

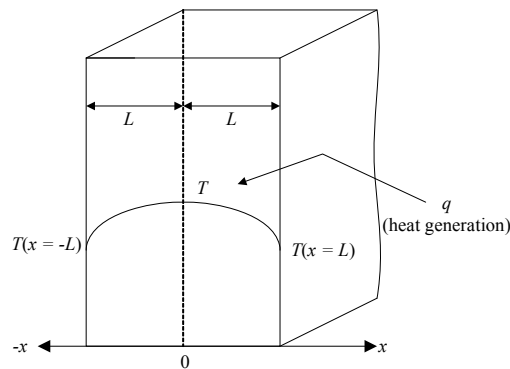
# DIFFERENTIAL EQUATIONS, PROBLEM

# BOUNDARY VALUE

## 5.1 INTRODUCTION

As it has been noted in the previous chapter, boundary value problems (BVP) for ordinary differential equations have boundary conditions specified at more than one point of the independent variable. Boundary value problems are quite common in chemical engineering applications. Problems where the independent variable is the position rather than time are often described in terms of ordinary differential equations with conditions imposed at more than one point. Examples of the BVP include the steady-state distribution of temperature and concentration in plug flow systems.

Consider the problem of temperature distribution inside a slab solid (with thermal conductivity  $k$ ) heated by a constant uniform heat source  $q$  (Figure 5.1). Assuming that the heat flows only on the axial direction  $x$ ,. Using the microscopic energy balance, the steady state energy equation is:



**Figure 0-1: Slab heated with constant source**

$$\frac{d^2T}{dx^2} = \frac{q}{k} \quad (5.1)$$

The  $x$ -axis is chosen so that the distance  $x$  is bounded by  $-L$  and  $L$  (See Figure 5.1). Various boundary conditions for this problem are possible:

- The surface temperatures at  $x = -L$  and  $x = L$  can be constant,

$$T(-L) = T_w \quad (5.2)$$

$$T(L) = T_w \quad (5.3)$$

- The temperature at one side, say  $x = -L$  can be constant while the surface on the other side is insulated. The flux  $\phi$ , given by Fourier law, is thus zero at this end. In this case the boundary conditions are:

$$T(-L) = T_w \quad (5.4)$$

$$-k \frac{\partial T}{\partial x} \Big|_{x=L} = 0 \quad (5.5)$$

- The temperature at one side, say  $x = -L$  can be constant while a cooling mechanism exists at the other end  $x = L$ . The boundary conditions at this end can be expressed by equating the flux, given by Fourier law, with the heat absorbed by the cooling mechanism

$$T(-L) = T_w \quad (5.6)$$

$$\phi \Big|_{x=L} = -k \frac{\partial T}{\partial x} \Big|_{x=L} = h(T - T_\infty) \quad (5.7)$$

where  $h$  is the heat transfer coefficient.

Our standard form for a boundary value problem is the second order ordinary differential equation of the form:

$$x''(t) = f(t, x, x') \quad t \in [a, b] \quad (5.8)$$

The associated boundary conditions at  $t = a$  and  $t = b$  have the general form

$$g_1(x, x') = 0 \text{ at } t = a \quad (5.9)$$

and

$$g_2(x, x') = 0 \text{ at } t = b \quad (5.10)$$

In most chemical engineering problems using transport equations (mass, energy and momentum),  $g_1$  and  $g_2$  have much simpler forms. Let the quantity ( $S$ ) designates the concentration ( $C$ ), temperature ( $T$ ) or velocity ( $v$ ) and let ( $\phi$ ) designates the flux of mass, energy or momentum. Some of the most common boundary conditions are the following:

1. The value of ( $S$ ) at the boundary is specified and it has a constant value  $S_0$ ,

$$S_{\text{boundary}} = S_0 \quad (5.11)$$

These boundaries of type 1 are constant-value boundaries. Examples of these type of boundaries include constant concentration  $C = C_0$ , constant surface temperature  $T = T_0$  and constant velocity  $v = v_0$ .

2. The values of  $S$  at both sides of the boundary are equal or related functionally

$$S_{\text{left}} = S_{\text{right}} \quad (5.12)$$

Or

$$S_{\text{left}} = F(S_{\text{right}}) \quad (5.13)$$

Boundaries of type 2 are constant-value boundaries that are continuous across the boundary

3. The flux at the boundary has a constant value  $\phi_0$ :

$$\phi_{\text{boundary}} = \phi_0 \quad (5.14)$$

Boundaries of type 3 represent cases where flux is specified at a boundary. Examples of this boundary include the case where the rate of a reaction at a boundary surface is specified, It includes the examples of thermal insulating surface where the heat flux  $\phi = -kdT/dx$  is zero. It also includes the example where the momentum flux at a gas-liquid interface is assumed zero.

4. The flux at a boundary is continuous, i.e., the flux of both sides of the boundary are equal.

$$\phi_{\text{left}} = \phi_{\text{right}} \quad (5.15)$$

Boundaries of type 4 represent cases of continuation of flux (heat, mass and momentum) across a boundary.

5. The flux at the boundary is empirically determined

$$\phi_{\text{boundary}} = f(S) \quad (5.16)$$

Boundaries of type 5 represent cases of mass, heat and momentum transport across a boundary layer .The mass or heat flux for instance from a bulk fluid in motion to a solid surface with temperature  $T_s$  and concentration  $c^*$  can be described by heat or mass transfer coefficient,  $k$  and  $h$

$$N_A = k(c - c^*) \quad (5.17)$$

$$q_A = h(T - T_s) \quad (5.18)$$

## 5.2 NUMERICAL METHODS FOR THE SOLUTION OF BVP PROBLEMS

To appreciate the difference between a boundary value problem (BVP) and an initial value problem (IVP) consider the following BVP in standard form and with constant-boundary conditions

$$\begin{aligned}x''(t) &= f(t,x,x'), & t \in [a,b] \\x(a) &= \alpha, & x(b) = \beta\end{aligned}\tag{5.19}$$

and let consider the following IVP

$$\begin{aligned}x''(t) &= f(t,x,x') & t \in [a,b] \\x(a) &= \alpha & x'(a) = \gamma\end{aligned}\tag{5.20}$$

Note that the differential equation and the first boundary condition are the same for both problems. Only the second boundary condition is different. The important distinction between the initial value problem (Eq 5.20) and the boundary value problem (Eq 5.19) is that in the first case the integration starts from the initial value and continues towards the ending point. In the BVP case a solution that satisfies the boundary condition at the starting point will not necessarily satisfy the boundary condition at the ending point. For this reason the methods used for initial value problems can not be used directly for the solution of BVP. In the following two major methods that are used for the solution of the BVP are presented.

- Shooting methods
- Finite difference methods

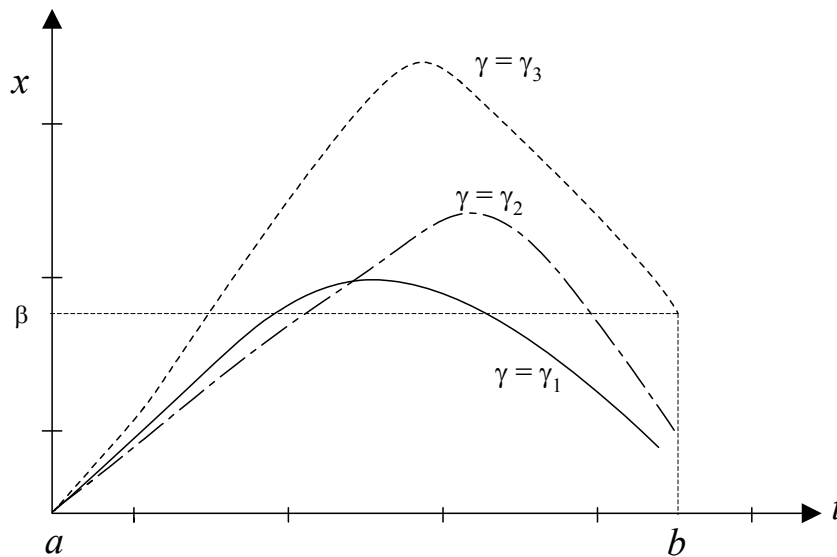
### 5.2.1 Shooting Method

Shooting method consists in converting the BVP into an iterative initial value problem. Consider the BVP with constant-boundary conditions (Eq. 5.19). Consider also the initial value problem (Eq 5.20), associated with the BVP problem where  $\gamma$  is a guessed value of  $x'(a)$ . This initial value problem can be integrated using any method presented in earlier chapter to obtain a solution  $x(t)$ . This solution will be the solution of the BVP (Eq 5.19) if it satisfies the condition  $x(b) = \beta$ . This is unlikely since the value  $\gamma$

was chosen arbitrarily. However, if the guessed value of  $\gamma = x'(a)$  is updated in a rational way, the procedure can be repeated until convergence. This process is called shooting as it can be seen graphically in Figure (5.2). The problem of updating the guessed value  $\gamma$  in a suitable way is the subject of the following section.

The solution  $x(t)$  of the initial-value problem, (Eq. 5.20), depends explicitly on the value of  $\gamma$  and, thus, it will be denoted  $x_\gamma(t)$ . The objective of the shooting method is to select  $\gamma$  so that

$$x_\gamma(b) = \beta \tag{5.21}$$



**Figure 0-2: Graphical interpretation of the shooting method;  $\gamma=\gamma_1$ : the first shot;  $\gamma=\gamma_2$ : the second shot;  $\gamma=\gamma_3$ : the final shot**

This is equivalent to solving the following algebraic equation for  $\gamma$

$$\phi(\gamma) := x_\gamma(b) - \beta = 0 \tag{5.22}$$

The algebraic equation can be solved by any of the methods studied earlier in Chapter 3. Newton-Raphson iteration, for instance, applied to Eq 5.22 yields the following iteration scheme:

$$\gamma_{n+1} = \gamma_n - \frac{\phi(\gamma_n)}{\phi'(\gamma_n)} \quad (5.23)$$

That is

$$\gamma_{n+1} = \gamma_n - \frac{x_{\gamma_n}(b) - \beta}{\phi'(\gamma_n)} \quad (5.24)$$

This iteration scheme will update the value of  $\gamma$  provided that the derivative term  $\phi'(\gamma_n)$  is known. In the following section, a way to determine this term is shown .

Let us differentiate partially with respect to  $\gamma$  both sides of Eq(5.20). This yields:

$$\frac{dx_{\gamma}''}{d\gamma} = \frac{df}{dt} \frac{dt}{d\gamma} + \frac{df}{dx_{\gamma}} \frac{dx_{\gamma}}{d\gamma} + \frac{df}{dx'_{\gamma}} \frac{dx'_{\gamma}}{d\gamma} \quad (5.25)$$

The same is done for the boundary conditions of Eq. (5.20) to yield

$$\frac{dx_{\gamma}(a)}{d\gamma} = 0 \quad (5.26)$$

$$\frac{dx'_{\gamma}(a)}{d\gamma} = 1 \quad (5.27)$$

Introducing the auxiliary variable  $v = dx_{\gamma}/d\gamma$  and noting that  $dt/d\gamma = 0$ , Eq. (5.25) becomes:

$$v'' = \frac{df}{dx_{\gamma}} v + \frac{df}{dx'_{\gamma}} v' \quad (5.28)$$

with the following initial conditions

$$v(a) = 0 \quad v'(a) = 1 \quad (5.29)$$

This is an initial value problem and it is called *the first variational equation*. The solution of this initial value problem will yield the value of  $v(b)$ . The term  $\phi'(\gamma)$  can then be computed since

$$v(b) = \frac{dx_\gamma(b)}{d\gamma} = \phi'(\gamma) \quad (5.30)$$

Knowing the value of the derivative  $\phi'(\gamma)$ , the iterations of the Newton-Raphson method (Eq. 5.24) can proceed until the convergence. As it can be seen, the shooting method is best applied to cases of constant-value boundary conditions. The shooting method can be costly in computational effort since each value of the function  $\phi(\gamma)$  is obtained by solving two initial-value problems (Eq 5.20) and (Eq. 5.28).

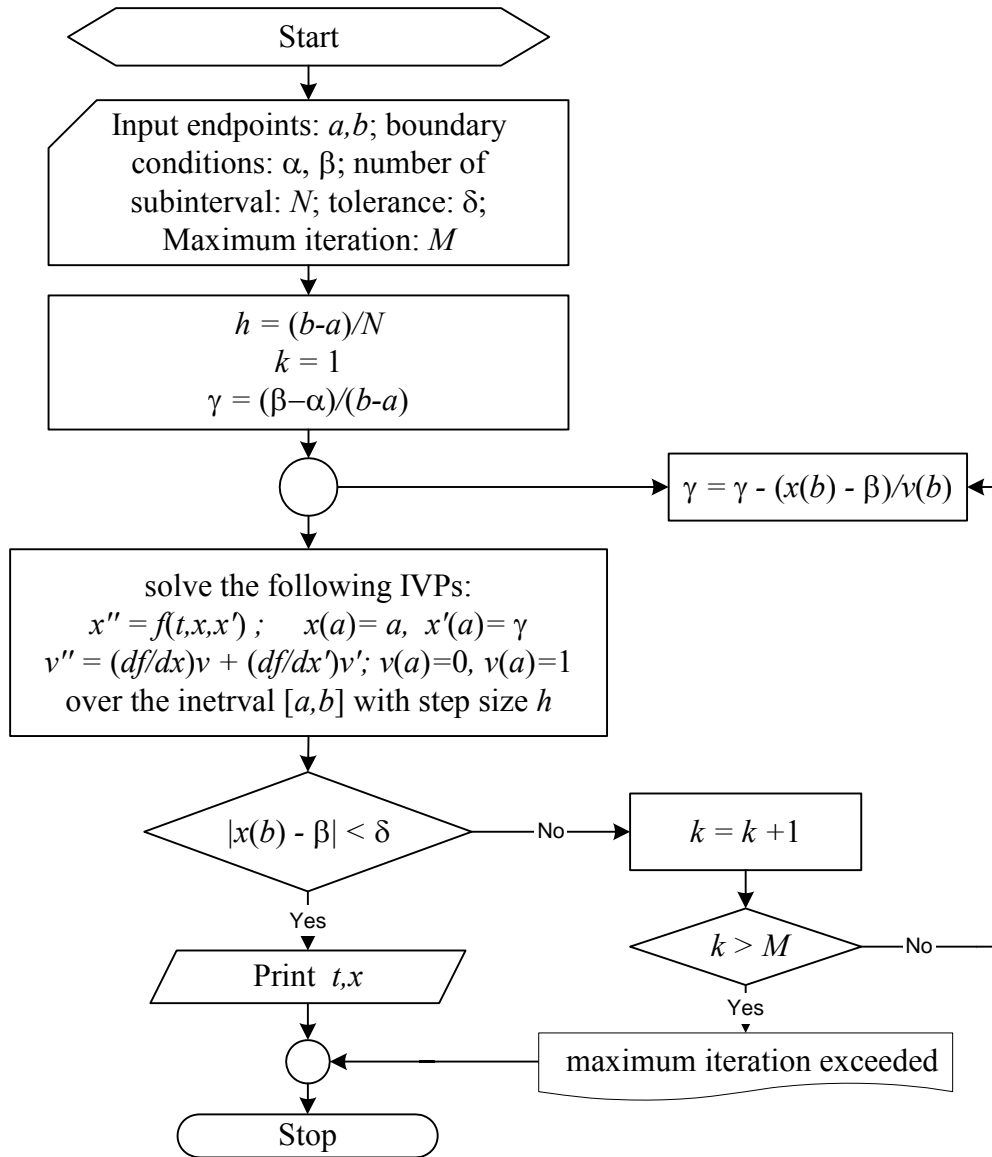
### **Organigram 5.1: The Shooting Method**

The shooting algorithm for solving BVP problem of the form of Eq (5.19) is shown in Figure (5.3). The algorithm terminates if one of the following criteria is met:

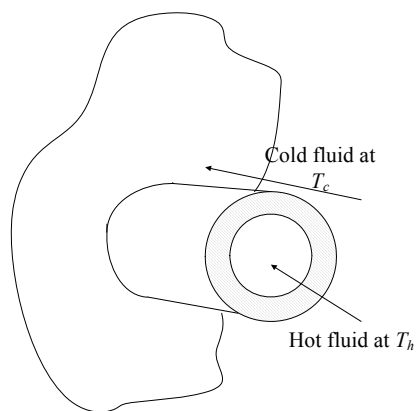
- The solution at the boundary point is within specific tolerance of the boundary value, i.e.,  $|x_\gamma(b) - \beta| \leq \delta$
- The number of iterations exceeded the maximum value.

### **Example 5.1: Temperature distribution in a pipe wall**

Consider the problem of finding the steady state temperature distribution in a wall of pipe where a hot liquid flowing inside the pipe is heating a cold liquid flowing outside of the pipe. The inner  $r_i$  and outer  $r_o$  surfaces of the pipe are assumed to be at constant temperatures  $T_h$  and  $T_c$ . The heat flux is assumed to occur radially. Performing a steady state microscopic energy balance on an element of the pipe as shown by figure 5.4, the temperature on the wall of the pipe satisfies the following differential equation



**Figure 0-3: Shooting method for boundary value problem**



**Figure 0-4: Temperature distribution in a pipe wall**

$$\frac{d}{dr}\left(r \frac{dT}{dr}\right) = 0 \quad (5.31)$$

which is equivalent to

$$\frac{d^2T}{dr^2} + \frac{1}{r} \frac{dT}{dr} = 0 \quad (5.32)$$

with the boundary conditions

$$T(r_i) = T_h \quad (5.33)$$

$$T(r_o) = T_c \quad (5.34)$$

Let  $r_i = 0.05$  cm,  $r_o = 0.1$  cm,  $T_h = 300$  °C and  $T_c = 100$  °C. The analytical solution of Eq. (5.32) can be easily obtained (by making change of variable  $w = T$ ) to yield:

$$T(r) = C_1 \ln(r) + C_2 \quad (5.35)$$

The constants  $C_1$  and  $C_2$  are determined by imposing the boundary conditions of Eqs.5.33-5.34 to yield

$$T(r) = \frac{T_h - T_c}{\ln\left(\frac{r_i}{r_o}\right)} \ln\left(\frac{r}{r_i}\right) + T_h \quad (5.36)$$

For the numerical solution of the problem, we apply the steps of the algorithm. At each iteration (k) the following IVP is solved:

$$T''(r) = -1/r T'(r) \quad (5.37)$$

With

$$\begin{aligned} T(r_i) &= T_h \\ T'(r_i) &= \gamma_k \end{aligned} \quad (5.38)$$

Because of the simplicity of the problem, this IVP can also be solved analytically to yield

$$T_{\gamma}(r) = \gamma_k r_i \ln\left(\frac{r}{r_i}\right) + T_h \quad (5.39)$$

The second IVP is constructed as follows: Since  $f(r, T, T') = -1/r T'(r)$ , it follows that  $\partial f / \partial T = 0$  and  $\partial f / \partial T' = -1/r$ . Thus Eq. (5.28) becomes

$$v'' = \frac{\partial f}{\partial T} v + \frac{\partial f}{\partial v'} v' = -\frac{1}{r} v' \quad (5.40)$$

with

$$v(r_i) = 0 \text{ and } v'(r_i) = 1 \quad (5.41)$$

In this simple example the second IVP can also be solved analytically again to yield

$$v(r) = r_i \ln\left(\frac{r}{r_i}\right) \quad (5.42)$$

The algorithm goes then as follows:

*Step 1:* Assume a value for  $\gamma_1$ , e.g.,  $\gamma_1 = 1$ , The IVP (Eq. 5.37-5.38) is solved (Eq. 5.39) to yield  $T(0.1) = 300.034$ , a value which is far from the given boundary condition 100.0

*Step 2:* The second IVP (Eq. 5.40-5.41) is solved (Eq. 5.42) to yield  $v(0.1) = 0.03465$

*Step 3:* The value of  $\gamma_1$  is updated by Eq. (5.24) to yield

$$\gamma_2 = \gamma_1 - \frac{T(0.1) - \beta}{v(0.1)} \quad (5.43)$$

and upon substitution yields

$$\gamma_2 = -5771.987 \quad (5.44)$$

Steps 1 through 3 are repeated. The algorithm converges in three iterations as shown in Table (5.1).

**Table 0-1: Shooting method iterations for example 5.1**

<i>Iteration k</i>	$\gamma_k$	$T(0.1)_{calc.}$	$ boundary - T(0.1)_{calc.} $
1	1	300.0340	200.034
2	-5771.9871	99.9580	0.042
3	-5770.7742	100.0002	0.0002

### 5.2.2 Finite-Difference Methods

Another approach to the solution of the boundary value problem consists in using finite difference approximations of the derivatives to represent the governing differential equations and the equations for the boundary conditions. This results in a set of linear or nonlinear algebraic equations. Taylor series expansions are used to develop difference approximations for the first and second derivatives of a function  $x(t)$ .

- A forward finite difference approximation of first order is given by:

$$x'(t_i) = \frac{x(t_{i+1}) - x(t_i)}{\Delta t} \quad (5.45)$$

$$x''(t_i) = \frac{x(t_i) - 2x(t_{i+1}) + x(t_{i+2}))}{\Delta t^2} \quad (5.46)$$

with

$$\Delta t = t_{i+1} - t_i \quad (5.47)$$

- A back finite difference approximation of first order is:

$$x'(t_i) = \frac{x(t_i) - x(t_{i-1})}{\Delta t} \quad (5.48)$$

$$x''(t_i) = \frac{x(t_i) - 2x(t_{i-1}) + x(t_{i-2}))}{\Delta t^2} \quad (5.49)$$

- A central finite difference yields

$$x'(t_i) = \frac{x(t_{i+1}) - x(t_{i-1}))}{2\Delta t} \quad (5.50)$$

$$x''(t_i) = \frac{x(t_{i+1}) - 2x(t_i) + x(t_{i-1}))}{\Delta t^2} \quad (5.51)$$

A better approximation is to use a second order approximation for the first and the second derivatives.

- A forward finite difference approximation of the second order is:

$$x'(t_i) = \frac{-3x(t_i) + 4x(t_{i+1}) - x(t_{i+2}))}{2\Delta t} \quad (5.52)$$

$$x''(t_i) = \frac{2x(t_i) - 5x(t_{i+1}) + 4x(t_{i+2}) - x(t_{i+3}))}{\Delta t^2} \quad (5.53)$$

- A back finite difference of the second order is:

$$x'(t_i) = \frac{-3x(t_i) - 4x(t_{i-1}) + x(t_{i-2}))}{2\Delta t} \quad (5.54)$$

$$x''(t_i) = \frac{2x(t_i) - 5x(t_{i-1}) + 4x(t_{i-2}) - x(t_{i+3}))}{\Delta t^2} \quad (5.55)$$

For considerations of simplicity and stability, the first order central finite difference scheme is preferred. In the first step of the implementation of the finite-difference method the interval  $[a, b]$  is divided into  $(N+1)$  equal subintervals whose endpoints are the mesh points  $t_i = a + ih$  for  $i = 0, 1, \dots, N+1$  where  $h = (b - a)/(N+1)$ .

Let the approximate value of  $x(t_i)$  be denoted by  $x_i$  and define the boundary conditions of Eq. (5.19) by

$$x_0 = \alpha, \quad x_{N+1} = \beta \quad (5.56)$$

Applying the central-difference formula to equation (5.19) yields:

$$-\frac{x_{i+1} - 2x_i + x_{i-1}}{h^2} + f(t_i, x_i, \frac{x_{i+1} - x_{i-1}}{2h}) = 0, \quad i = 1, 2, \dots, N \quad (5.57)$$

Writing this equation for each  $i = 1, 2, \dots, N$ , then the following  $N \times N$  nonlinear system is obtained :

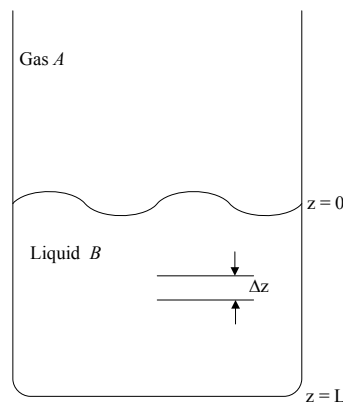
$$\begin{cases} 2x_1 - x_2 + h^2 f(t_1, x_1, \frac{x_2 - \alpha}{2h}) - \alpha = 0 \\ -x_1 + 2x_2 - x_3 + h^2 f(t_2, x_2, \frac{x_3 - x_1}{2h}) = 0 \\ \vdots \\ -x_{N-2} + 2x_{N-1} - x_N + h^2 f(t_{N-1}, x_{N-1}, \frac{x_N - x_{N-2}}{2h}) = 0 \\ -x_{N-1} + 2x_N + h^2 f(t_N, x_N, \frac{\beta - x_{N-1}}{2h}) - \beta = 0 \end{cases} \quad (5.58)$$

The unknowns are  $x_1, x_2, \dots, x_N$ . The Newton's method can be used for the solutions of this system of nonlinear algebraic equations. However the number of equations can be large and so is the number of initial guesses. A safe but slow procedure is to start with

a 2x2 system. Solve it and then use its results as initial guesses for the 4x4 system and so on.

**Example 5.2: Diffusion and a second order reaction**

Consider the problem of diffusion and a homogenous reaction of second order of a component  $A$  in a dilute liquid phase of component  $B$  (Figure 5.4). The liquid phase is stagnant, thus, mass is only transported by diffusion and not by bulk flow. The steady state equation for the diffusion of  $A$  in the  $z$ -direction can be obtained by directly applying the component balance equation to yield:



**Figure 0-5: Diffusion into a stagnant fluid**

$$\frac{dc_A^2}{dz^2} = \frac{k}{D_{AB}} c_A^2 \tag{5.56}$$

with boundary conditions

$$\begin{aligned} c_A &= c_{A1} \text{ at } z = 0 \\ c_A &= c_{A2} \text{ at } z = L \end{aligned} \tag{5.57}$$

This is a non linear BVP with

$$f(z, C_A, \frac{dC_A}{dz}) = \frac{k}{D_{AB}} C_A^2 \tag{5.58}$$

Applying the finite difference method to Eq. (5.58), the following system of nonlinear algebraic equations is obtained:

$$\left\{ \begin{array}{l} 2C_{A1} - C_{A2} + h^2 \frac{k}{D_{AB}} C_{A1}^2 - \alpha = 0 \\ -C_{A1} + 2C_{A2} - C_{A3} + h^2 \frac{k}{D_{AB}} C_{A2}^2 = 0 \\ \vdots \\ -C_{A(N-2)} + 2C_{A(N-1)} - C_{AN} + h^2 \frac{k}{D_{AB}} C_{A(N-1)}^2 = 0 \\ -C_{A(N-1)} + 2C_{AN} + h^2 \frac{k}{D_{AB}} C_{AN}^2 - \beta = 0 \end{array} \right. \quad (5.59)$$

Solution of this system is listed in Table (5.2), for  $k=10$ ,  $D_{AB} = 1.5 \times 10^{-5}$ ,  $N = 9$ ,  $L=0.0005$ ,  $C_{A1}=0.1$  and  $C_{A2}=0.02$ .

**Table 0-2: Non-linear finite difference method iterations for example 5.2**

$Z$	$C_A$
0.0000	0.10000
0.0005	0.08856
0.0010	0.07843
0.0015	0.06933
0.0020	0.06103
0.0025	0.05335
0.0030	0.04615
0.0035	0.03930
0.0040	0.03271
0.0045	0.02629
0.0050	0.02000

### 5.2.3 Finite-Difference Methods for Linear Problems

For a linear BVP the function  $f$  is linear in  $x$  and  $x'$  and can be represented by the general form

$$f(t,x,x') = w(t)x'(t) + v(t)x(t) + u(t) \quad (5.60)$$

Applying the finite-difference method (Eq. 5.57) results in the following equations

$$\frac{2x_i - x_{i+1} - x_{i-1}}{h^2} + w(x_i) \frac{x_{i+1} - x_{i-1}}{2h} + v(x_i)x_i = -u(x_i) \quad (i = 1, 2, \dots, N) \quad (5.61)$$

with the boundary conditions

$$x_0 = \alpha, \quad x_{N+1} = \beta \quad (5.62)$$

Equations (5.61) are rearranged to become:

$$(-1 - h/2w(x_i))x_{i-1} + (2 + (h^2v(x_i)))x_i + (-1 + h/2w(x_i))x_{i+1} = h^2u(x_i) \quad (5.63)$$

The resulting system of equations is a tridiagonal system of the form

$$Ax=b \quad (5.64)$$

With

$$A = \begin{bmatrix} 2 + h^2v(x_1) & -1 + \frac{h}{2}w(x_1) & 0 & \dots & 0 \\ -1 - \frac{h}{2}w(x_2) & 2 + h^2v(x_2) & -1 + \frac{h}{2}w(x_2) & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & -1 + \frac{h}{2}w(x_{n-1}) \\ 0 & \dots & 0 & -1 - \frac{h}{2}w(x_n) & 2 + h^2v(x_n) \end{bmatrix} \quad (5.65)$$

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} \quad (5.66)$$

and

$$b = \begin{bmatrix} -h^2 u(x_1) + (1 + \frac{h}{2} w(x_1)) x_0 \\ -h^2 u(x_2) \\ \vdots \\ -h^2 u(x_{n-1}) \\ -h^2 u(x_n) + (1 - \frac{h}{2} w(x_n)) x_{n+1} \end{bmatrix} \quad (5.67)$$

The tridiagonal system can be solved by the methods presented in Chapter 2. It can be proved that if  $v(x) \geq 0$  on the interval  $[a, b]$ , then the linear system has a unique solution provided that

$$h < \frac{L}{2} \quad (5.68)$$

Where

$$L = \max_{a \leq x \leq b} |w(x)| \quad (5.69)$$

### Example 5.3: Diffusion and first order reaction

Consider the previous example of diffusion and homogenous reaction. Assume the reaction is of first order. Then the mass balance equation is

$$\frac{dc_A^2}{dz^2} = \frac{k}{D_{AB}} c_A \quad (5.70)$$

with boundary conditions

$$\begin{aligned} c_A &= c_{A1} \text{ at } z = 0 \\ c_A &= c_{A2} \text{ at } z = L \end{aligned} \quad (5.71)$$

This linear BVP can be solved analytically to yield

$$c_A = \frac{c_{A2} \sinh\left(\sqrt{\frac{k}{D_{AB}}}z\right) + c_{A1} \sinh\left(\sqrt{\frac{k}{D_{AB}}}(L-z)\right)}{\sinh\left(\sqrt{\frac{k}{D_{AB}}}L\right)} \quad (5.72)$$

The equation (Eq. 5.70-5.71) can be solved using the algorithm described in the previous section. The differential equation is put under the form of Eq(5.60)

$$\frac{dc_A^2}{dz^2} = w(z)\frac{dc_A}{dz} + v(z)c_A + u(z) \quad (5.73)$$

where  $w(z) = 0$ ,  $v(z) = k/D_{AB}$  and  $u(z) = 0$ . The matrix  $A$  and vector  $b$  take in this case the simpler form of

$$A = \begin{bmatrix} 2 + h^2 \frac{k}{D_{AB}} & -1 & 0 & \dots & 0 \\ -1 & 2 + h^2 \frac{k}{D_{AB}} & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & -1 \\ 0 & \dots & 0 & -1 & 2 + h^2 \frac{k}{D_{AB}} \end{bmatrix} \quad (5.74)$$

$$b = \begin{bmatrix} x_0 \\ 0 \\ \vdots \\ 0 \\ x_{n+1} \end{bmatrix} \quad (5.75)$$

This can be solved using a linear system routine. Table (5.3) shows the results for the same values as in the previous example. The comparison between the numerical solution and the actual solution is also provided.

**Table 0-3: Linear finite difference method iterations for example 5.3**

$z$	$(C_A)_{\text{calc.}}$	$(C_A)_{\text{Anal.}}$	$ (C_A)_{\text{calc.}} - (C_A)_{\text{Anal.}} $
0.0000	0.10000	0.10000	0.00000
0.0005	0.06693	0.06674	0.00019
0.0010	0.04501	0.04476	0.00025
0.0015	0.03060	0.03034	0.00026
0.0020	0.02129	0.02105	0.00023
0.0025	0.01553	0.01532	0.00020
0.0030	0.01236	0.01218	0.00017
0.0035	0.01124	0.01110	0.00014
0.0040	0.01201	0.01190	0.00011
0.0045	0.01477	0.01470	0.00006
0.0050	0.02000	0.02000	0.00000

### 5.3 HANDLING DIFFERENT TYPES OF BOUNDARY CONDITIONS

The finite difference method is useful in handling different types of boundary value besides the constant-value boundary problems discussed before. Consider, for instance, the boundary value problem of type 2 applied to the example of Figure (5.1). For this type of BVP we have:

$$q_x = -k \frac{dT}{dx} = 0 \quad \text{at} \quad x = -L \quad (5.76)$$

Expressing the derivative as a second-order forward finite difference equation (Eq. 5.52) and denoting  $T(x=-L)=T_0$ , leads to

$$-k \left( \frac{-3T_0 + 4T_1 - T_2}{2\Delta x} \right) = 0 \quad (5.77)$$

This equation results in the following expression for the boundary point  $T_0$

$$T_0 = (4T_1 - T_2)/3 \quad (5.78)$$

The boundary condition (Type 5) can also be expressed in the same way. For this case, assuming a cooling mechanism, the boundary condition is given by

$$q = -k \frac{dT}{dx} = h(T_0 - T_\infty) \quad \text{at} \quad x = -L \quad (5.79)$$

Using again Eq.(5.52) to approximate the derivative yields the following equation for  $T_0$

$$T_0 = \frac{4T_1 - T_2 - \frac{2h\Delta x}{k} T_\infty}{3 - \frac{2h\Delta x}{k}} \quad (5.80)$$

These expressions for the boundary condition can be, therefore, integrated in the finite-difference scheme.

#### 5.4 OTHER SOLUTION TECHNIQUES

The shooting method discussed in this chapter can be improved by dividing the original interval  $[a,b]$  into smaller intervals and solve the BVP into pieces. This technique is called multiple shootings techniques.

Let recast the BVP in its standard form

$$x''(t) = f(t, x(t), x'(t)) \quad (5.81)$$

$$x(a) = \alpha \quad \text{and} \quad x(b) = \beta \quad (5.82)$$

Let divide the interval  $[a,b]$  into two subintervals  $[a,c]$  and  $[c,b]$ .

Let us define two IVP's as follows

IVP#1 defined for  $a \leq t \leq c$

$$x_1''(t) = f(t, x_1(t), x_1'(t)) \quad (5.83)$$

$$x_1(a) = \alpha \quad \text{and} \quad x_1(b) = \gamma_1 \quad (5.84)$$

IVP#2 defined for  $c \leq t \leq b$

$$x_2''(t) = f(t, x_2(t), x_2'(t)) \quad (5.85)$$

$$x_2(a) = \alpha \quad \text{and} \quad x_2(b) = \gamma_1 \quad (5.86)$$

The solution of the BVP is composed of the solutions of two IVPs in this way

$$x(t) = \begin{cases} x_1(t) & a \leq t \leq c \\ x_2(t) & c \leq t \leq b \end{cases} \quad (5.87)$$

To ensure continuity of both  $x(t)$  and  $x_2(t)$  at  $t = c$  we require then that

$$\begin{cases} x_1(c) = x_2(c) \\ x_1'(c) = x_2'(c) \end{cases} \quad (5.88)$$

These are two nonlinear algebraic equations for which the unknowns are  $\gamma_1$  and  $\gamma_2$ . They can be solved by Newton method. This procedure can be extended by dividing the original interval  $[a, b]$  many subintervals. Check references [56] for some details.

### 5.5 IMSL ROUTINES

Some IMSL routines to solve ODE-BVP are as follows:

<b>Routine</b>	<b>Features</b>
BVPFD	Solve a system of differential equations with boundary conditions at two points, based on finite difference method.
BVPMS	Solve a system of differential equations with boundary conditions at two points, using a multiple-shooting method.

