2+x_i^2 + d^3) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ -\ 2h^2(d_2x_i^2 + d_3) - (2d_1 - h\frac{(x_i - x_i^3 - d_1)}{xi}\theta_o \end{bmatrix} \qquad (3.21)$$

3.2 The Existence and Uniqueness of the solution

The following theorem gives condition under which the equations (3.3) and (3.9) have unique solutions.

Theorem 3.1: Consider the boundry-value problem of the form

$$y'' = p(x)\,y' + q(x)y + r(x),\ a\le x\le b$$
$$y(a) = \alpha\ ,\ y(b) = \beta \qquad (3.22)$$

Suppose that p(x), q(x) and r(x) are continuous on [a,b].

If $q(x) \geq o$ on [a,b] the equation (3.13) has a unique solution provided that

$$h < 2/L, \quad \text{where } L = \max_{a\le x\le b} |p(x)|$$

Remark: Equations (3.3) and (3.9) are of the form equation (3.22), hence, Theorem (3.1) is applicabale to these equations

Proof:

a. For existence of solutions

By Theorem (3.1), p(x), q(x), r(x) must be continuous on (a,b) for a solution to exist.

Recall equation (3.9)

$$\therefore \frac{d^2y}{dx^2} = \frac{b\,y}{a}$$

$p(x) = 0$, $q(x) = \dfrac{b}{a}$ and $r(x) = 0$, for $a \neq 0$, p(x), q(x) and r(x) are continuous on (0,1). Hence, the existence of the solution.

b. **For uniqueness of solution**

The proof of Theorem (3.1) is a consequence of the theorem below.

Theorem 3.2:(Burdens and Faires(1985))

In tridiagonal systems (3.15), (3.19) with

$a_{i,i+1}, a_{i,i+1} \neq 0$, for each $i = 2,3, \ldots, n-1$

If $|a_{11}| > |a_{12}|$, $|a_{ii}| \geq |a_{i,i+1}|$, for each $i = 1, \ldots n-1$ and $|a_{nn}| > |a_{n,n-1}|$, then A is non-singular and the values of l_{ii} in LU factorization given as:

$$L_{11} = a_{11}$$

$$U_{12} = a_{12}/L_{11}$$

for $i = 2,3,\ldots,n-1$

Set $L_{i,i-1} = a_{i,i-1}$

$${}_{i,i} = a_{i,i} - L_{i,i-1}\, U_{i-1,i}$$

$$U_{i,i+1} = a_{i,i+1}/L_{i,i}$$

$$L_{n,n-1} - a_{n,n-1}$$

$$L_{n,n} = a_{n,n} - L_{n,n-1}$$

where L - Lower tiangular matrix and

U - Upper triangular matrix

are nonzero for each $i = 1,2,\ldots m$.

Proof:

Claims:

a. To prove that A in equations (3.18) and (3.21) is non-singular.

. To prove that Gaussian elimination can be performed on A in equations (3.18) and (3.21) without row interchanges. That is, we show that each of the matrices $A^{(2)}, A^{(3)}, \ldots, A^{(n-1)}$ generated by the Gaussian elimination process is strictly diagonally dominant.

We prove by contradiction, to show that A is non-singular.

Consider $A\underline{y} = 0$ (3.23)

where A and $\underline{y}$ are as defined in equations (3.18) and (3.21).

Suppose that there exists a non-zero solutions $y = (y_i)$ and $\theta = (\theta_i)$ to equations (3.18) and (3.21) respectively which implies that these equations are consistent for a strictly diagonally dominant, matrix A

Let us consider equation (3.18).

Let k be an index for which

$$0 < |y_k| = \underset{1 \le j \le n}{\text{Max}} |y_j| \tag{3.24}$$

By Bundens as Faires (1985).

$$\sum_{j \le i-1} a_{ij} y_j = 0, \text{ for each } i = 2,3,\ldots,n-1$$

if i = k, we have

$$a_{kk} y_k = - \sum_{\substack{j=1 \\ j \ne k}}^{k+1} a_{ij} y_j, \quad i \le j \le i \tag{3.25}$$

$$|a_{ii}|\,|y_i| \le \sum_{\substack{j=1 \\ j \ne k}}^{k+1} |a_{kj}|\,|y_j| \tag{3.27}$$

Simplifying, we obtain

$$|a_{kk}| \le \sum_{\substack{j=1 \\ j \ne k}}^{k+1} \frac{|a_{kj}|\,|y_j|}{|y_k|}$$

using Equation (3.24),

$$|a_{kk}| \quad \leq \quad \sum_{\substack{j=1 \\ j\neq k}}^{k+1} |a_{kj}| \tag{3.28}$$

This contradicts the *strict diagonal dominance* of A. Consequently, the only solution to equation(3.23) is $\underline{y} = 0$, which satisfies the condition that the equation $A\underline{y} = 0$ has the unique solution $\underline{y} = 0$. This concludes proof for claim (a).

Proof of Claim (b). Since A in equation (3.18) is *strictly diagonally dominant* $a_n \neq o$ and $A^{(2)}$ can be formed for i = 2, since matrix A (see equation 3.18) is tridiagonal, we eliminate y_1 from equation 2 of (3.18) only, y_2 from equation 3 only and so on to y_{n-1} from equation n only.

Generally, by Gaussian elimination

$$a^1_{ii} = a_{ii} - \frac{a_{i-1,i}\ a_{i,i-1}}{a_{i-1,i-1}}$$

Since A (equation 3.18) is strictly diagonally dominant $a_{11} \# 0$ and $A^{(2)}$ can be formed. For each j = 2,3, ..., n

$$a_{2j}^{(2)} = a_{2j}^{(1)} - \frac{a_{1j}^{(1)}a_{21}^{(1)}}{a_{11}^{(1)}}$$

By elimination $a_{21}^{(2)} = 0$

$$\sum_{\substack{j=2 \\ j\neq 2}}^{n} |a_{2j}^{(2)}| = \sum_{\substack{j=2 \\ j\neq 2}}^{n} \left| a_{2j}^{(1)} - \frac{a_{1j}^{(1)}a_{21}^{(1)}}{a_{11}^{(1)}} \right| \tag{3.29}$$

$$\le \sum_{\substack{j=2\\ j\neq 2}}^{n} |a_{2j}^{(1)}| + \sum_{\substack{j=2\\ j\neq 2}}^{n} \left|\frac{a_{1j}^{(1)}a_{21}^{(1)}}{a_{11}^{(1)}}\right| .$$

$$< |a_{22}^{(1)}| - | a_{21}^{(1)}| + \frac{|a_{21}^{(1)}|}{|a_{11}^{(1)}|} \sum_{\substack{j=1\\ j\neq 2}}^{n} |a_{1j}^{(1)}|$$

$$= |a_{22}^{(1)}| - \frac{|a_{21}^{(1)}||a_{12}^{(1)}|}{|a_{11}^{(1)}|}$$

$$\therefore \sum_{\substack{j=2\\ j\neq 2}}^{n} |a_{2j}^{(2)}| \le \left|a_{22}^{(1)} - \frac{a_{21}^{(1)}a_{12}^{(1)}}{a_{11}^{(1)}}\right| = |a_{22}^{(2)}| \qquad (3.23)$$

Hence, the strict diagonal dominance is established for row 2: Since, the first rows of $A^{(2)}$ and A are same, $A^{(2)}$ is strictly diagonally dominant.

This process is done for $A^{(3)}$, $A^{(4)}$ up to $A^{(n-1)}$. The upper-triangular and strictly diagonally dominant $A^{(n)}$ are obtained. This implies that all the diagonal element are non-zero.

Hence, Gaussian elimination can be performed without row intrchanges.

This completes the proof of Theorem (3.2) hence, the proof of Theorem (3.1) follows:

It is now established that the tridiagonal linear system (3.15) has a unique solution. Same can be said of equation (3.19)

Now that it has been established that the tridiagonal linear system (3.15) has a unique solution. The value of h-mesh size which will be used to solve equations (3.15), (3.16), (3.19) and (3.20), is to be determined.

3.4 To determine the value of h that gives unique solutions

Recall,

$$\frac{d^2y}{dx^2} = \frac{(x - x^3 - a)}{ax}\frac{dy}{dx} + \frac{by}{a}$$

$$y(0) = 0 \; , \; y(1) = 1 \qquad (3.22)$$

By Theorem 3.1, equation (3.31) has a unique solution provided $h < 2/L$ or $(h/2)L < 1$.

where $L = \underset{a \le x \le b}{\mathrm{Max}} |P(x)|$

Comparing equation (3.33) with equation (3.31)

$$P(x) = \frac{x - x^3 - a}{ax}$$

Hence $L = \underset{0 \le x \le 1}{\mathrm{Max}} \frac{|x - x^3 - a|}{|ax|}$

This is determined based on the following theorem.

Theorem 3.3: If $P(x)$ is twice-differentiable on a small interval $(0,1)$ at x and if $p'(x_0) = 0$ and $P''(x_0) < 0$, then $P(x)$ has a maximum at x_0.

Claim.

$P(x)$ is continuous and $P'(x)$ exists. With the derivatives defined everywhere, the maximum on $(0,1)$ occurs at endpoints $x = 0$ or $x = 1$, or at a stationery point, where $P'(x) = 0$.

Hence, to determine the maximum of $P(x)$, we have

$$P'(x) = \frac{[x(1-3x^2) - (x - x^3 - a)]}{ax^2}$$

Simplifying to get

$$P'(x) = \frac{-2x^3 - a}{ax^2}$$

At stationery point

$$-2x^3 + a = 0$$

$$\therefore \quad x = \sqrt[3]{(\tfrac{1}{2}a)}$$

By Theorem (3.3)

$$P''(x) = \frac{-2(x^3 + a)}{ax^3}$$

$$\therefore \quad P''(a/2)^{\frac{1}{3}} = \frac{-6}{a} \quad , \text{ provided } a \neq 0$$

Hence, P(x) is maximum for some a > 0.

$$\therefore \text{ Max } |P(x)| = \frac{|((\tfrac{1}{2})^{\frac{1}{3}} - \tfrac{1}{2}a - a)|}{|a(\tfrac{1}{2}a)^{\frac{1}{3}}|}$$

$$= \frac{|(\tfrac{1}{2}a)^{\frac{1}{3}} - 3(a/2)\ |}{|a(\tfrac{1}{2}a)^{\frac{1}{3}}|}$$

$$\therefore \quad L = |(1/a)(1 - 3(\tfrac{1}{2}a)^{\frac{1}{3}})|$$

Since $h < \dfrac{2}{L}$

$$\therefore \quad h < \frac{2}{|(1/a) - 3a(\tfrac{1}{2}a)^{\frac{1}{3}}|} \qquad (3.23)$$

Similarly, equation (3.12) has a unique solution provided that $h < 2/L$.

where $$L = \max_{0<x<1} \frac{|x-x^3-d_1|}{|d_1x|} .$$

Hence, the value of h is determined thus:

Let $$P(x) = \frac{x-x^3-d_1}{d_1x}$$

$$P'(x) = \frac{(1-3x^2)d_1x-d_1(x-x^3d_1)}{d_1{}^2x^2}$$

$$\therefore \quad P'(x) = \frac{-2x^3 + d_1}{d_1x}$$

At turning point $P'(x) = 0$

$$-2x^3 + d_1 = 0.$$

$$\therefore \quad x = (\tfrac{1}{2}d_1)^{\frac{1}{3}}$$

Also

$$P''(x) = \frac{-2x^3 - 2d_1}{d_1x^3}$$

By Theorem (3.3) $P(x)$ has a maximum when

$$P''(x) < 0.$$

$$P''(\tfrac{1}{2}d_1) = -6/d_1, \text{ provided } d_1 \neq 0.$$

satisfied Theorem (3.3) for all $d_1 > 0$.

$P(x)$ has a maximum at $x = (\tfrac{1}{2}d_1)^{\frac{1}{3}}$.

Hence, the $\text{Max}|P(x)|$ is given as

$$\text{Max}|P(x)| = \left|\frac{(1/d_1-3(\tfrac{1}{2}d_1)^{2/3})}{d_1}\right| .$$

Hence, $$h < \frac{2}{|1/d_1 - 3d_1(\tfrac{1}{2}d_1)^{2/3}|} \qquad (3.33)$$

The choice of h-mesh size for the two equations are now determined.

Now that it has been established that the tridiagonal linear system (3.15) and (3.19) have unique solutions and the choice of h determined. We can now solve equations (3.15) and (3.19) together with the boundary conditions $y(0) = 0$ and $y(0) = 0$, and $\theta(0) = 0$ and $\theta(1) = 1$ respectively. The algorithms and some other programming tools which implement this method are discussed in chapter four.

3.3 SHOOTING METHOD

The basic philosophy behind shooting method for solution of a two-point Boundary-value problem is that we embed the solution of an initial-value problem within an equation solving routine which is then used to find the appropriate initial conditions so that the final Boundary conditions are also satisfied.

The solution of this initial-value problem is then the solution of the original Boundary-value problem. The details will vary depending on the particular type of problem to be solved.

Generally, suppose that we wish to solve the two-point boundary-value problem of the form

$$y'' = f(x,y,y')$$

$$y(a) = \alpha, \; y(b) = \beta \qquad (3.34)$$

By shooting method, equation (3.34) becomes the Initial-value problem

$$y'' = f(x,y,y')$$

$$y(a) = \alpha,\ y'(a) = r \qquad (3.35)$$

We wish to find this value of r for which

$$y_r(b) = \beta$$

To carry out the shooting method, we introduce the error function

$$E(x) = y_r(b) - \beta \qquad (3.35)$$

The value of E(x) is the amount by which $y_r(b)$ misses the 'target' $y(b) = \beta$. We try different potential values for r with the aim of finding the one which hits the 'target' $y(b) = \beta$. To guess values for $y'(a)$ is to find a root r of $E(x) = 0$. Once $y'(a)$ has been found, the desired $y(x)$ is $y_r(x)$.

The evaluation of E(x) requires a lot of work. $E(x) = 0$ can be solved by some numerical techniques. We adopt the Secant Method to find a root of E(x).

Now, equation (3.5) given as

$$\frac{d^2y}{dx^2} = \frac{(x - x^3 - a)}{ax}\frac{dy}{dx} + \frac{by}{a} = f(x, y, y')$$

$$y(0) = 0\ ,\ y(1) = 1$$

By shooting method, this equation becomes the Initial-value problem

$$\frac{d^2y}{dx^2} = \frac{(x - x^3 - a)}{ax}\frac{dy}{dx} + \frac{by}{a} = f(x, y, y')$$

$$y(0) = 0\ ,\ y'(0) = r(\text{unknown to be found}) \qquad (3.37)$$

We which to find this value of r for which $y_r(1) = 1$

Similarly, equation (3.5) given as

$$\frac{d^2\theta}{dx^2} = \frac{(x - x - d_1)}{d_1x}\frac{d\theta}{dx} - \frac{d_2x^2}{d_1} - \frac{d_3}{d_1} = f(x, \theta, \theta')$$

$$\theta(0) = 0 , \quad \theta(1) = 1$$

becomes

$$\frac{d^2\theta}{dx^2} = \frac{(x - x - d_1)}{d_1x}\frac{d\theta}{dx} - \frac{d_2x^2}{d_1} - \frac{d_3}{d_1} = f(x, \theta, \theta')$$

$$\theta(0) = 0 , \quad \theta'(1) = r(\text{unknown to be found}) \qquad (3.38)$$

We which to find this value of r for which $\theta_r(1) = 1$

The algorithm and some other programming tools which implement this method are discussed in chapter four.

CHAPTER FOUR

COMPUTER IMPLEMENTATION AND RESULTS

In this chapter, the programming tools used for the implementation of Finite difference and Shooting methods are discussed. These include algorithms, flow Charts and programs.

Algorithm 1: (For Finite difference method)

To solve equations (3.16) and (3.20) for x closed to zero and equations (3.15) and (3.19) otherwise, we adopt the Finite difference formular, which is pseudo coded in the algorithm below.

To approximate the solution of the boundary value problem of the form

$$y'' = (P(x)\ y' + q(x)\ y + r(x), \quad a < x < b$$

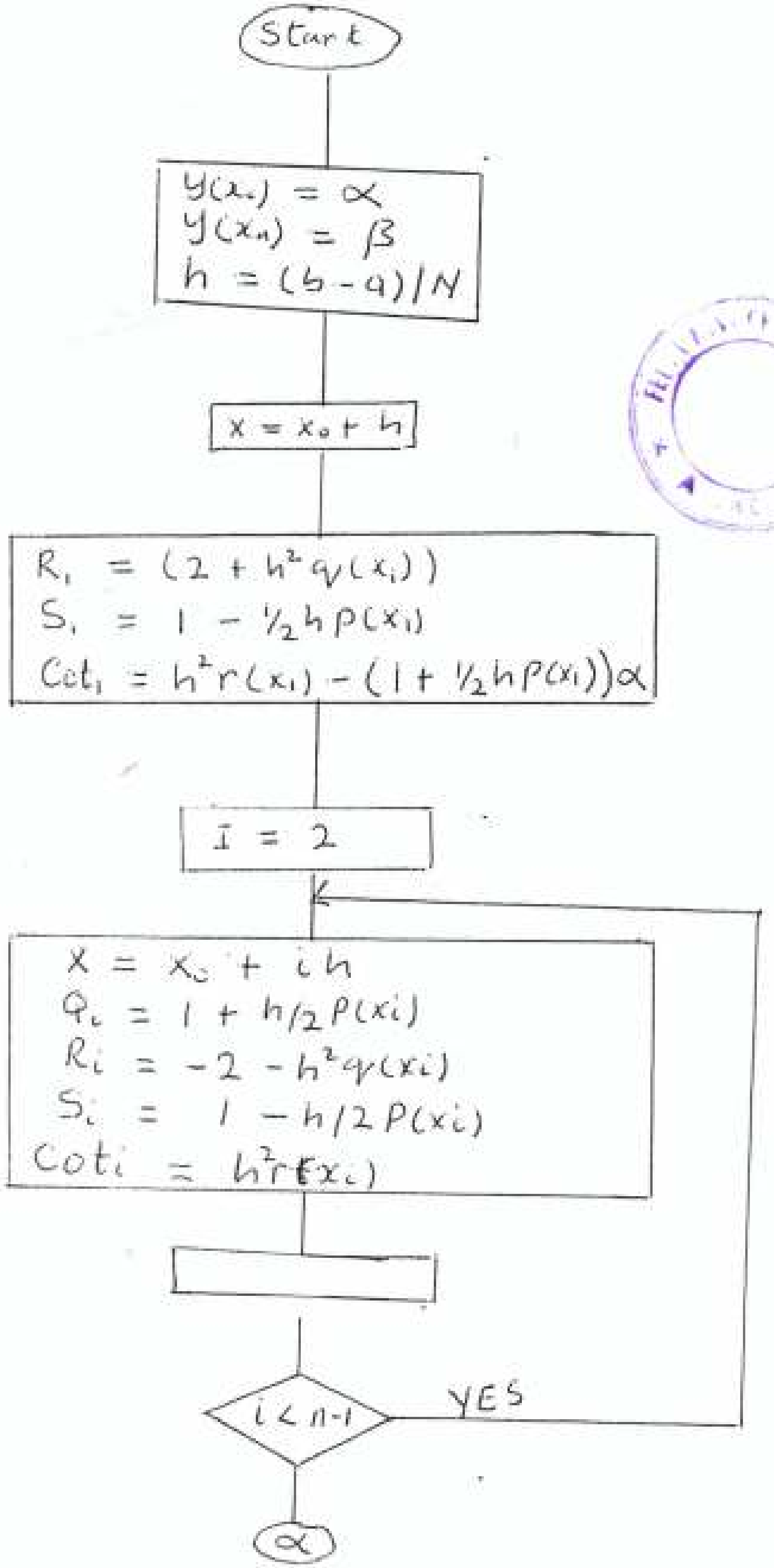
$$y(a) = \alpha\ ,\ y(b) = \beta \qquad (3.39).$$

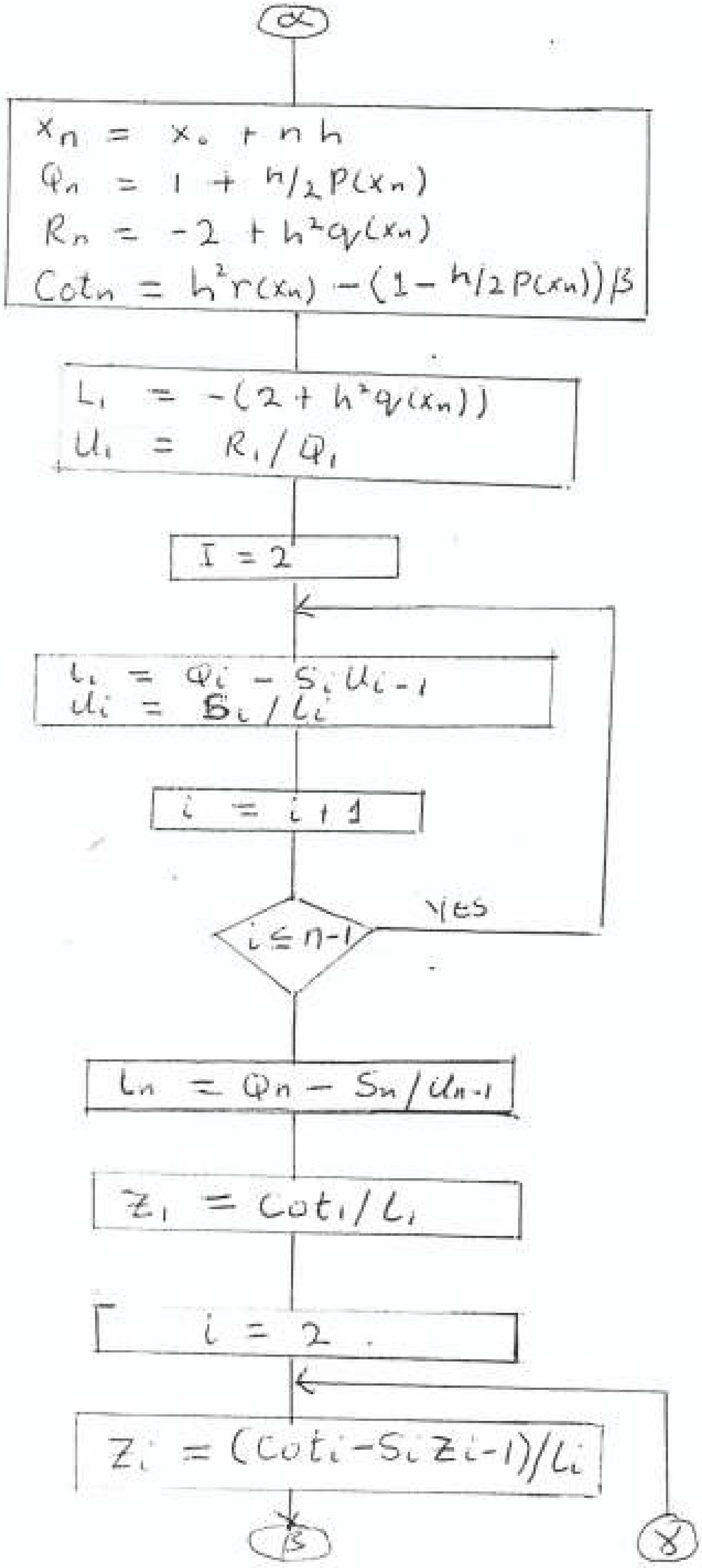
with the finite difference method.

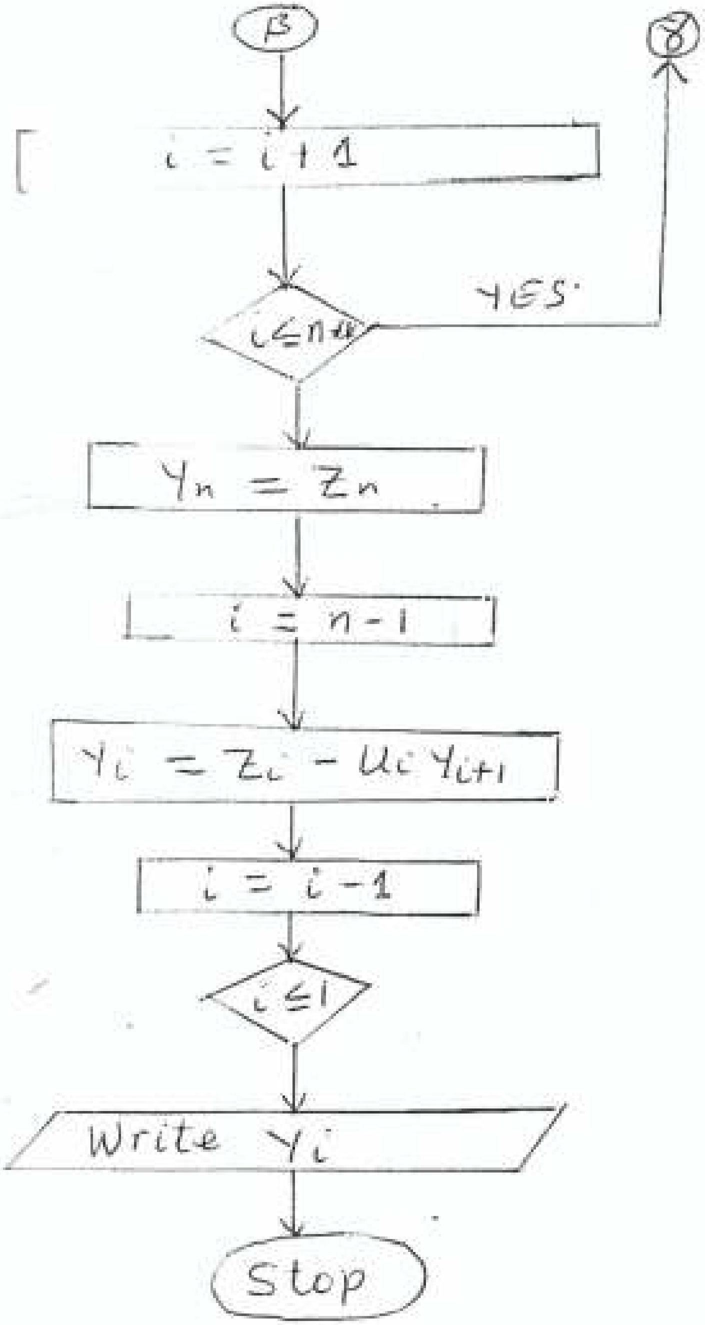
```
Step 1:  Set $h = (b - a)/n+1)$
             $x = x + h$
             $R_1 = -(2 + h^2 q(x_1))$
             $S_1 = 1 - \frac{1}{2}hp(x_1)$
             $COT_1 = h^2 r(x_1) - (1 + (\frac{1}{2}h)P(x_1))\alpha$
Step 2:  For $i = 2, \ldots, n-1$
         Set $x = x + ih$
             $Q_i = 1 + (\frac{1}{2}h)P(x_i)$
             $R_i = -(2 + h^2 q(x_i))$
             $S_i = (1 - \frac{1}{2}h)P(x_i))$
```

```
             $COT_1 = h^2r(x)$
Step 3:    Set $x = x + nh$
             $Q_n = 1 + (\frac{1}{2}h)P(x_n)$
             $R_n = -(2 = h^2q(x_n))$
             $COT_n = h^2r(x_n) - (1 - (\frac{1}{2}h)P(x_n)\beta$
Step 4:    Set $l_1 = -(2 + h^2q(x_1)$
           (Steps 4 - 10 solve a tridiagonal linear system using
            LU - decomposion))
              $U_1 = R_1/Q_1$
Step 5:    For $i = 2, \ldots, n - 1$
             $l_i = Q_i - S_iU_{i-1}$
             $U_i = b_i/l_i$
Step 6:    Set $l_n = Q_n - S_nU_{n-1}$
Step 7:    Set $Z_1 = COT_1/l_1$
Step 8:    For $i = 2, \ldots n$
           Set $Z_i = (COT_i - S_iZ_{i-1})/l_i$
Step 9:    Set $Y_0 = \alpha$
              $y_1 = \beta$
              $Y_n = Z_n$
Step 10:   For $i = n - 1, \ldots 1$
           Set $Y_i = Z_i - U_iY_{i+1}$
Step 11:   For $i = 0, \ldots, n+1$
           Set $x = a + ih$
           Output $(x, y_i)$
Step 12:   Stop.
```

Flow chart 1: for algorithm(1)




α
$x_n = x_0 + nh$
$Q_n = 1 + h/2\,p(x_n)$
$R_n = -2 + h^2 q(x_n)$
$Cot_n = h^2 r(x_n) - (1 - h/2\,p(x_n))\beta$
$L_1 = -(2 + h^2 q(x_n))$
$U_1 = R_1/Q_1$
$I = 2$
$l_i = Q_i - S_i U_{i-1}$
$u_i = B_i/l_i$
$i = i + 1$
$i \le n-1$
Yes
$L_n = Q_n - S_n/u_{n-1}$
$Z_1 = Cot_1/L_1$
$i = 2$.
$Z_i = (Cot_i - S_i Z_{i-1})/L_i$
β
γ



The above algorithm(1) was implemented with FORTRAN 77 to solve the equations (3.15) and (3.16), (3.19) and (3.20) for some varying values of parameters a and b, d_1, d_2 and d_3 respectively. The FORTRAN 77 programs can be found in the appendix and the results are discussed in chapter five.

<u>**Algorithm 2**</u> (Algorithm for the Shooting Method).

To solve the Second-order Boundary-value problem (3.3) and (3.5). The method requires solving the associated initial-value problems.

Consider the general form of BVP

$$y'' = f(x,y,y'),$$

$$y(a) = \alpha,\ y(b) = \beta$$

We consider the associated $(IVP)_r$

$$y'' = f(x,x,y')$$

$$y(a) = \alpha,\ y'(a) = r$$

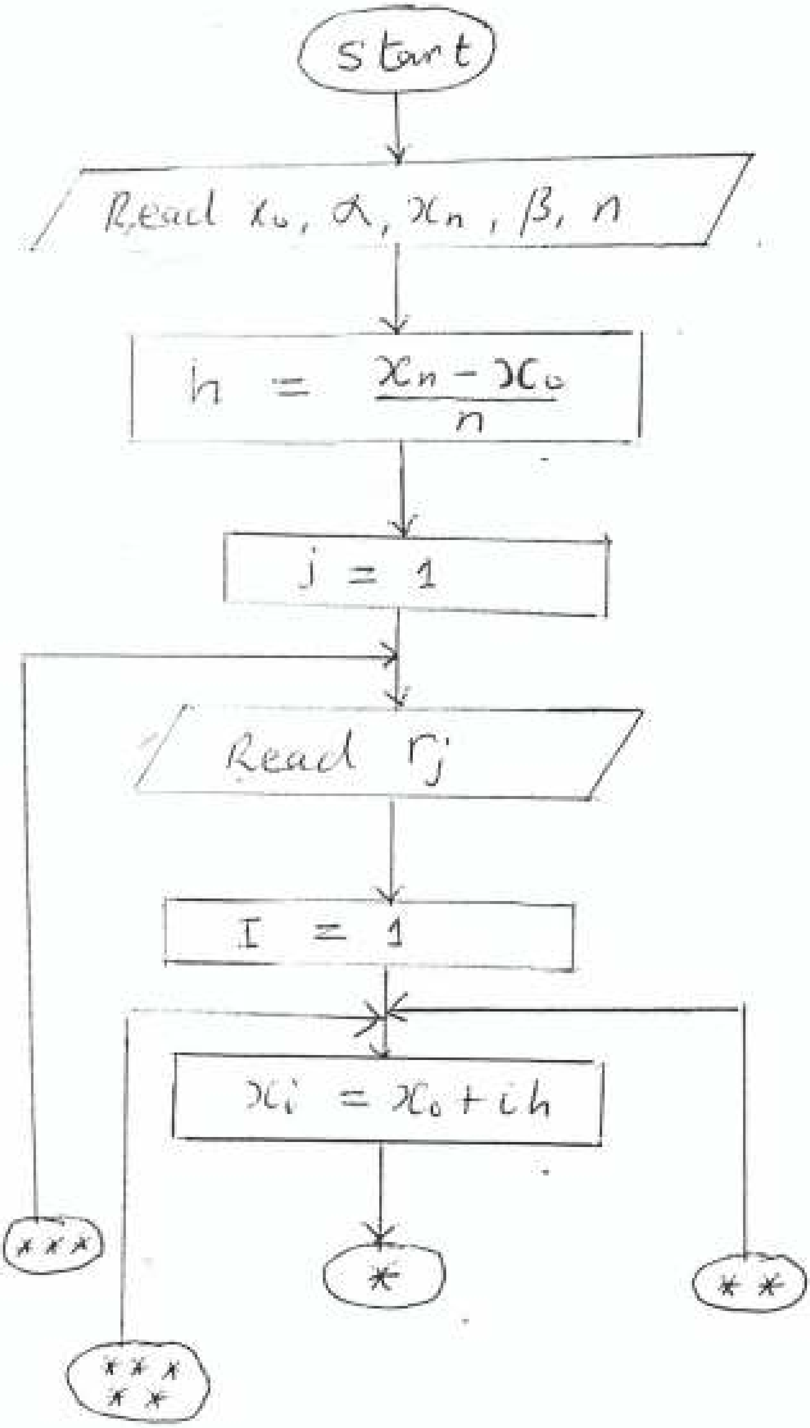
for $y_r(b) = \beta$. The Secant Method is used to get r as a root of E(x)

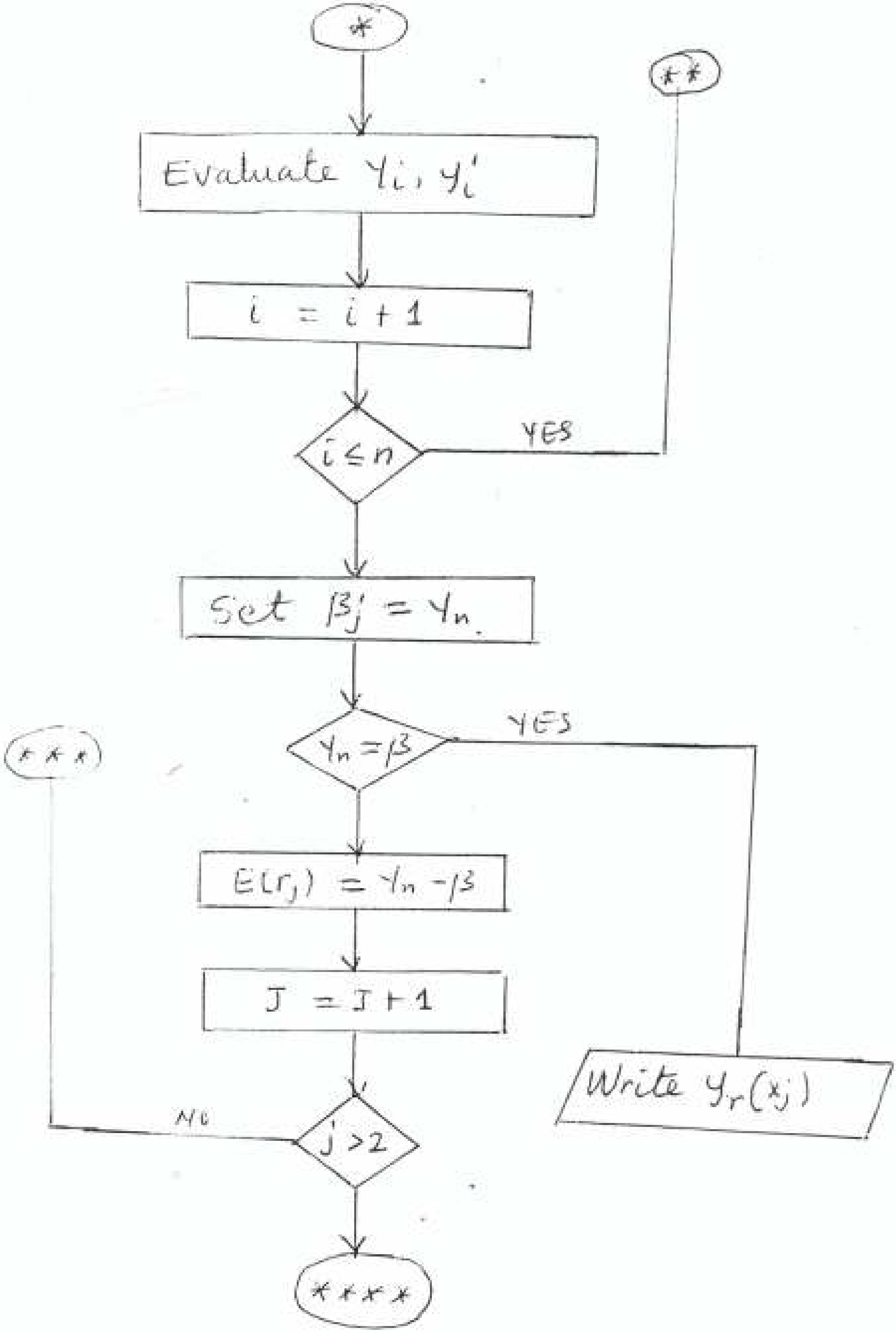
```
Given: $f(x,y,y')$, $a_1$, $\alpha$, $b_1$, $\beta$, n, $r_1$, $r_2$
Set $h = (b_1 - a_1)/(n+1)$
Repeat for j = 1, 2, 3..
For i = 1, 2, ... n
Set $x_i = a_i + ih$
Evaluate $y_i$, $y_i'$ (by solving the system:
     $y' = yp$    ,  $y(a) = 0$
     $yp = f(x,y,y')$  $yp(a) = rj$)
Set $\beta_j = y_n$
If j > 2, then
Set $r_{j+1} = r_j - \dfrac{E(r_j)(r_j - r_{j-1})}{E(r_j) - E(r_{j-1})}$
```

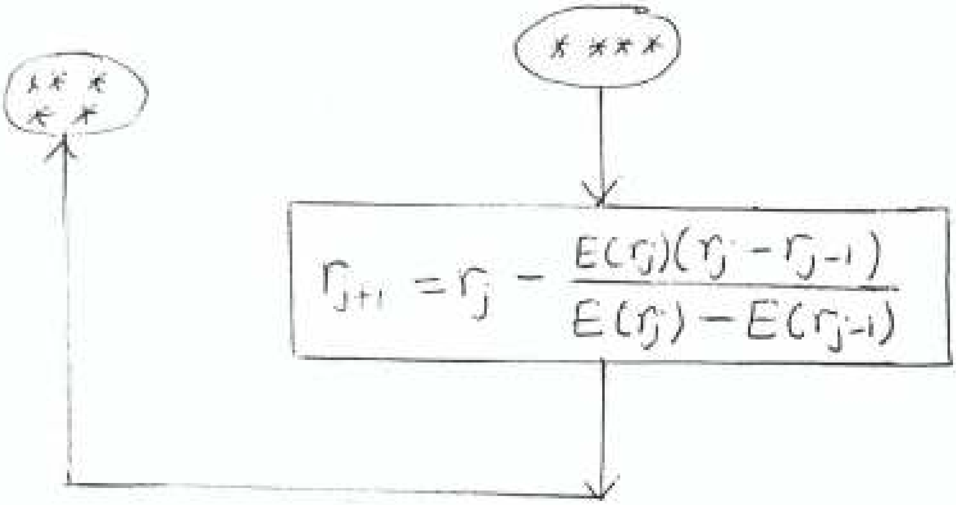
Until convergence

Output ('Solution', (x_j, $y_r(x_j)$, for x_j = a_1 to b_1

Flow chart 2: for the algorithm(2)




*
**
Evaluate y_i, y_i'
$i = i+1$
$i \le n$
YES
Set $\beta_j = y_n$
$y_n = \beta$
YES
***
$E(r_j) = y_n - \beta$
$J = J+1$
Write $y_r(x_j)$
NO
$j > 2$
****



The above algorithm (2) that uses Runge-Kutta Fourth order method as its integrator was implemented with FORTRAN 77 to solve the equations (3.3) and (3.5) for some varying values of parameters a and b, and d_1, d_2 and d_3 respectively. The FORTRAN 77 programs can be found in the appendix and the results obtained shall be discussed in the next chapter.

RESULTS

```
Results of Fin. diff. method for proplem 1

      for  A = 1.00    B = 1.00
    X                    Y
  .0000              .000000000
  .0196              .062042360
  .0392              .124108300
  .0588              .186222400
  .0784              .248407700
  .0980              .310688600
  .1176              .356982000
  .1373              .376763800
  .1569              .395444000
  .1765              .413208700
  .1961              .430205900
  .2157              .446555700
  .2353              .462356700
  .2549              .477691100
  .2745              .492628200
  .2941              .507226800
  .3137              .521537600
  .3333              .535604300
  .3529              .549465100
  .3725              .563153600
  .3922              .576699000
  .4118              .590127700
  .4314              .603462800
  .4510              .616725000
  .4706              .629933000
  .4902              .643103400
  .5098              .656251300
  .5294              .669389900
  .5490              .682531500
  .5686              .695687100
  .5882              .708866300
  .6078              .722078100
  .6275              .735330200
  .6471              .748629500
  .6667              .761982300
  .6863              .775394000
  .7059              .788869100
  .7255              .802411900
  .7451              .816025600
  .7647              .829713100
  .7843              .843476700
  .8039              .857317800
  .8235              .871237700
  .8431              .885236800
  .8627              .899315300
  .8824              .913472900
  .9020              .927708600
  .9216              .942021300
  .9412              .956409100
  .9608              .970869900
  .9804              .985401200
 1.0000             1.000000000
```

for A = 1.00 B = 2.00

X	Y
.0000	.000000000
.0196	.054702840
.0392	.109416300
.0588	.164150400
.0784	.218916400
.0980	.273724400
.1176	.310912900
.1373	.326985200
.1569	.342292000
.1765	.356983200
.1961	.371179100
.2157	.384978000
.2353	.398461400
.2549	.411698300
.2745	.424747100
.2941	.437658500
.3137	.450476700
.3333	.463240400
.3529	.475984000
.3725	.488738500
.3922	.501531500
.4118	.514388300
.4314	.527331500
.4510	.540382300
.4706	.553559700
.4902	.566881700
.5098	.580364600
.5294	.594023900
.5490	.607873500
.5686	.621926800
.5882	.636196200
.6078	.650693000
.6275	.665427900
.6471	.680410700
.6667	.695651000
.6863	.711157100
.7059	.726936900
.7255	.742997800
.7451	.759346400
.7647	.775988900
.7843	.792930600
.8039	.810176300
.8235	.827730400
.8431	.845596500
.8627	.863777600
.8824	.882276200
.9020	.901094200
.9216	.920232900
.9412	.939693000
.9608	.959474600
.9804	.979577400
1.0000	1.000000000

for A = 2.00 B = 1.00

X	Y
.0000	.000000000
.0196	.073282810
.0392	.146621800
.0588	.220073600
.0784	.293694700
.0980	.367541600
.1176	.422690300
.1373	.445799000
.1569	.467339700
.1765	.487555600
.1961	.506639800
.2157	.524748100
.2353	.542008300
.2549	.558526300
.2745	.574391100
.2941	.589678000
.3137	.604451500
.3333	.618767000
.3529	.632672500
.3725	.646210300
.3922	.659417000
.4118	.672325600
.4314	.684964700
.4510	.697360100
.4706	.709534900
.4902	.721509800
.5098	.733303300
.5294	.744932500
.5490	.756412400
.5686	.767757000
.5882	.778978600
.6078	.790088900
.6275	.801098100
.6471	.812015800
.6667	.822850800
.6863	.833611100
.7059	.844303800
.7255	.854935800
.7451	.865513100
.7647	.876041100
.7843	.886525000
.8039	.896969600
.8235	.907379000
.8431	.917757000
.8627	.928107000
.8824	.938432300
.9020	.948735600
.9216	.959019400
.9412	.969286000
.9608	.979537100
.9804	.989774600
1.0000	1.000000000

for A = 2.00 B = 2.00

X	Y
.0000	.000000000
.0196	.062042360
.0392	.124108300
.0588	.186222400
.0784	.248407700
.0980	.310688600
.1176	.363663400
.1373	.385946900
.1569	.406782000
.1765	.426403000
.1961	.444996300
.2157	.462713000
.2353	.479677200
.2549	.495992000
.2745	.511744400
.2941	.527008400
.3137	.541847300
.3333	.556316200
.3529	.570462800
.3725	.584329200
.3922	.597952500
.4118	.611365900
.4314	.624598600
.4510	.637677000
.4706	.650625000
.4902	.663464100
.5098	.676213900
.5294	.688892300
.5490	.701515500
.5686	.714098400
.5882	.726654700
.6078	.739197000
.6275	.751737000
.6471	.764285300
.6667	.776851800
.6863	.789445800
.7059	.802075600
.7255	.814749100
.7451	.827473700
.7647	.840256200
.7843	.853102600
.8039	.866018800
.8235	.879010000
.8431	.892081400
.8627	.905237300
.8824	.918481800
.9020	.931818800
.9216	.945251800
.9412	.958783700
.9608	.972417500
.9804	.986155500
1.0000	1.000000000

Results of Fin. diff. method for problem 2

for $d_1 = 2.00$ $d_2 = 2.00$ $d_3 = 2.00$

X	θ
.0000	.000000000
.0196	.026330850
.0392	.051890200
.0588	.076674390
.0784	.100678600
.0980	.123896800
.1176	.241876200
.1373	.290518500
.1569	.335312200
.1765	.376794900
.1961	.415392300
.2157	.451447500
.2353	.485240500
.2549	.517002800
.2745	.546928100
.2941	.575179900
.3137	.601897400
.3333	.627199900
.3529	.651190600
.3725	.673959100
.3922	.695584100
.4118	.716134400
.4314	.735671200
.4510	.754248500
.4706	.771914400
.4902	.788712300
.5098	.804681000
.5294	.819855500
.5490	.834267500
.5686	.847945700
.5882	.860916500
.6078	.873203800
.6275	.884829700
.6471	.895814400
.6667	.906176600
.6863	.915933500
.7059	.925101600
.7255	.933695600
.7451	.941729800
.7647	.949217400
.7843	.956170700
.8039	.962601700
.8235	.968521500
.8431	.973941000
.8627	.978870200
.8824	.983319100
.9020	.987297200
.9216	.990813700
.9412	.993877500
.9608	.996497300
.9804	.998681700
1.0000	1.000000000

for $d_1 = 2.00$ $d_2 = 1.00$ $d_3 = 2.00$

X	θ
.0000	.000000000
.0196	.025513860
.0392	.050256220
.0588	.074223410
.0784	.097410610
.0980	.119811800
.1176	.238051200
.1373	.286804600
.1569	.331703200
.1765	.373285700
.1961	.411978700
.2157	.448125900
.2353	.482007800
.2549	.513856500
.2745	.543866200
.2941	.572200500
.3137	.598998800
.3333	.624380900
.3529	.648450100
.3725	.671296200
.3922	.692997900
.4118	.713624400
.4314	.733236700
.4510	.751889200
.4706	.769630000
.4902	.786502500
.5098	.802545600
.5294	.817794400
.5490	.832280800
.5686	.846033300
.5882	.859078500
.6078	.871440400
.6275	.883141000
.6471	.894200500
.6667	.904637800
.6863	.914470000
.7059	.923713600
.7255	.932383400
.7451	.940493700
.7647	.948057600
.7843	.955087600
.8039	.961595600
.8235	.967592700
.8431	.973089700
.8627	.978096800
.8824	.982623900
.9020	.986680600
.9216	.990275900
.9412	.993418800
.9608	.996118100
.9804	.998382200
1.0000	1.000000000

for $d_1 = 2.00$ $d_2 = 2.00$ $d_3 = 1.00$

X	θ
.0000	.000000000
.0196	.023786340
.0392	.047186930
.0588	.070199940
.0784	.092822950
.0980	.115053000
.1176	.219882000
.1373	.263314300
.1569	.303455400
.1765	.340776400
.1961	.375650200
.2157	.408377500
.2353	.439203700
.2549	.468331800
.2745	.495931700
.2941	.522146600
.3137	.547098800
.3333	.570892800
.3529	.593619200
.3725	.615356600
.3922	.636173900
.4118	.656131700
.4314	.675283400
.4510	.693676400
.4706	.711352700
.4902	.728350300
.5098	.744703100
.5294	.760441600
.5490	.775593300
.5686	.790183100
.5882	.804233900
.6078	.817766300
.6275	.830799200
.6471	.843349800
.6667	.855434000
.6863	.867066500
.7059	.878260900
.7255	.889029500
.7451	.899384100
.7647	.909335500
.7843	.918893600
.8039	.928068000
.8235	.936867500
.8431	.945300500
.8627	.953374900
.8824	.961098000
.9020	.968477000
.9216	.975518800
.9412	.982229800
.9608	.988616200
.9804	.994684000
1.0000	1.000000000

for $d_1 = 1.00$ $d_2 = 1.00$ $d_3 = 1.00$

X	θ
.0000	.000000000
.0196	.027190820
.0392	.054185480
.0588	.080979760
.0784	.107569200
.0980	.133949000
.1176	.238792600
.1373	.282602300
.1569	.323285800
.1765	.361276400
.1961	.396916600
.2157	.430481600
.2353	.462195600
.2549	.492243100
.2745	.520777900
.2941	.547929400
.3137	.573806900
.3333	.598503900
.3529	.622100400
.3725	.644665800
.3922	.666260100
.4118	.686935700
.4314	.706738400
.4510	.725708400
.4706	.743881300
.4902	.761288700
.5098	.777958400
.5294	.793915300
.5490	.809181800
.5686	.823777800
.5882	.837721300
.6078	.851028900
.6275	.863715000
.6471	.875793300
.6667	.887276100
.6863	.898174800
.7059	.908500100
.7255	.918261800
.7451	.927469400
.7647	.936131800
.7843	.944257400
.8039	.951854300
.8235	.958930400
.8431	.965493500
.8627	.971551100
.8824	.977110700
.9020	.982179800
.9216	.986766300
.9412	.990877600
.9608	.994521400
.9804	.997705800
1.0000	1.000000000

for $d_1 = 2.00$ $d_2 = 1.00$ $d_3 = 1.00$

X	θ
.0000	.000000000
.0196	.022969350
.0392	.045552950
.0588	.067748960
.0784	.089554980
.0980	.110968000
.1176	.216057100
.1373	.259600400
.1569	.299846400
.1765	.337267200
.1961	.372236600
.2157	.405055900
.2353	.435971100
.2549	.465185600
.2745	.492869800
.2941	.519167200
.3137	.544200200
.3333	.568073700
.3529	.590878600
.3725	.612693500
.3922	.633587700
.4118	.653621600
.4314	.672848800
.4510	.691317000
.4706	.709068200
.4902	.726140400
.5098	.742567700
.5294	.758380500
.5490	.773606500
.5686	.788270700
.5882	.802395900
.6078	.816002800
.6275	.829110300
.6471	.841735800
.6667	.853895100
.6863	.865602900
.7059	.876872700
.7255	.887717200
.7451	.898147900
.7647	.908175600
.7843	.917810400
.8039	.927061700
.8235	.935938500
.8431	.944449100
.8627	.952601300
.8824	.960402700
.9020	.967860300
.9216	.974981000
.9412	.981771100
.9608	.988236900
.9804	.994384500
1.0000	1.000000000

```
Results of Shooting method for problem 1

for  A = 1.00   B = 2.00

      M1 = 2.3368

        X            Y
     .00000       .02291
     .01961       .04584
     .03922       .06879
     .05882       .09178
     .07843       .11481
     .09804       .13789
     .11765       .17430
     .13725       .20640
     .15686       .23529
     .17647       .26170
     .19608       .28616
     .21569       .30905
     .23529       .33067
     .25490       .35124
     .27451       .37094
     .29412       .38992
     .31373       .40830
     .33333       .42618
     .35294       .44365
     .37255       .46078
     .39216       .47763
     .41176       .49425
     .43137       .51071
     .45098       .52702
     .47059       .54325
     .49020       .55941
     .50980       .57554
     .52941       .59167
     .54902       .60783
     .56863       .62402
     .58824       .64029
     .60784       .65664
     .62745       .67309
     .64706       .68966
     .66667       .70636
     .68627       .72322
     .70588       .74023
     .72549       .75741
     .74510       .77477
     .76471       .79233
     .78431       .81008
     .80392       .82805
     .82353       .84622
     .84314       .86462
     .86275       .88325
     .88235       .90211
     .90196       .92120
     .92157       .94054
     .94118       .96011
     .96078       .97993
     .98039      1.00000
```

```
for  A = 1.00   B = 1.00

      M1 = 2.6556

        X               Y
     .00000          .02604
     .01961          .05208
     .03922          .07814
     .05882          .10422
     .07843          .13033
     .09804          .15646
     .11765          .19767
     .13725          .23394
     .15686          .26650
     .17647          .29620
     .19608          .32361
     .21569          .34916
     .23529          .37318
     .25490          .39592
     .27451          .41758
     .29412          .43833
     .31373          .45829
     .33333          .47757
     .35294          .49627
     .37255          .51446
     .39216          .53220
     .41176          .54956
     .43137          .56659
     .45098          .58332
     .47059          .59980
     .49020          .61605
     .50980          .63211
     .52941          .64801
     .54902          .66376
     .56863          .67939
     .58824          .69492
     .60784          .71036
     .62745          .72573
     .64706          .74105
     .66667          .75631
     .68627          .77154
     .70588          .78674
     .72549          .80193
     .74510          .81710
     .76471          .83227
     .78431          .84745
     .80392          .86263
     .82353          .87782
     .84314          .89302
     .86275          .90824
     .88235          .92348
     .90196          .93874
     .92157          .95402
     .94118          .96933
     .96078          .98465
     .98039         1.00000
```

```
for  A = 2.00   B = 2.00

     M1 = 2.9654

        X              Y
     .00000         .02907
     .01961         .05816
     .03922         .08726
     .05882         .11639
     .07843         .14554
     .09804         .17472
     .11765         .22056
     .13725         .26050
     .15686         .29601
     .17647         .32808
     .19608         .35739
     .21569         .38445
     .23529         .40966
     .25490         .43331
     .27451         .45564
     .29412         .47684
     .31373         .49706
     .33333         .51644
     .35294         .53507
     .37255         .55306
     .39216         .57048
     .41176         .58739
     .43137         .60386
     .45098         .61994
     .47059         .63567
     .49020         .65110
     .50980         .66625
     .52941         .68116
     .54902         .69586
     .56863         .71038
     .58824         .72473
     .60784         .73894
     .62745         .75302
     .64706         .76700
     .66667         .78089
     .68627         .79471
     .70588         .80846
     .72549         .82217
     .74510         .83584
     .76471         .84948
     .78431         .86310
     .80392         .87672
     .82353         .89033
     .84314         .90395
     .86275         .91758
     .88235         .93124
     .90196         .94492
     .92157         .95863
     .94118         .97238
     .96078         .98617
     .98039        1.00000
```

```
for  A = 2.00   B = 1.00

     M1 = 3.1680

       X            Y
    .00000       .03106
    .01961       .06213
    .03922       .09320
    .05882       .12429
    .07843       .15539
    .09804       .18651
    .11765       .23538
    .13725       .27793
    .15686       .31571
    .17647       .34978
    .19608       .38086
    .21569       .40951
    .23529       .43613
    .25490       .46104
    .27451       .48449
    .29412       .50667
    .31373       .52775
    .33333       .54787
    .35294       .56714
    .37255       .58566
    .39216       .60350
    .41176       .62073
    .43137       .63743
    .45098       .65363
    .47059       .66939
    .49020       .68475
    .50980       .69973
    .52941       .71438
    .54902       .72873
    .56863       .74279
    .58824       .75659
    .60784       .77016
    .62745       .78351
    .64706       .79665
    .66667       .80961
    .68627       .82240
    .70588       .83502
    .72549       .84750
    .74510       .85984
    .76471       .87205
    .78431       .88414
    .80392       .89612
    .82353       .90800
    .84314       .91978
    .86275       .93147
    .88235       .94308
    .90196       .95460
    .92157       .96606
    .94118       .97744
    .96078       .98875
    .98039      1.00000
```

Results of Shooting method for problem 2

for $d_1 = 2.00$ $d_2 = 2.00$ $d_3 = 2.00$

M1 = .2910

X	θ
.0000	.005320
.0196	.009862
.0392	.013618
.0588	.016577
.0784	.018727
.0980	.020057
.1176	.021248
.1373	.023012
.1569	.025398
.1765	.028443
.1961	.032184
.2157	.036652
.2353	.041875
.2549	.047878
.2745	.054685
.2941	.062318
.3137	.070798
.3333	.080145
.3529	.090377
.3725	.101511
.3922	.113567
.4118	.126560
.4314	.140508
.4510	.155427
.4706	.171336
.4902	.188249
.5098	.206186
.5294	.225162
.5490	.245197
.5686	.266309
.5882	.288517
.6078	.311839
.6275	.336298
.6471	.361913
.6667	.388706
.6863	.416702
.7059	.445922
.7255	.476393
.7451	.508140
.7647	.541190
.7843	.575573
.8039	.611317
.8235	.648455
.8431	.687018
.8627	.727042
.8824	.768562
.9020	.811617
.9216	.856245
.9412	.902489
.9608	.950392
.9804	1.000000

for d_1 = 2.00 d_2 = 1.00 d_3 = 2.00

M1 = .3061

X	θ
.0000	.005617
.0196	.010457
.0392	.014512
.0588	.017773
.0784	.020230
.0980	.021874
.1176	.023406
.1373	.025557
.1569	.028370
.1765	.031882
.1961	.036125
.2157	.041128
.2353	.046915
.2549	.053509
.2745	.060930
.2941	.069196
.3137	.078325
.3333	.088331
.3529	.099230
.3725	.111034
.3922	.123758
.4118	.137413
.4314	.152011
.4510	.167565
.4706	.184087
.4902	.201587
.5098	.220079
.5294	.239573
.5490	.260081
.5686	.281618
.5882	.304194
.6078	.327823
.6275	.352520
.6471	.378298
.6667	.405173
.6863	.433160
.7059	.462275
.7255	.492537
.7451	.523962
.7647	.556571
.7843	.590383
.8039	.625420
.8235	.661704
.8431	.699259
.8627	.738109
.8824	.778282
.9020	.819804
.9216	.862706
.9412	.907017
.9608	.952771
.9804	1.000001

for d_1 = 2.00 d_2 = 2.00 d3 = 1.00

M1 = .2746

X	θ
.0000	.005191
.0196	.009993
.0392	.014401
.0588	.018407
.0784	.022004
.0980	.025184
.1176	.028486
.1373	.032457
.1569	.037114
.1765	.042471
.1961	.048542
.2157	.055338
.2353	.062868
.2549	.071142
.2745	.080169
.2941	.089957
.3137	.100514
.3333	.111848
.3529	.123967
.3725	.136878
.3922	.150590
.4118	.165112
.4314	.180451
.4510	.196618
.4706	.213622
.4902	.231474
.5098	.250184
.5294	.269763
.5490	.290224
.5686	.311580
.5882	.333844
.6078	.357031
.6275	.381156
.6471	.406236
.6667	.432288
.6863	.459330
.7059	.487382
.7255	.516464
.7451	.546598
.7647	.577807
.7843	.610115
.8039	.643547
.8235	.678131
.8431	.713895
.8627	.750869
.8824	.789084
.9020	.828573
.9216	.869372
.9412	.911517
.9608	.955046
.9804	1.000001

for $d_1 = 1.00$ $d_2 = 1.00$ $d_3 = 1.00$

M1 = .2155

X	θ
.0000	.004033
.0196	.007673
.0392	.010913
.0588	.013743
.0784	.016154
.0980	.018135
.1176	.020231
.1373	.023004
.1569	.026489
.1765	.030713
.1961	.035699
.2157	.041466
.2353	.048030
.2549	.055402
.2745	.063596
.2941	.072620
.3137	.082484
.3333	.093194
.3529	.104759
.3725	.117185
.3922	.130479
.4118	.144649
.4314	.159702
.4510	.175645
.4706	.192486
.4902	.210234
.5098	.228900
.5294	.248492
.5490	.269023
.5686	.290506
.5882	.312953
.6078	.336380
.6275	.360802
.6471	.386239
.6667	.412708
.6863	.440231
.7059	.468830
.7255	.498530
.7451	.529358
.7647	.561341
.7843	.594510
.8039	.628898
.8235	.664541
.8431	.701476
.8627	.739744
.8824	.779388
.9020	.820455
.9216	.862995
.9412	.907061
.9608	.952709
.9804	1.000000

for $d_1 = 2.00$ $d_2 = 1.00$ $d_3 = 1.00$

M1 = .2897

X	θ
.0000	.005488
.0196	.010588
.0392	.015295
.0588	.019603
.0784	.023507
.0980	.027000
.1176	.030645
.1373	.035002
.1569	.040086
.1765	.045910
.1961	.052482
.2157	.059813
.2353	.067908
.2549	.076773
.2745	.086414
.2941	.096835
.3137	.108041
.3333	.120034
.3529	.132820
.3725	.146400
.3922	.160781
.4118	.175964
.4314	.191954
.4510	.208756
.4706	.226373
.4902	.244812
.5098	.264076
.5294	.284173
.5490	.305108
.5686	.326888
.5882	.349521
.6078	.373015
.6275	.397378
.6471	.422621
.6667	.448754
.6863	.475788
.7059	.503735
.7255	.532607
.7451	.562420
.7647	.593187
.7843	.624924
.8039	.657649
.8235	.691380
.8431	.726135
.8627	.761935
.8824	.798803
.9020	.836760
.9216	.875832
.9412	.916044
.9608	.957424
.9804	1.000000

CHAPTER FIVE

ANALYSIS OF RESULTS

I will now discuss the results with particular reference to the objective.

The mathematical equations for the problem have been formulated. The problem of singularities treated.

The existence and uniqueness of the solutions of the equations formulated have been investigated

The key parameters for equation (3.3) are

$$a = \frac{D}{VR} \quad \text{- modified diffusion coefficient}$$

and $$b = \frac{\beta}{RPV} \quad \text{- modified pre-exponential factor,}$$

and that of equation 3.5 are

$$d_1 = \frac{k}{\rho CVR} \quad \text{- modified thermal conductivity}$$

$$d_2 = \frac{wVE\mu}{RR_oT_o^2} \quad \text{- modified viscosity}$$

and $$d_3 = \frac{REQ\beta}{VR_oT_o^2} \quad \text{- modified Heat Release}$$

Solutions of Equation (3.3) exist for all times when parameter $a > o$ and mesh-size

$$h < \frac{2}{|1/a - 3a(\tfrac{1}{2}a)^{2/3}|}$$

and also solutions of equation (3.5) occur for all times when

parameter $d_1 > o$ and meshsize
$$h < \frac{2}{|1/d_1-3d_1(\frac{1}{2}d_1)^{2/3}|}$$

The exact solutions of equations (3.3) and (3.5) do not exist. For the purpose of comparison between the Finite-difference and shooting methods with respect to the exact solutions, we considered two test cases whose exact solutions are known

Case 1:
$$y'(t) = -y$$
$$y(0) = 1$$
$$y(\Pi/2) = 3$$

Exact solution: $y = \text{Cos}t + 3\text{Sin}t$

Case 2:
$$\theta''(t) = t$$
$$\theta(0) = 1$$
$$\theta(1) = 0$$

Exact solution: $\theta(t) = 1/6t^3 - 7/6t + 1$

The results are summarized thus:

Table 1: Results of test case 1

t	Exact Solution (θ)	Shooting method (θ_1)	Fin. Diff. method (θ_2)	$/\theta-\theta_1/$	$/\theta-\theta_2/$
0	1.000	1.000	1.000	0.000	0.000
$\Pi/6$	2.366	2.433	2.389	0.067	0.023
$\Pi/3$	3.098	3.181	3.122	0.083	0.024
$\Pi/2$	3.000	3.000	3.000	0.000	0.000

Table 2: Results of test case 2

t	Exact Solution (θ)	Shooting Method (θ_1)	Fin. Diff. Method (θ_2)	$/\theta-\theta_1/$	$/\theta-\theta_2/$
0.00	1.000	1.000	1.000	0.000	0.000
0.25	0.711	0.718	0.710	0.007	0.001
0.50	0.438	0.432	0.437	0.006	0.001
0.75	0.195	0.187	0.195	0.008	0.000
1.00	0.000	0.000	0.000	0.000	0.000

From the above tables ,the results of the Finite difference mothod is closer to the exact solutions compared with the results of the Shooting method. This shows things could be said of results of equation (3.3) and (2.5) provided by these methods.

Figures (4), (5), (6) and (7) represent the graphs of the result for the methods, -Shooting and Finite difference schemes for equation (3.3). Also, Figures (8), (9), (10), (11) and (12) represent the graph of the results of the methods for equation (3.5).

From the graphs, the results of finite difference method is closer to the exact solutions than that of the shooting method. Finite difference scheme takes shorter time because we guess values for initial condition in shooting method and is more accurate than the shooting method.

The physical implications of our results

The effects of the parameters a and b on temperature. For a constant value of the parameter a, there is a decrease in temperature as parameter b increases (see Figs. (4) and (5), also Figs. (6) and (7)).

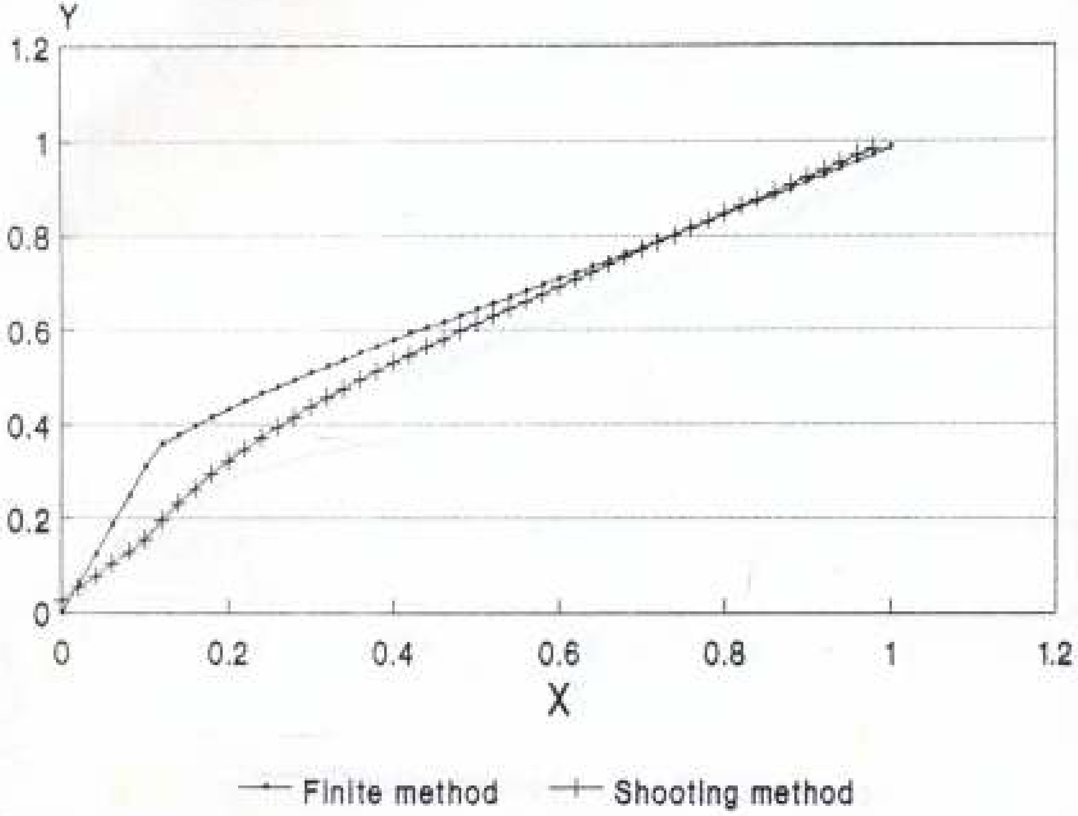
The effects of the parameters d_1, d_2 and d_3 on temperature. for constant values of d_1 and d_2, (i.e. $d_1,d_2 = 2.00$), there is an increase in temperature for an increase in parameter d_3 (see Figs. (9) and (11)).

Also temperature decreases as parameter d_1 increases (i e d_1 from 1.00 to 2.00) for constant d_2 and d_3 (i e $d_2,d_3 = 1.00$) see Figs. (8) and (10).

Lastly, increase in parameter d_2 (d_2 changes form 1.00 to 2.00) causes increase in temperature when parameters d_1 and d_2 are constants (i,e $d_2,d_3 = 1.00$) (See Figs. (11) and (12))

The effect of viscosity on temperature . Since viscosity is directly proportional to parameter d_2, therefore, Figs.(11) and (12) shows that increase in viscosity causes increase in temperature and verse visa.

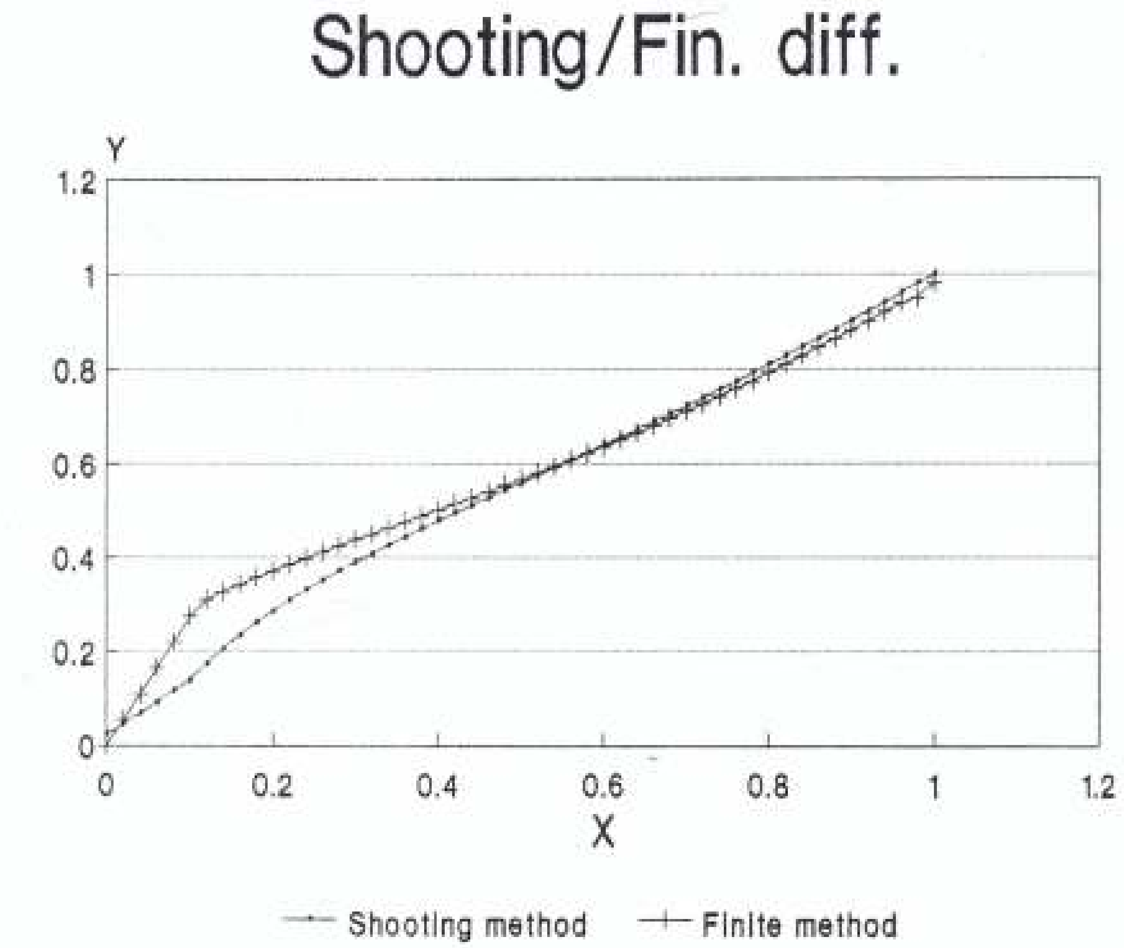
Conclusively, the above results, most especially the relationships, between the heat release and temperature, and between the viscosity and temperature would be found useful in the medical and engineering fields.



Shooting/Fin. diff.

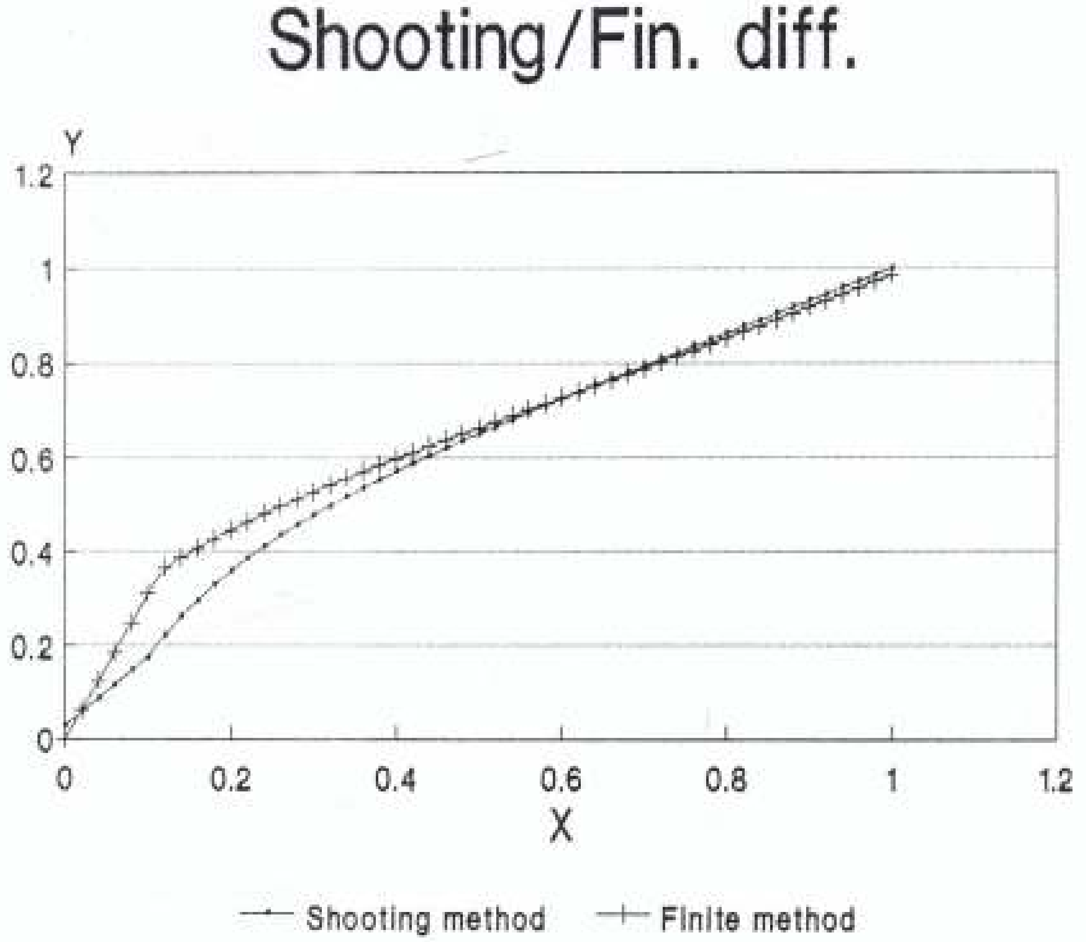
A = 1.00, B = 1.00

Figure 4



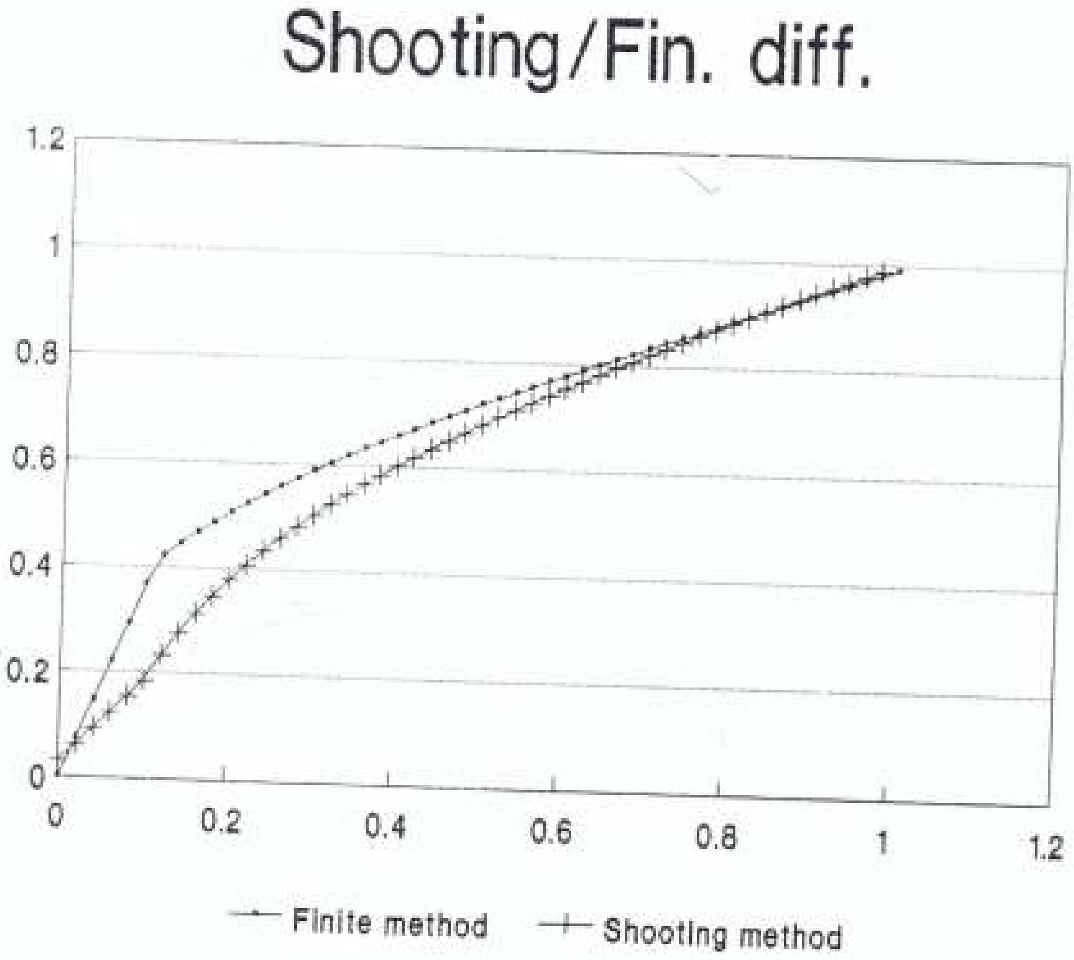
A = 1.00, B = 2.00

Figure 5



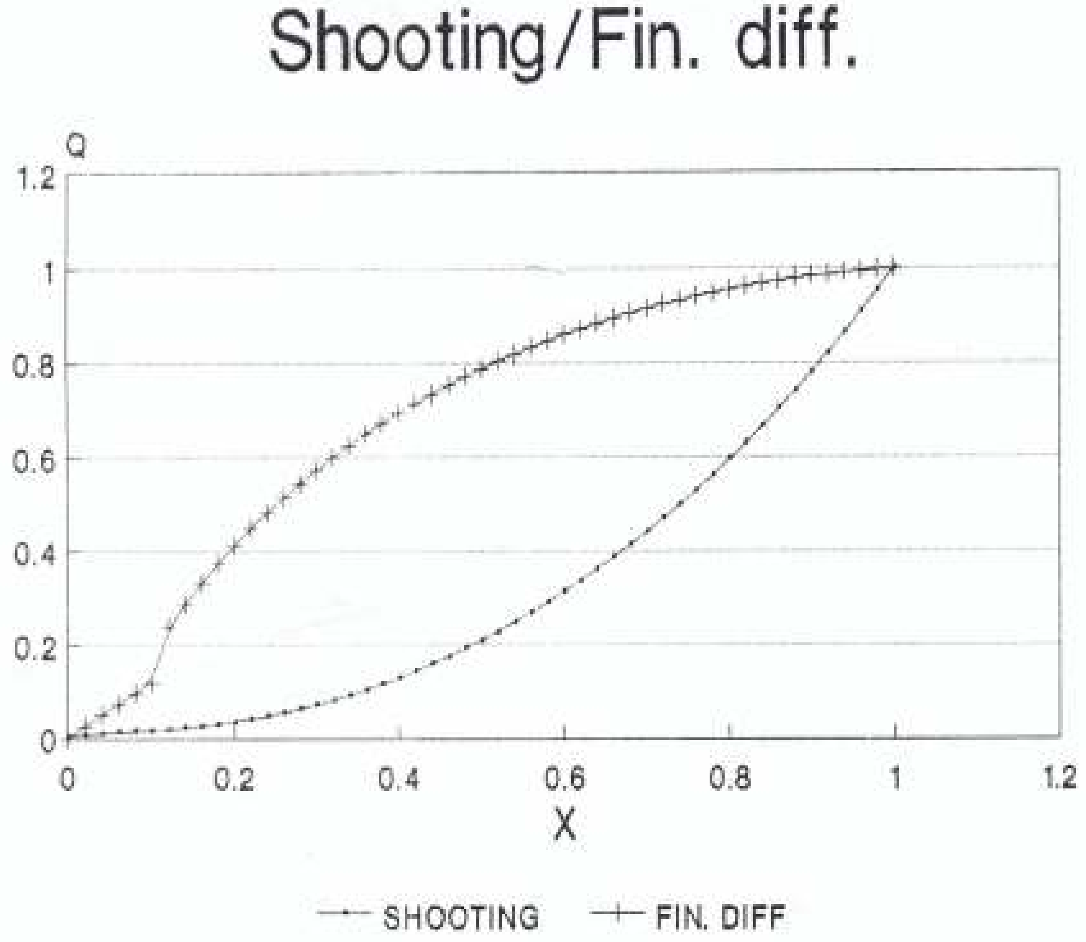
A • 2.00, B • 2.00

Figure 6



A = 2.00, B = 1.00

Figure 7



D1 = 1.00, D2 = 1.00, D3 = 1.00

Figure 8

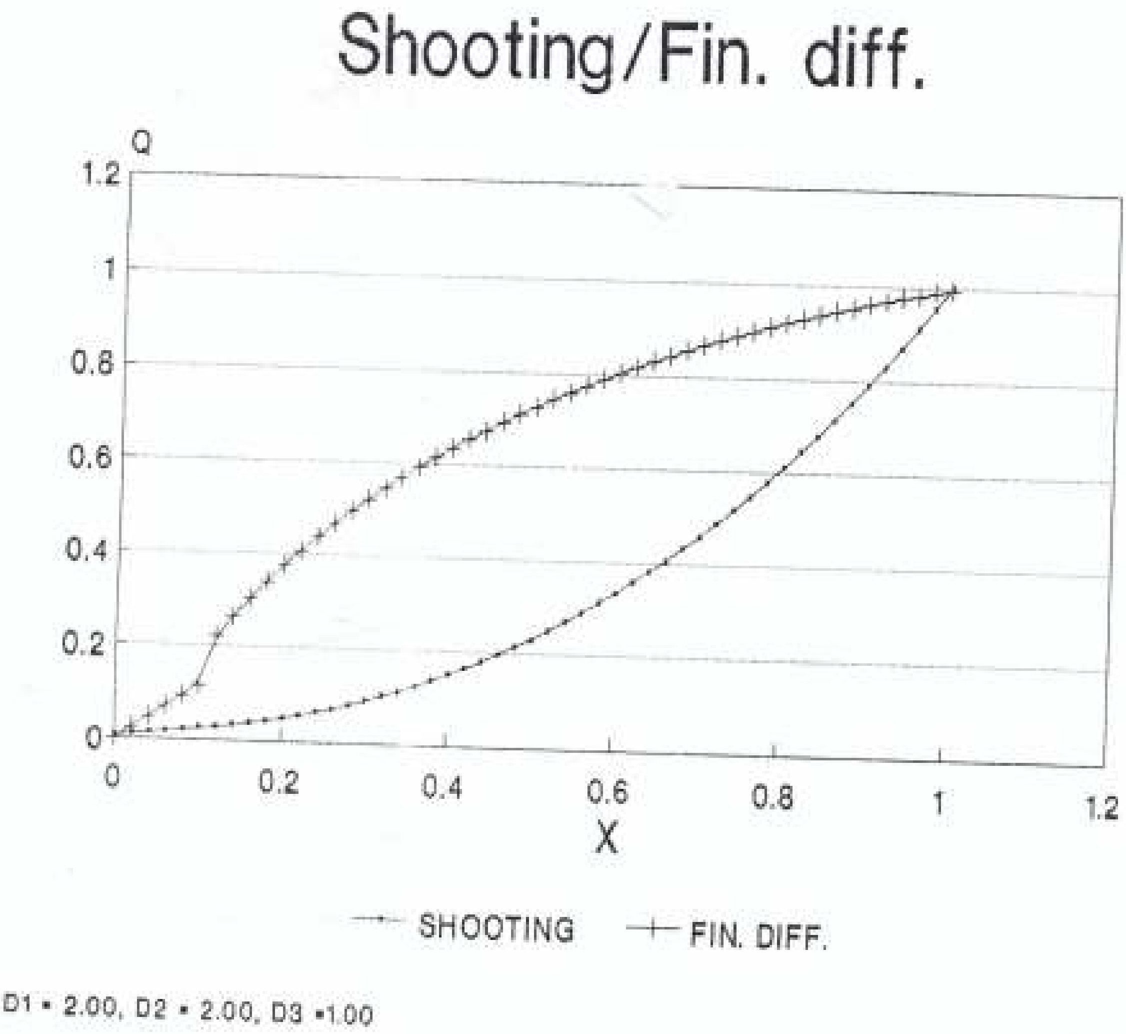
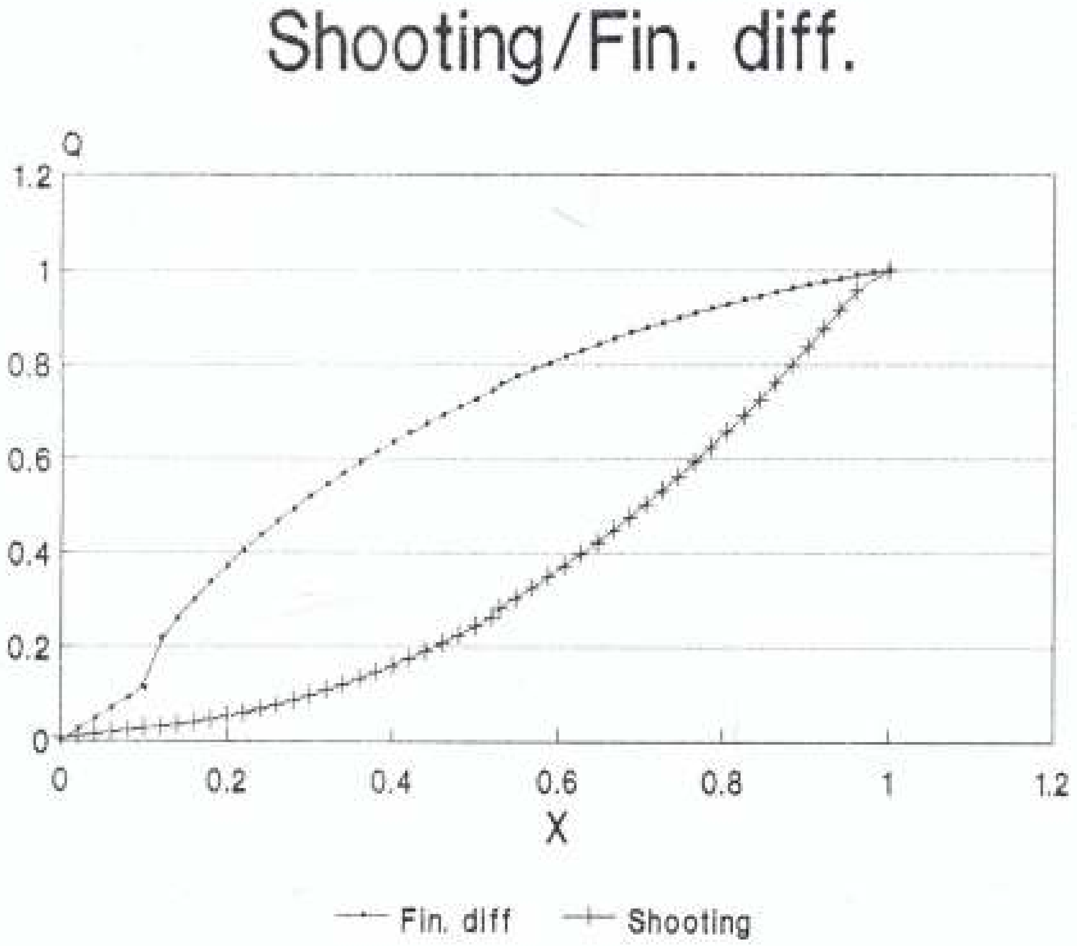
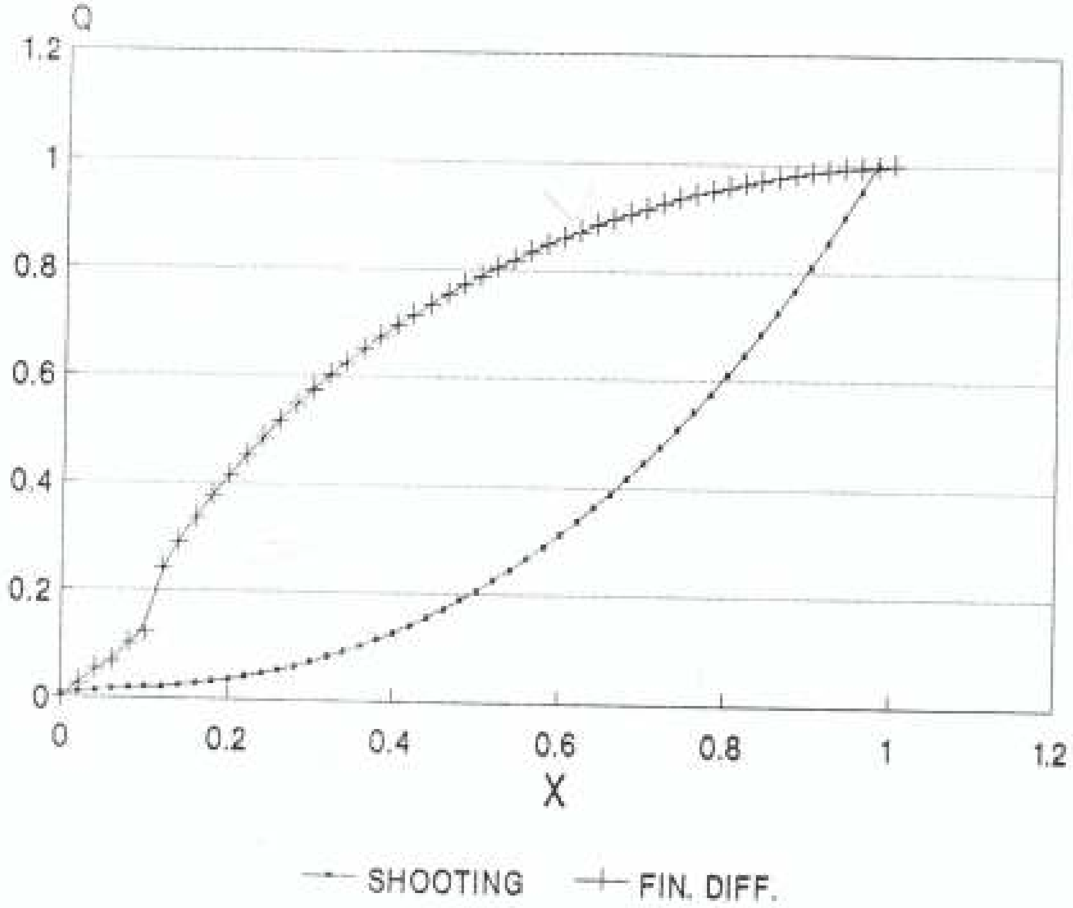

Shooting/Fin. diff.
Q
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2
X
SHOOTING
FIN. DIFF.
D1 = 2.00, D2 = 2.00, D3 =1.00

Figure 9



D1 = 2.00, D2 = 1.00, D3 = 1.00

Figure 10



D1 = 2.00, D2 = 2.00, D3 = 2.00

Figure 11

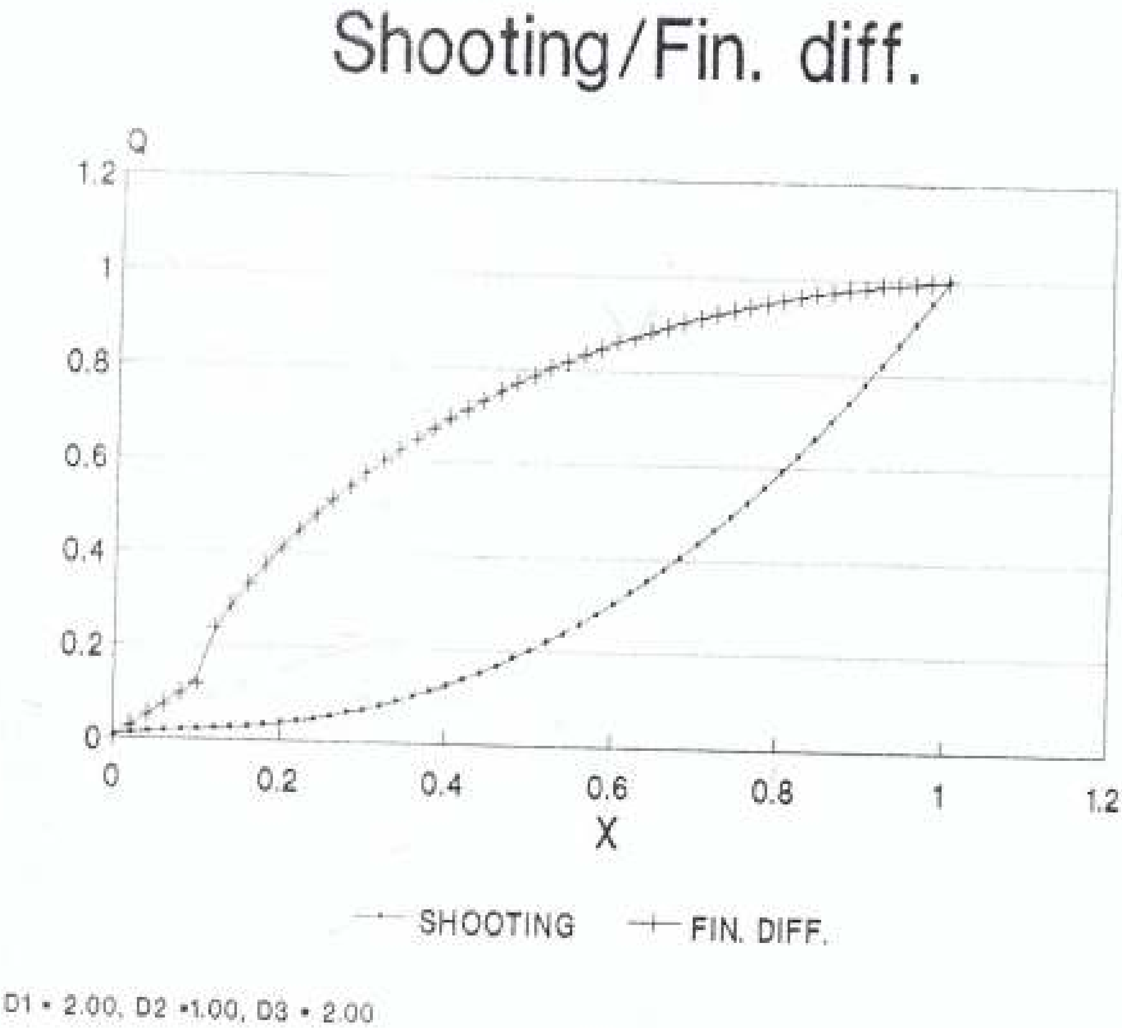

Shooting/Fin. diff.
Q
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2
X
SHOOTING
FIN. DIFF.
D1 = 2.00, D2 =1.00, D3 = 2.00

Figure 12

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APPENDIX

Programs 1

```
C     PROGRAM TO SOLVE STEADY CASE PROBLEM
C     (1.0-X*X)DY/DX = A/X(D/DX(XDY/DX)) - B*Y
C     USING FINITE DIFFERENT METHOD
      REAL X1,XN,XF,YN,YF,AL,AU,Z,Y,Y1
      INTEGER N,K,N1,R,IR
      DIMENSION C(50,50),AL(50,50),AU(50,50),Z(50),Y(50)
      DIMENSION D(50),X(50),X1(50),Y1(50)
      OPEN(UNIT=1,FILE='FIN1.IN')
      OPEN(UNIT=2,FILE='FIN1.OUT')
      XN = 0.0
      XF = 1.0
      YN = 0.0
      YF = 1.0
      N = 50
      N1 = N+1
      H = (XF-XN)/FLOAT(N+1)
      DO 5 K = 1,4
     READ(1,7)A,B
     WRITE(2,9)A,B
     WRITE(2,10)
     R = 0
     IR = 0
 4      X(R) = XN + R*H
     IF(X(R) .LT. 0.1)THEN
       BA = SQRT(B/A)
       E1 = EXP(BA)
       E2 = EXP(2.0*BA)
       EA = BA*X(R)
       E3 = EXP(EA)
       E4 = EXP(-EA)
       Y(R) = (E1/(1.0-E2))*(-E3 + E4)
       WRITE(2,18)X(R),Y(R)
       X1(R) = X(R)
       R = R+1
       IR = R
       GO TO 4
     END IF
      R = IR-1
      C(R,R) = -(H**2)*(B/A)-2.0
      C(R,R+1) = 1.0-(H/(2.0*A*X1(R)))*(X1(R)-X1(R)**3-A)
      D(R) = -(1.0+(H/(2.0*A*X1(R)))*(X1(R)-X1(R)**3-A))*Y(R)
      DO 13 I = R+1,N-1
     X1(I) = X1(R)+I*H
     C(I,I-1) = 1.0+(H/(2.0*A*X1(I)))*(X1(I)-X1(I)**3-A)
     C(I,I) = -(H**2*B/A)-2.0
     C(I,I+1) = 1.0-(H/(2.0*A*X1(I)))*(X1(I)-X1(I)**3-A)
     D(I) = 0.0
 13   CONTINUE
     X1(N) = X1(N-1)+ H
     C(N,N-1) = 1.0+(H/(2.0*A*X1(N)))*(X1(N)-X1(N)**3-A)
     C(N,N) = -(H**2*B/A)-2.0
     D(N) = -(1.0-(H/(2.0*A*X1(N)))*(X1(N)-X1(N)**3-A))*YF
C   DECOMPOSE MATRIX C INTO LOWER AND UPPER TRIANGULAR                C
MATRICES (I.E.(A=LU)
```

```
     AL(R,R) = C(R,R)
     AU(R,R+1) = C(R,R+1)/AL(R,R)
     AU(R,R) = 1.0
     DO 15 I = R+1,N-1
       AL(I,I-1) = C(I,I-1)
       AL(I,I) = C(I,I)-AL(I,I-1)*AU(I-1,I)
       AU(I,I) = 1.0
       AU(I,I+1) = C(I,I+1)/AL(I,I)
 15     CONTINUE
     AL(N,N-1) = C(N,N-1)
     AL(N,N) = C(N,N)-AL(N,N-1)*AU(N-1,N)
     AU(N,N) = 1.0
C   SOLVE THE SYSTEM LZ = D
     Z(R) = D(R)/AL(R,R)
     DO 17 I = R+1,N
       Z(I) = (D(I)-AL(I,I-1)*Z(I-1))/AL(I,I)
 17     CONTINUE
C   SOLVE THE SYSTEM UY1 = Z
     Y1(N) = Z(N)
     DO 20 I = N-1,R,-1
       Y1(I) = Z(I)-AU(I,I+1)*Y1(I+1)
 20       CONTINUE
       DO 22 I = IR,N,1
       X1(I) = X1(I-1)+H
       WRITE(2,18)X1(I),Y1(I)
 22     CONTINUE
       WRITE(2,18)XF,YF
 7    FORMAT(2(F4.2))
 9    FORMAT(/,3X,'A = ',F4.2,3X,'B = ',F4.2)
 10   FORMAT(3X,'     X                Y ')
 18   FORMAT(5X,F6.4,8X,F14.9)
 5    CONTINUE
      STOP
      END
```

Program 2

```
C     PROGRAM TO SOLVE STEADY CASE PROBLEM
C     (1.0-X*X)DQ/DX = D1/X(D/DX(XDQ/DX)) - D2*X*X+ D3
C     USING FINITE DIFFERENCE METHOD
      REAL X1,XN,XF,QN,QF,AL,AU,Z,Q,Q1
      INTEGER N,N1,R,IR
      DIMENSION C(50,50),AL(50,50),AU(50,50),Z(50),Q(50)
      DIMENSION D(50),X(50),X1(50),Q1(50),Y(50)
      OPEN(UNIT=1,FILE='FIND2.IN')
      OPEN(UNIT=2,FILE='FIND2.OUT')
      XN = 0.0
      XF = 1.0
      QN = 0.0
      QF = 1.0
      N = 50
      N1 = N+1
      H = (XF-XN)/FLOAT(N+1)
      DO 5 K = 1,7
        READ(1,7)D1,D2,D3
        WRITE(2,9)D1,D2,D3
```

```
         WRITE(2,10)
         R = 0
         IR = 0
 4       X(R) = XN + R*H
         IF(X(R) .LT. 0.1)THEN
           TERM1 = (D3*X(R)**5)/(40.0*(D1**2))
           TERM2 = (D2*X(R)**4)/(12.0*D1)
           TERM3 = (D3*X(R)**3)/(12.0*(D1**2))
           TERM4 = (D3*(X(R)**2))/(4.0*D1)
           NUM1 = 120.0*(D1**2)
           NUM2 = (7.0*D3)+(10.0*D1*D2)
           NUM3 = 30.0*D1*D3
           NUM  = NUM1+NUM2+NUM3
           DEN = 120.0*(D1**2)
           TERM5 = (NUM/DEN)*X(R)
           Q(R) = TERM1-TERM2-TERM3-TERM4+TERM5
           WRITE(2,18)X(R),Q(R)
           X1(R) = X(R)
           R = R+1
           IR = R
           GO TO 4
         END IF
 12      R = IR-1
         C(R,R) = -4.0*D1
         C(R,R+1) = 2.0*D1-(H/X1(R))*(X1(R)-X1(R)**3-D1)
         D(R) = -2.0*H*H*(D2*(X1(R)**2)+D3)-
      *         ((2.0*D1+(H/X1(R))*(X1(R)-X1(R)**3-D1))*Q(R))
         DO 13 I = R+1,N-1
          X1(I) = X1(R)+I*H
          C(I,I-1) = 2.0*D1+(H/X1(I))*(X1(I)-X1(I)**3-D1)
          C(I,I) = -4.0*D1
          C(I,I+1) = 2.0*D1-(H/X1(I))*(X1(I)-X1(I)**3-D1)
          D(I) = -2.0*H*H*(D2*X1(R)**2+D3)
 13      CONTINUE
         X1(N) = X1(N-1)+ H
         C(N,N-1) = 2.0*D1+(H/X1(N))*(X1(N)-X1(N)**3-D1)
         C(N,N) = -4.0*D1
         D(N) = -2.0*H*H*(D2*X1(N)**2+D3)-
      *         ((2.0*D1-(H/X1(N))*(X1(N)-X1(N)**3-D1))*QF)
C   DECOMPOSE MATRIX C INTO LOWER AND UPPER TRIANGULAR
MATRICES(I.E.(A=LU)
         AL(R,R) = C(R,R)
         AU(R,R+1) = C(R,R+1)/AL(R,R)
         AU(R,R) = 1.0
         DO 15 I = R+1,N-1
           AL(I,I-1) = C(I,I-1)
           AL(I,I) = C(I,I)-AL(I,I-1)*AU(I-1,I)
           AU(I,I) = 1.0
           AU(I,I+1) = C(I,I+1)/AL(I,I)
 15      CONTINUE
         AL(N,N-1) = C(N,N-1)
         AL(N,N) = C(N,N)-AL(N,N-1)*AU(N-1,N)
         AU(N,N) = 1.0
C   SOLVE THE SYSTEM LZ = D
         Z(R) = D(R)/AL(R,R)
         DO 17 I = R+1,N
           Z(I) = (D(I)-AL(I,I-1)*Z(I-1))/AL(I,I)
 17      CONTINUE
```

```
C   SOLVE THE SYSTEM UQ1 = Z
        Q1(N) = Z(N)
        DO 20 I = N-1,R,-1
          Q1(I) = Z(I)-AU(I,I+1)*Q1(I+1)
 20       CONTINUE
        DO 22 I = IR,N,1
          X1(I) = X1(I-1)+H
          WRITE(2,18)X1(I),Q1(I)
 22     CONTINUE
          WRITE(2,18)XF,QF
 7    FORMAT(3(F4.2))
 9    FORMAT(/,3X,'D1 =',F4.2,3X,'D2 =',F4.2,3X,'D3 = ',F4.2)
 10   FORMAT(3X,'          X                 Q  ')
 18   FORMAT(3X,F6.4,8X,F9.6)
 5    CONTINUE
      STOP
      END
```

Program 3

```
C     PRODRAM TO SOLVE STEADY CASE PROBLEM
C     (1.0-X*X)DY/DX = A/X(D/DX(X DY/DX)) - B*Y
C     USING SHOOTING METHOD
      REAL M1,KE1,KE2,KE3,SET,MI,MP,M2,KEP1,
     1 KEP2,KEP3,KEP4,NUM1,NUM2,NUM3
      OPEN(UNIT=4,FILE='SHOT1.IN')
      OPEN(UNIT=5,FILE='SHOT1.OUT')
      XN = 0.0
      XF = 1.0
      YN = 0.0
      YF = 1.0
      N = 50
      N1 = N-1
      H=(XF-XN)/FLOAT(N+1)
  6   READ(4,7)A,B
      J = 0
      K = 1
 7    FORMAT(2(F4.2))
      WRITE(5,9)A, B
 9    FORMAT(//,3X,'A=',F4.2,3X,'B=',F4.2)
      WRITE(5,10)
 10   FORMAT(5X,'  X               Y  ')
 11   J = J+1
      READ(4,12)M1, M2
 12   FORMAT(2(F4.2))
 15   Y = YN
      WRITE(5,13)M1
 13   FORMAT(//,5X,'M1 = ',F6.4)
      YP = M1
      X  = XN
      DO 20 I = 1,N + 1
        X = XN + (I-1)*H
        HA = H/A
        IF(X .LT. 0.1)THEN
          KE1  = H * YP
          KEP1 = HA*B*Y
```

```
         KE2  = H*(YP*KEP1/2.0)
         KEP2 = HA*B*(Y+KE1/2.0)
         KE3  = H*(YP+KEP2/2.0)
         KEP3 = HA*B*(Y+KE2/2.0)
         KE4  = H*(YP+KEP3)
         KEP4 = HA*B*(Y+KE3)
         ELSE
           XE1  = X*X*X
           XE2  = X+H/2.0
           XE3  = X+H
           XE4  = XE2*XE2*XE2
           XE5  = XE3*XE3*XE3
           NUM1 = (X-XE1-A)/X
           NUM2 = (XE2-XE4-A)/XE2
           NUM3 = (XE3-XE5-A)/XE3
           KE1  = H*YP
           KEP1 = HA*(NUM1*YP+B*Y)
           KE2  = H*(YP+KEP1/2.0)
           KEP2 = HA*(NUM2*(YP+KEP1/2.0)+B*(Y+KE1/2.0))
           KE3  = H*(YP+KEP2/2.0)
           KEP3 = HA*(NUM2*(YP+KEP2/2.0)+B*(Y+KE2/2.0))
           KE4  = H*(YP+KEP3)
           KEP4 = HA*(NUM3*(YP+YEP3)+B*(Y+KE3))
       END IF
       Y = Y+(KE1+2.0*KE2+2.0*KE3+KE4)/6.0
       YP = YP+(KEP1+2.0*KEP2+2.0*KEP3+KEP4)/6.0
       WRITE(5,35)X, Y
       X =XN + I*H
20   CONTINUE
      ERRF = Y-YF
      IF(ABS(ERRF) .LE. 0.0000001) THEN
          GO TO 29
         ELSE
          IF(J .GE. 2) THEN
            MP = M1
            M1 = M1 - (ERRF * (M1 - MI))/(ERRF - ERRI)
            MI = MP
            J = J + 1
            ERRI = ERRF
            GO TO 15
           ELSE
             ERRI = ERRF
             MI = M1
             M1 = M2
             J = J + 1
             GO TO 15
          END IF
     END IF
29   K = K+1
     IF(K .GE. 4) THEN
      GO TO 33
      ELSE
       GO TO 6
     END IF
35   FORMAT(3X,F7.5,5X,F7.5)
33   STOP
     END
```

Program 4

```
C     PROGRAM TO SOLVE STEADY CASE PROBLEM
C     (1.0-X*X)DQ/DX = D1/X(D/DX(XDQ/DX)) + D2*X*X + D3
C     USING SHOOTING METHOD
      REAL X1,X2,X3,X4,X5,X,Y,YP,M1,M2,YN,YF,H,K1,K2,K3,
     1 K4,KP1,KP2,KP3,KP4,ERRF,ERRI,MI,MP,NUM1,NUM2,NUM3
      OPEN(UNIT=4,FILE='SHOT2.IN')
      OPEN(UNIT=5,FILE='SHOT2.OUT')
      XN = 0.0
      XF = 1.0
      YN = 0.0
      YF = 1.0
      N = 50
      N1 = N-1
      H=(XF-XN)/FLOAT(N)
 6    READ(4,7)D1,D2,D3
      J = 0
       K = 1
 7    FORMAT(3(F4.2))
      WRITE(5,9)D1,D2,D3
 9    FORMAT(//,3X,'D1=',F4.2,3X,'D2=',F4.2,3X,'D3=',F4.2)
C      WRITE(5,10)
 10   FORMAT(5X,'  X               Y   ')
 11   J = J+1
      READ(4,12) M1,M2
 12   FORMAT(2(F4.2))
 15   Y = YN
      WRITE(5,13)M1
 13   FORMAT(//,5X,'M1 = ',F6.4)
      WRITE(5,10)
      YP = M1
      X  = XN
      DO 20 I = 1,N+1
        HD = -H/D1
        X1 = X*X*X
        X2 = X + H/2.0
        X3 = X + H
        X4 = X2*X2*X2
        X5 = X3*X3*X3
        X6 = (X+H/2.0)*(X+H/2.0)
        X7 = (X+H)*(X+H)
        IF(X .LE. 0.1)THEN
          NUM1 = X-X1-D1
          NUM2 = X2-X4-D1
          NUM3 = X3-X5-D1
          K1   = H*YP
          KP1  = HD*(NUM1*D3+D2*X*X+D3)
          K2   = H*(YP+KP1/2.0)
          KP2  = HD*(NUM2*D3+D2*X6+D3)
          K3   = H*(YP+KP2/2.0)
          KP3  = HD*(NUM2*D3+D2*X6+D3)
          K4   = H*(YP+KP3)
          KP4  = HD*(NUM3*D3+D2*X7+D3)
          ELSE
            NUM1 = (X-X1-D1)/X
            NUM2 = (X2-X4-D1)/X2
```

```
           NUM3 = (X3-X5-D1)/X3
           K1   = H*YP
           KP1  = HD*(NUM1*YP-D2*X*X-D3)
           K2   = H*(YP+KP1/2.0)
           KP2  = HD*(NUM2*(YP+KP1/2.0)-D2*X6-D3)


           K3   = H*(YP+KP2/2.0)
           KP3  = HD*(NUM2*(YP+KP2/2.0)-D2*X6-D3)
           K4   = H*(YP+KP3)
           KP4  = HD*(NUM3*(YP+YP3)-D2*X7-D3)
       END IF
       Y  = Y+(K1+2.0*K2+2.0*K3+K4)/6.0
       YP = YP+(KP1+2.0*KP2+2.0*KP3+KP4)/6.0
       WRITE(5,35) X,Y
       X  = XN + I*H
20     CONTINUE
        ERRF = Y-YF
        IF(ABS(ERRF) .LE. 0.0001) THEN
          GO TO 29
          ELSE
            IF(J .GE. 2) THEN
              MP   = M1
              M1   = M1 - (ERRF * (M1 - MI))/(ERRF - ERRI)
              MI   = MP
              J    = J + 1
              ERRI = ERRF
              GO TO 15
             ELSE
               ERRI = ERRF
               MI   = M1
               M1   = M2
               J    = J + 1
                GO TO 15
            END IF
        END IF
29      K = K + 1
        IF(K .GE. 4) THEN
          GO TO 33
          ELSE
           GO TO 6
        END IF
35     FORMAT(3X,F7.5,5X,F7.5)
33     STOP
       END
```