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INTRODUCTION TO NUMERICAL METHODS IN CHEMICAL ENGINEERING

$$\frac{dC_j}{dx} = 0,\ j = A,B,C,D$$

$$A+B \xrightarrow{k_1} C$$

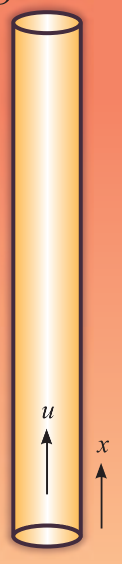
$$B+C \xrightarrow{k_2} D$$

$$D\frac{d^2C_A}{dx^2} - u\frac{dC_A}{dx} - k_1C_AC_B = 0$$

$$D\frac{d^2C_B}{dx^2} - u\frac{dC_B}{dx} - k_1C_AC_B - k_2C_BC_C = 0$$

$$D\frac{d^2C_C}{dx^2} - u\frac{dC_C}{dx} + k_1C_AC_B - k_2C_BC_C = 0$$

$$D\frac{d^2C_D}{dx^2} - u\frac{dC_D}{dx} + k_2C_BC_C = 0$$



$$D\frac{d^2C_i}{dx^2} = D\frac{C_{i+1} - 2C_i + C_{i-1}}{x^2}$$

$$u\frac{dC_i}{dx} = u\frac{C_i - C_{i-1}}{x}$$

$$uC_{j,in} = uC_j - D\frac{dC_j}{dx}$$

Pradeep Ahuja

Introduction to
Numerical Methods in Chemical Engineering

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To
my Mother
Kamla Ahuja
and
All my Students

Contents

Preface

This book entitled *Introduction to Numerical Methods in Chemical Engineering* is designed for a course on Numerical Methods in Chemical Engineering and the associated Computer Applications Laboratory course offered as part of undergraduate programmes in chemical engineering. Also, for the courses on Chemical Engineering Mathematics or Applied Mathematics in Chemical Engineering, this book can be used for the numerical solution aspects of chemical engineering problems.

The computer programs are listed in C++. The author assumes that the students are at least moderately familiar with the C++ language. In addition to the computer examples, there are several much shorter examples appearing throughout the text. These shorter examples usually illustrate a particular point by means of hand calculations. 33 sample programs in C++, arranged by chapter, are presented in the Appendix and about 148 exercises (including chapter-end exercises with answers) are solved. The numerical solutions of algebraic (linear and nonlinear) and differential (ordinary and partial) equations encountered in subjects such as General Chemical Engineering, Chemical Engineering Thermodynamics, Chemical Reaction Engineering, and Heat Transfer are discussed using introductory but efficient numerical methods. The students can also use the programs and build up their own programs to solve specific Design Project problems in chemical engineering. The author feels that before using chemical engineering software (which use advanced numerical methods), the students should have some hands-on experience on small programs and introductory numerical methods as well as their usage in chemical engineering. The experience gained from using these programs helps in the development of basic understanding of numerical methods and confidence in handling numerical techniques. Some problems whose analytical solutions are available are also solved and the numerical and analytical results are compared. By changing various parameters the student can find out the conditions under which correct results are obtained as well as those under which correct results are not obtained.

For the solution of linear algebraic equations, the tridiagonal matrix algorithm (TDMA), Gauss elimination, and Gauss–Seidel methods are discussed. For the solution of nonlinear equation(s), Newton's method is discussed and for initial value problems in ordinary differential equations the Runge–Kutta fourth order method is discussed. For the solution of boundary value problems the Finite Difference method is used. The Finite Difference method is a simple yet very powerful tool for the solution of boundary value problems, but requires a structured grid. It is the basis for the Advanced Finite Volume and Finite Element methods. In this book the following Finite Difference methods are discussed: Central Difference Scheme (CDS) for discretization of diffusion terms, Upwind Difference Scheme (UDS) for discretization of convection terms, Forward in Time and Central in Space (FTCS) difference scheme for discretization of the one-dimensional transient conduction/diffusion equation adopting the Explicit, Implicit and Crank–Nicolson methods, and the Alternating Direction Implicit (ADI) method for the numerical solution of two-dimensional steady and transient heat conduction.

Chapter 1 contains an introduction to the numerical solution of a system of linear algebraic equations. The numerical solution of a single as well as two (simultaneous) nonlinear algebraic equation(s) and the calculation of pressure drop in a pipe under nonlaminar conditions, minimum fluidization velocity and terminal velocity are all discussed in Chapter 2. The numerical solution of computer-oriented problems in Chemical Engineering Thermodynamics is discussed in Chapter 3. Various problems in vapour–liquid and chemical reaction equilibria are discussed. Vapour–liquid equilibrium calculations are done for systems following Raoult's law, modified Raoult's law, Gamma–Phi approach and Phi–Phi approach. The numerical solution of initial value problems in ordinary differential equations, along with the initial value problems in double pipe heat exchanger and stirred tanks with coil heater, and in batch, stirred and plug flow reactors are discussed in Chapter 4. The numerical solution of boundary value problems in ordinary differential equations and convection–diffusion problems are discussed in Chapters 5 and 6 respectively. The numerical solution of tubular reactors with axial dispersion and simultaneous chemical reaction and diffusion in spherical catalyst pellets are discussed in Chapters 7 and 8 respectively. The numerical solution of one-dimensional transient heat conduction/diffusion is discussed in Chapter 9, and that of two-dimensional steady and transient heat conduction is discussed in Chapter 10. The Finite Difference method is used for the solution of boundary value problems in Chapters 5–10.

The books referred to by the author for the preparation of class notes, on which the contents of this book are principally based, is given in the Bibliography. The author expresses his thanks to all those authors, too numerous to acknowledge individually. The author is indebted to all his colleagues for many positive interactions and discussions and also to all his friends for their constant appreciation, invaluable advice and encouragement. The author would like to thank the Department of Science and Technology, New Delhi, for providing partial financial support and Prof. S.N. Upadhyay, Director, Institute of Technology, Banaras Hindu University, Varanasi, for providing the major part of the funds for the purchase of Fluent 25 Users Perpetual License software in the Department of Chemical Engineering and Technology, which proved immensely useful in the process of writing this book.

The author is also thankful to all his B.Tech. Chemical Engineering students who have taken up the Computer Laboratory course and various computational and other chemical engineering courses so enthusiastically and helped in many ways in developing this work. Their inquisitive questions and enthusiasm towards the numerical solution of algebraic and differential equations in chemical engineering inspired the author to create a work of this kind, in which the numerical solution of various equations in chemical engineering is provided under one cover. Feedback from students has critically guided the development and evolution of the book, taking it from a handwritten collection of notes to the present form. The book is thus dedicated to all his students. The author is grateful to Mr. Sudarshan Das, Mr. Abhjit Baroi and Mr. Pankaj Manohar of PHI Learning for their cooperation.

The author is indebted and extremely thankful to his mother Kamla Ahuja, to his father A.D. Ahuja, and his wife Preeti Bala Ahuja, for their care, help and understanding, as without their support this work could never have been completed.

In spite of all efforts to the contrary, some errors might have crept into the book. The author would be rather grateful if such errors are pointed out. He would also very much appreciate any criticism or suggestion for improvement of the contents of the book from the readers.

Pradeep Ahuja

Chapter 1

Linear Algebraic Equations

A system of linear algebraic equations can be solved by direct or iterative methods. The direct methods discussed in this chapter are the TriDiagonal Matrix Algorithm (TDMA) and Gauss Elimination methods, and the iterative method discussed is the Gauss-Seidel method.

A tridiagonal or block tridiagonal set of linear algebraic equations is formed during the discretization of ordinary and partial differential equations. The discretization of differential equations using the finite difference method is discussed in Chapters 5 to 10. All types of linear algebraic equations can be solved using the Gauss Elimination method, but if the equations are of tridiagonal type, then TDMA is very fast as compared to the Gauss Elimination method. The Gauss–Seidel method is used for the solution of two-dimensional steady heat transfer, which is discussed in Chapter 10.

1.1 Tridiagonal Matrix Algorithm (TDMA)

TDMA is a direct method. Consider the following tridiagonal set of linear algebraic equations:

$$\begin{bmatrix} b_1 & c_1 & & & & & & & \\ a_2 & b_2 & c_2 & & & & & & \\ & a_3 & b_3 & c_3 & & & & & \\ & & a_4 & b_4 & c_4 & & & & \\ & & & \cdots & \cdots & \cdots & & & \\ & & & & \cdots & \cdots & \cdots & & \\ & & & & & \cdots & \cdots & \cdots & \\ & & & & & & a_{N-1} & b_{N-1} & c_{N-1} \\ & & & & & & & a_N & b_N \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \cdots \\ \cdots \\ \cdots \\ x_{N-1} \\ x_N \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ \cdots \\ \cdots \\ \cdots \\ d_{N-1} \\ d_N \end{bmatrix} \tag{1.1}$$

N linear algebraic equations can be written in the form $Ax = d$. The matrix A contains elements on the diagonal (b_i, $i = 1$ to N), sub-diagonal (a_i, $i = 2$ to N), and super-diagonal (c_i, $i = 1$ to $N - 1$), and thus is called a *tridiagonal matrix*. The algorithm for the solution of this sort of linear algebraic equation is called the TriDiagonal Matrix Algorithm or the Thomas algorithm.

The equations are of the type

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = d_i \qquad \text{where } a_1 = 0,\ c_N = 0 \tag{1.2}$$

Let us write the solution at x_i in terms of x_{i+1} as

$$x_i = \gamma_i - \frac{c_i x_{i+1}}{\beta_i} \tag{1.3a}$$

Then we can also write

$$x_{i-1} = \gamma_{i-1} - \frac{c_{i-1} x_i}{\beta_{i-1}} \tag{1.3b}$$

where β_i and γ_i are obtained by substituting Eq. (1.3b) into Eq. (1.2). Thus we get

$$a_i \left(\gamma_{i-1} - \frac{c_{i-1} x_i}{\beta_{i-1}} \right) + b_i x_i + c_i x_{i+1} = d_i$$

The above equation can be written as

$$\left(b_i - \frac{a_i c_{i-1}}{\beta_{i-1}} \right) x_i = d_i - a_i \gamma_{i-1} - c_i x_{i+1}$$

Thus

$$x_i = \frac{d_i - a_i \gamma_{i-1}}{\left(b_i - \dfrac{a_i c_{i-1}}{\beta_{i-1}} \right)} - \frac{c_i}{\left(b_i - \dfrac{a_i c_{i-1}}{\beta_{i-1}} \right)} x_{i+1}$$

Comparing with Eq. (1.3a), we get

$$\beta_i = b_i - \frac{a_i c_{i-1}}{\beta_{i-1}} \tag{1.4}$$

$$\gamma_i = \frac{d_i - a_i \gamma_{i-1}}{\left(b_i - \dfrac{a_i c_{i-1}}{\beta_{i-1}} \right)} = \frac{d_i - a_i \gamma_{i-1}}{\beta_i} \tag{1.5}$$

$a_1 = 0$; therefore

$$\beta_1 = b_1 \tag{1.6}$$

and

$$\gamma_1 = \frac{d_1}{b_1} \tag{1.7}$$

The algorithm for the solution of a tridiagonal set of linear algebraic equations is given below:

(i) Calculate β_i and γ_i for $i = 1$ to N.

(ii) Calculate $x_N = \gamma_N - \dfrac{c_N x_{N+1}}{\beta_N}$. Since $c_N = 0$, therefore $x_N = \gamma_N$.

(iii) Calculate $x_i = \gamma_i - \dfrac{c_i x_{i+1}}{\beta_i}$ for $i = N-1, N-2, \ldots, 3, 2, 1$.

EXAMPLE 1.1 Solve the following set of linear algebraic equations using TDMA

$$\begin{bmatrix} -2 & 1 & & & & & \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & 1 & -2 & 1 & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & 1 \\ & & & & & 1 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{bmatrix} = \begin{bmatrix} -240 \\ -40 \\ -40 \\ -40 \\ -40 \\ -40 \\ -60 \end{bmatrix}$$

Solution We have

$$\beta_1 = b_1 = -2$$

$$\gamma_1 = \frac{d_1}{b_1} = \frac{-240}{-2} = 120$$

$$\beta_2 = b_2 - \frac{a_2 c_1}{\beta_1} = -2 - \frac{1}{-2} = -\frac{3}{2}$$

$$\gamma_2 = \frac{d_2 - a_2\gamma_1}{\beta_2} = \frac{-40 - 1 \times 120}{-\frac{3}{2}} = \frac{-160}{-\frac{3}{2}} = \frac{320}{3}$$

$$\beta_3 = b_3 - \frac{a_3 c_2}{\beta_2} = -2 - \frac{1}{-\frac{3}{2}} = -\frac{4}{3}$$

$$\gamma_3 = \frac{d_3 - a_3\gamma_2}{\beta_3} = \frac{-40 - \frac{320}{3}}{-\frac{4}{3}} = 110$$

$$\beta_4 = b_4 - \frac{a_4 c_3}{\beta_3} = -2 - \frac{1}{-\frac{4}{3}} = -\frac{5}{4}$$

$$\gamma_4 = \frac{d_4 - a_4\gamma_3}{\beta_4} = \frac{-40 - 110}{-\frac{5}{4}} = 120$$

$$\beta_5 = b_5 - \frac{a_5 c_4}{\beta_4} = -2 - \frac{1}{-\frac{5}{4}} = -\frac{6}{5}$$

$$\gamma_5 = \frac{d_5 - a_5\gamma_4}{\beta_5} = \frac{-40 - 120}{-\frac{6}{5}} = \frac{400}{3}$$

$$\beta_6 = b_6 - \frac{a_6 c_5}{\beta_5} = -2 - \frac{1}{-\frac{6}{5}} = -\frac{7}{6}$$

$$\gamma_6 = \frac{d_6 - a_6\gamma_5}{\beta_6} = \frac{-40 - \frac{400}{3}}{-\frac{7}{6}} = \frac{1040}{7}$$

$$\beta_7 = b_7 - \frac{a_7 c_6}{\beta_6} = -2 - \frac{1}{-\frac{7}{6}} = -\frac{8}{7}$$

$$\gamma_7 = \frac{d_7 - a_7\gamma_6}{\beta_7} = \frac{-60 - \frac{1040}{7}}{-\frac{8}{7}} = \frac{365}{2}$$

Now let us compute the solution starting with x_7.

$$x_7 = \gamma_7 = \frac{730}{4} = 182.5$$

$$x_6 = \gamma_6 - \frac{c_6 x_7}{\beta_6} = \frac{1040}{7} + \frac{730}{4} \times \frac{6}{7} = 305$$

$$x_5 = \gamma_5 - \frac{c_5 x_6}{\beta_5} = \frac{400}{3} + \frac{305 \times 5}{6} = 387.5$$

$$x_4 = \gamma_4 - \frac{c_4 x_5}{\beta_4} = 120 + \frac{387.5 \times 4}{5} = 430$$

$$x_3 = \gamma_3 - \frac{c_3 x_4}{\beta_3} = 110 + \frac{430 \times 3}{4} = 432.5$$

$$x_2 = \gamma_2 - \frac{c_2 x_3}{\beta_2} = \frac{320}{3} + \frac{432.5}{1.5} = 395$$

$$x_1 = \gamma_1 - \frac{c_1 x_2}{\beta_1} = 120 + \frac{395}{2} = 317.5$$

Program 1.1 uses the above method for solving the tridiagonal system of linear algebraic equations and is given in the Appendix.

1.2 Gauss Elimination Method

Gauss Elimination is a direct method. The Gauss Elimination method reduces the system of equations to an upper triangular system which can then be solved by back substitution. Consider the following system of three linear algebraic equations:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = d_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = d_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = d_3$$

The augmented matrix is

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & d_1 \\ a_{21} & a_{22} & a_{23} & d_2 \\ a_{31} & a_{32} & a_{33} & d_3 \end{array}\right] \tag{1.8}$$

Take the element a_{11} as the pivot. Multiply the first equation by $-\frac{a_{21}}{a_{11}}$ and then add it to the second equation, which then becomes

$$\left(a_{22} - \frac{a_{21}a_{12}}{a_{11}}\right)x_2 + \left(a_{23} - \frac{a_{21}a_{13}}{a_{11}}\right)x_3 = d_2 - \frac{a_{21}}{a_{11}}d_1$$

Thus x_1 is eliminated from the second equation. Similarly, eliminate x_1 from the third equation by multiplying the first equation by $-\frac{a_{31}}{a_{11}}$ and then adding it to the third equation. At the end of the first stage the augmented matrix becomes

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & d_1 \\ 0 & a'_{22} & a'_{23} & d'_2 \\ 0 & a'_{32} & a'_{33} & d'_3 \end{array}\right] \tag{1.9}$$

Now take the element a'_{22} as the new pivot. Multiply the second equation by $-\frac{a'_{32}}{a'_{22}}$ and then add it to the third equation. Thus x_2 is eliminated from the third equation. At the end of the second stage the augmented matrix becomes

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & d_1 \\ 0 & a'_{22} & a'_{23} & d'_2 \\ 0 & 0 & a''_{33} & d''_3 \end{array}\right] \tag{1.10}$$

The values of x_1, x_2, and x_3 can be obtained by back substitution. The pivots should be chosen in such a way that they are nonzero. Rows can be exchanged so that the pivot is nonzero. This procedure is called *partial pivoting*.

EXAMPLE 1.2 Solve the following set of three linear algebraic equations in three variables using the Gauss Elimination method:

$$10x_1 + x_2 + 2x_3 = 44$$

$$2x_1 + 10x_2 + x_3 = 51$$

$$x_1 + 2x_2 + 10x_3 = 61$$

Solution The augmented matrix is

$$\left[\begin{array}{ccc|c} 10 & 1 & 2 & 44 \\ 2 & 10 & 1 & 51 \\ 1 & 2 & 10 & 61 \end{array}\right]$$

Multiply the first equation by $-\frac{2}{10}$ and then add it to the second equation. We get

$$\left[\begin{array}{ccc|c} 10 & 1 & 2 & 44 \\ 0 & 9.8 & 0.6 & 42.2 \\ 1 & 2 & 10 & 61 \end{array}\right]$$

Multiply the first equation by $-\frac{1}{10}$ and then add it to the third equation. We get

$$\left[\begin{array}{ccc|c} 10 & 1 & 2 & 44 \\ 0 & 9.8 & 0.6 & 42.2 \\ 0 & 1.9 & 9.8 & 56.6 \end{array}\right]$$

This completes the first stage. Multiply the second equation by $-\frac{1.9}{9.8}$ and then add it to the third equation. We get

$$\left[\begin{array}{ccc|c} 10 & 1 & 2 & 44 \\ 0 & 9.8 & 0.6 & 42.2 \\ 0 & 0 & 9.68367 & 48.418367 \end{array}\right]$$

From the previous equation we get

$$9.68367x_3 = 48.418367$$

Solving, we get $x_3 = 5$.
From the second equation we get

$$9.8x_2 + 0.6x_3 = 42.2$$

Thus $$x_2 = \frac{42.2 - 0.6 \times 5}{9.8} = 4$$

From the first equation we get

$$10x_1 + x_2 + 2x_3 = 44$$

Thus $$x_1 = \frac{44 - 4 - 2 \times 5}{10} = 3.$$

Program 1.2 uses the Gauss elimination method for solving a system of linear algebraic equations and is given in the Appendix.

EXAMPLE 1.3 Solve the following set of three linear algebraic equations in three variables using the Gauss Elimination method:

$$\begin{aligned} 3x_1 + x_2 - 2x_3 &= 9 \\ -x_1 + 4x_2 - 3x_3 &= -8 \\ x_1 - x_2 + 4x_3 &= 1 \end{aligned}$$

Solution The augmented matrix is

$$\left[\begin{array}{rrr|r} 3 & 1 & -2 & 9 \\ -1 & 4 & -3 & -8 \\ 1 & -1 & 4 & 1 \end{array}\right]$$

Multiply the first equation by $\frac{1}{3}$ and then add it to the second equation. We get

$$\left[\begin{array}{lrr|r} 3 & 1 & -2 & 9 \\ 0 & 4.3333 & -3.6667 & -5 \\ 1 & -1 & 4 & 1 \end{array}\right]$$

Multiply the first equation by $-\frac{1}{3}$ and then add it to the third equation. We get

$$\left[\begin{array}{lrr|r} 3 & 1 & -2 & 9 \\ 0 & 4.3333 & -3.6667 & -5 \\ 0 & -1.3333 & 4.6667 & -2 \end{array}\right]$$

Multiply the second equation by 0.3076923 and then add it to the third equation. We get

$$\left[\begin{array}{lrr|r} 3 & 1 & -2 & 9 \\ 0 & 4.3333 & -3.6667 & -5 \\ 0 & 0 & 3.5384 & -3.5384 \end{array}\right]$$

From the previous equation, we get

$$3.5384x_3 = -3.5384$$

Solving, we get $x_3 = -1$.

From the second equation, we get

$$4.3333x_2 - 3.6667x_3 = -5$$

Thus
$$x_2 = \frac{-5 - 3.6667}{4.3333} = -2.$$

From the first equation, we get

$$3x_1 + x_2 - 2x_3 = 9$$

Thus
$$x_1 = \frac{9 + 2 - 2}{3} = 3.$$

EXAMPLE 1.4 Benzene (1), toluene (2), styrene (3), and xylene (4) are to be separated in the sequence of distillation columns shown in Fig. 1.1. Determine molar flow rates of streams D_1, B_1, D_2, and B_2. The composition of the feed stream and the streams D_1, B_1, D_2, and B_2 is shown in the figure. Also, determine the molar flow rates and compositions of streams B and D. The molar flow rate of the feed stream is 70 mol/min.

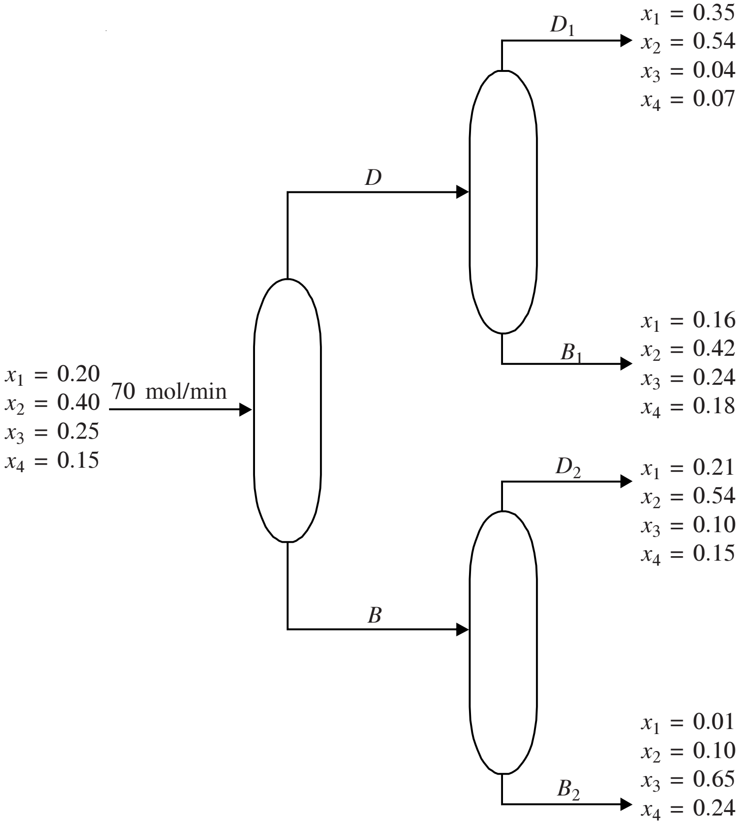

Fig. 1.1 Schematic diagram for Example 1.4.

Solution The material balance equations for benzene (1), toluene (2), styrene (3), and xylene (4) are given below.

$$0.20 \times 70 = 0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2$$

$$0.40 \times 70 = 0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2$$

$$0.25 \times 70 = 0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2$$

$$0.15 \times 70 = 0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2$$

The above equations can be written as

$$\begin{bmatrix} 0.35 & 0.16 & 0.21 & 0.01 \\ 0.54 & 0.42 & 0.54 & 0.10 \\ 0.04 & 0.24 & 0.10 & 0.65 \\ 0.07 & 0.18 & 0.15 & 0.24 \end{bmatrix} \begin{bmatrix} D_1 \\ B_1 \\ D_2 \\ B_2 \end{bmatrix} = \begin{bmatrix} 14 \\ 28 \\ 17.5 \\ 10.5 \end{bmatrix}$$

Solving by using the Gauss Elimination method, we get

D_1 = 26.25 mol/min

B_1 = 17.5 mol/min

D_2 = 8.75 mol/min

B_2 = 17.5 mol/min.

$B = D_2 + B_2 = 26.25$ mol/min.

The composition of stream B is given by

$$x_{1B} = \frac{0.21D_2 + 0.01B_2}{B} = 0.0767$$

$$x_{2B} = \frac{0.54D_2 + 0.10B_2}{B} = 0.2467$$

$$x_{3B} = \frac{0.10D_2 + 0.65B_2}{B} = 0.4667$$

$$x_{4B} = \frac{0.15D_2 + 0.24B_2}{B} = 0.21$$

$D = D_1 + B_1 = 43.75$ mol/min.

The composition of stream D is given by

$$x_{1D} = \frac{0.35D_1 + 0.16B_1}{D} = 0.274$$

$$x_{2D} = \frac{0.54D_1 + 0.42B_1}{D} = 0.492$$

$$x_{3D} = \frac{0.04D_1 + 0.24B_1}{D} = 0.120$$

$$x_{4D} = \frac{0.07D_1 + 0.18B_1}{D} = 0.114$$

Now, let us check the solution obtained. $B + D$ is 70 mol/min, which is correct. Now, let us back-calculate the feed composition.

$$\frac{Dx_{1D} + Bx_{1B}}{70} = 0.2$$

$$\frac{Dx_{2D} + Bx_{2B}}{70} = 0.4$$

$$\frac{Dx_{3D} + Bx_{3B}}{70} = 0.25$$

$$\frac{Dx_{4D} + Bx_{4B}}{70} = 0.15$$

1.3 Gauss–Seidel Method

Gauss–Seidel is an iterative method. Consider a system of N linear algebraic equations in N variables. The first equation can be written with variable x_1 on the left hand side and the rest of the terms on the right hand side. Similarly, the second equation can be written with variable x_2 on the left hand side and the rest of the terms on the right hand side, and so on. Now we can assume some values of the variables, and compute the new value of x_1 from the first equation and the new value of x_2 from the second equation, and so on. In the Gauss–Seidel method, when the new value of x_2 is computed from the second equation then on the right hand side for the variable x_1 the updated value calculated from the first equation, is used. Similarly, when the new value of x_3 is calculated from the third equation, then on the right hand side for the variables x_1 and x_2 the updated values calculated from the first and second equations are used. By doing this a higher convergence rate is obtained. So the latest values of the variables are always used.

In the above explanation it is assumed that in the first equation the coefficient of x_1 is the highest among the coefficients of the other variables, and in the second equation the coefficient of x_2 is the highest among the coefficients of the other variables. All the equations have many variables in them. A survey of the given system of linear algebraic equations is made and that variable which has the highest coefficient is kept on the left hand side. The variable whose coefficient is the largest is used to express that variable in terms of the others.

The Gauss–Seidel method has the disadvantage of not always converging to a solution and of sometimes converging very slowly. However, this method will always converge to a solution when the magnitude of the coefficient on the left hand side is sufficiently dominant with respect to the magnitudes of the other coefficients in that equation.

EXAMPLE 1.5 Solve the following set of three linear algebraic equations in three variables using the Gauss–Seidel method:

$$10x_1 + x_2 + 2x_3 = 44$$

$$2x_1 + 10x_2 + x_3 = 51$$

$$x_1 + 2x_2 + 10x_3 = 61$$

Solution It can be seen that the coefficient of x_1 is dominant in the first equation, and the coefficient of x_2 and x_3 are dominant in the second and third equations, respectively. Thus

$$x_1^{n+1} = \frac{44 - x_2^n - 2x_3^n}{10}$$

$$x_2^{n+1} = \frac{51 - 2x_1^{n+1} - x_3^n}{10}$$

$$x_3^{n+1} = \frac{61 - x_1^{n+1} - 2x_2^{n+1}}{10}$$

Let us assume $x_2 = 0$, $x_3 = 0$. The initial values used will not affect the converged solution, but will affect the number of iterations required for convergence.

First Iteration:

$$x_1 = \frac{44 - 0 - 0}{10} = 4.4$$

$$x_2 = \frac{51 - 2 \times 4.4 - 0}{10} = 4.22$$

$$x_3 = \frac{61 - 4.4 - 2 \times 4.22}{10} = 4.816$$

Second Iteration:

$$x_1 = \frac{44 - 4.22 - 2 \times 4.816}{10} = 3.0148$$

$$x_2 = \frac{51 - 2 \times 3.0148 - 4.816}{10} = 4.01544$$

$$x_3 = \frac{61 - 3.0148 - 2 \times 4.01544}{10} = 4.995432$$

The final converged solution is $x_1 = 3$, $x_2 = 4$, $x_3 = 5$.

Program 1.3 uses the Gauss–Seidel method for solving a system of linear algebraic equations and is given in the Appendix.

EXAMPLE 1.6 Solve the following set of three linear algebraic equations in three variables using the Gauss–Seidel method:

$$3x_1 + x_2 - 2x_3 = 9$$

$$-x_1 + 4x_2 - 3x_3 = -8$$

$$x_1 - x_2 + 4x_3 = 1$$

Solution Let us write the first, second and third equations in the form

$$x_1^{n+1} = \frac{9 - x_2^n + 2x_3^n}{3}$$

$$x_2^{n+1} = \frac{-8 + x_1^{n+1} + 3x_3^n}{4}$$

$$x_3^{n+1} = \frac{1 - x_1^{n+1} + x_2^{n+1}}{4}$$

Let us assume $x_2 = 0$, $x_3 = 0$.

First Iteration:

$$x_1 = \frac{9 - 0 + 0}{3} = 3$$

$$x_2 = \frac{-8 + 3 + 0}{4} = -1.25$$

$$x_3 = \frac{1 - 3 - 1.25}{4} = -0.8125$$

Second Iteration:

$$x_1 = \frac{9 + 1.25 - 2 \times 0.8125}{3} = 2.875$$

$$x_2 = \frac{-8 + 2.875 - 3 \times 0.8125}{4} = -1.8906$$

$$x_3 = \frac{1 - 2.875 - 1.8906}{4} = -0.9414$$

The final converged solution is $x_1 = 3$, $x_2 = -2$, $x_3 = -1$.

Exercises

1.1 Solve the following using TDMA:

$$\begin{bmatrix} 2 & -1 & & & & & & \\ -1 & 2 & -1 & & & & & \\ & -1 & 2 & -1 & & & & \\ & & -1 & 2 & -1 & & & \\ & & & -1 & 2 & -1 & & \\ & & & & -1 & 2 & -1 & \\ & & & & & -1 & 2 & -1 \\ & & & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{bmatrix} = \begin{bmatrix} 100 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 200 \end{bmatrix}$$

(**Ans:** $x_1 = 111.11$, $x_2 = 122.22$, $x_3 = 133.33$, $x_4 = 144.44$, $x_5 = 155.55$, $x_6 = 166.66$, $x_7 = 177.77$, $x_8 = 188.88$)

1.2 Solve the following linear algebraic equations using the Gauss elimination method:

$$\begin{aligned} 2x_1 - x_2 &= 100 \\ -x_1 + 2x_2 - x_3 &= 0 \\ -x_2 + 2x_3 - x_4 &= 0 \\ -x_3 + 2x_4 - x_5 &= 0 \\ -x_4 + 2x_5 - x_6 &= 0 \\ -x_5 + 2x_6 - x_7 &= 0 \\ -x_6 + 2x_7 - x_8 &= 0 \\ -x_7 + 2x_8 &= 200 \end{aligned}$$

Note that the augmented matrix for this problem is

$$\left[\begin{array}{rrrrrrrr|r} 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 100 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & 200 \end{array}\right]$$

(**Ans:** $x_1 = 111.11$, $x_2 = 122.22$, $x_3 = 133.33$, $x_4 = 144.44$, $x_5 = 155.55$, $x_6 = 166.66$, $x_7 = 177.77$, $x_8 = 188.88$)

1.3 Solve the equations in Problem 1.2 using the Gauss–Seidel method.
Note that the equations are expressed in the form

$$x_1^{n+1} = \frac{100 + x_2^n}{2}$$

$$x_2^{n+1} = \frac{x_1^{n+1} + x_3^n}{2}$$

$$x_3^{n+1} = \frac{x_2^{n+1} + x_4^n}{2}$$

$$x_4^{n+1} = \frac{x_3^{n+1} + x_5^n}{2}$$

$$x_5^{n+1} = \frac{x_4^{n+1} + x_6^n}{2}$$

$$x_6^{n+1} = \frac{x_5^{n+1} + x_7^n}{2}$$

$$x_7^{n+1} = \frac{x_6^{n+1} + x_8^n}{2}$$

$$x_8^{n+1} = \frac{200 + x_7^{n+1}}{2}$$

(**Ans:** $x_1 = 111.11$, $x_2 = 122.22$, $x_3 = 133.33$, $x_4 = 144.44$, $x_5 = 155.55$, $x_6 = 166.66$, $x_7 = 177.77$, $x_8 = 188.88$)

1.4 Solve the following linear algebraic equations using the Gauss elimination method:

$$4x_1 + 2x_2 + x_3 = 11$$

$$-x_1 + 2x_2 = 3$$

$$2x_1 + x_2 + 4x_3 = 16$$

Note that the augmented matrix is

$$\left[\begin{array}{rrr|r} 4 & 2 & 1 & 11 \\ -1 & 2 & 0 & 3 \\ 2 & 1 & 4 & 16 \end{array}\right]$$

(**Ans:** $x_1 = 1$, $x_2 = 2$, $x_3 = 3$)

1.5 Solve the linear algebraic equations of Problem 1.4 using the Gauss–Seidel method: Note that for Gauss–Seidel to converge the equations are expressed in the form

$$x_1^{n+1} = \frac{11 - 2x_2^n - x_3^n}{4}$$

$$x_2^{n+1} = \frac{3 + x_1^{n+1}}{2}$$

$$x_3^{n+1} = \frac{16 - 2x_1^{n+1} - x_2^{n+1}}{4}$$

(**Ans:** $x_1 = 1$, $x_2 = 2$, $x_3 = 3$)

1.6 Solve the following linear algebraic equations using the Gauss elimination method:

$$3x_1 - 2x_2 + 7x_3 = 20$$

$$x_1 + 6x_2 - x_3 = 10$$

$$10x_1 - 2x_2 + 7x_3 = 29$$

(**Ans:** $x_1 = 1.2857$, $x_2 = 1.9286$, $x_3 = 2.8571$)

1.7 Solve the linear algebraic equations of Problem 1.6 using the Gauss-Seidel method: Note that for Gauss–Seidel to converge the equations are expressed in the form

$$x_1^{n+1} = \frac{29 + 2x_2^n - 7x_3^n}{10}$$

$$x_2^{n+1} = \frac{10 - x_1^{n+1} + x_3^n}{6}$$

$$x_3^{n+1} = \frac{20 - 3x_1^{n+1} + 2x_2^{n+1}}{7}$$

(**Ans:** $x_1 = 1.2857$, $x_2 = 1.9286$, $x_3 = 2.8571$)

1.8 Solve the following linear algebraic equations using the Gauss elimination method:

$$\begin{bmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_{1,1} \\ T_{1,2} \\ T_{1,3} \\ T_{2,1} \\ T_{2,2} \\ T_{2,3} \\ T_{3,1} \\ T_{3,2} \\ T_{3,3} \end{bmatrix} = \begin{bmatrix} -40 \\ -20 \\ -420 \\ -20 \\ 0 \\ -400 \\ -40 \\ -20 \\ -420 \end{bmatrix}$$

Note that for using the Gauss elimination method the equations have to expressed in the form of augmented matrix as

$$\left[\begin{array}{ccccccccc|c} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -40 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & -20 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 & -420 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 & -20 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 & -400 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 & -40 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 & -20 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & -420 \end{array}\right]$$

(**Ans:** $T_{1,1} = 47.14$, $T_{1,2} = 91.25$, $T_{1,3} = 182.86$, $T_{2,1} = 57.32$, $T_{2,2} = 115.00$, $T_{2,3} = 220.18$, $T_{3,1} = 47.14$, $T_{3,2} = 91.25$, $T_{3,3} = 182.86$)

1.9 Solve the following linear algebraic equations using the Gauss–Seidel method:

$$-4T_{1,1} + T_{1,2} + T_{2,1} = -40$$
$$T_{1,1} - 4T_{1,2} + T_{1,3} + T_{2,2} = -20$$
$$T_{1,2} - 4T_{1,3} + T_{2,3} = -420$$
$$T_{1,1} - 4T_{2,1} + T_{2,2} + T_{3,1} = -20$$
$$T_{1,2} + T_{2,1} - 4T_{2,2} + T_{2,3} + T_{3,2} = 0$$
$$T_{1,3} + T_{2,2} - 4T_{2,3} + T_{3,3} = -400$$
$$T_{2,1} - 4T_{3,1} + T_{3,2} = -40$$
$$T_{2,2} + T_{3,1} - 4T_{3,2} + T_{3,3} = -20$$
$$T_{2,3} + T_{3,2} - 4T_{3,3} = -420$$

Note that for Gauss–Seidel to converge the equations are to be expressed in the form

$$T_{1,1}^{n+1} = \frac{40 + T_{1,2}^{n} + T_{2,1}^{n}}{4}$$

$$T_{1,2}^{n+1} = \frac{T_{1,1}^{n+1} + T_{1,3}^{n} + T_{2,2}^{n} + 20}{4}$$

$$T_{1,3}^{n+1} = \frac{T_{1,2}^{n+1} + T_{2,3}^{n} + 420}{4}$$

$$T_{2,1}^{n+1} = \frac{T_{1,1}^{n+1} + T_{2,2}^{n} + T_{3,1}^{n} + 20}{4}$$

$$T_{2,2}^{n+1} = \frac{T_{1,2}^{n+1} + T_{2,1}^{n+1} + T_{2,3}^{n} + T_{3,2}^{n}}{4}$$

$$T_{2,3}^{n+1} = \frac{T_{1,3}^{n+1} + T_{2,2}^{n+1} + T_{3,3}^{n} + 400}{4}$$

$$T_{3,1}^{n+1} = \frac{40 + T_{2,1}^{n+1} + T_{3,2}^{n}}{4}$$

$$T_{3,2}^{n+1} = \frac{T_{2,2}^{n+1} + T_{3,1}^{n+1} + T_{3,3}^{n} + 20}{4}$$

$$T_{3,3}^{n+1} = \frac{T_{3,2}^{n+1} + T_{2,3}^{n+1} + 420}{4}$$

(**Ans:** $T_{1,1} = 47.14$, $T_{1,2} = 91.25$, $T_{1,3} = 182.86$, $T_{2,1} = 57.32$, $T_{2,2} = 115.00$, $T_{2,3} = 220.18$, $T_{3,1} = 47.14$, $T_{3,2} = 91.25$, $T_{3,3} = 182.86$)

Chapter 2

Nonlinear Algebraic Equations

Newton's (or Newton–Raphson) method for the numerical solution of a nonlinear algebraic equation is described first in this chapter. Examples discussed include the calculation of pressure drop in a pipe in nonlaminar range, and the calculation of minimum fluidization velocity and terminal velocity. Thereafter the solution of two simultaneous nonlinear algebraic equations is discussed using Newton's method.

2.1 Newton's Method

The function f is formulated in such a way that the polynomial or the expression whose root is to be determined is of the form $f(x) = 0$. Newton's method is given by

$$x^{n+1} = x^n - \frac{f}{f'} \tag{2.1}$$

where x^n is the value of x at the start of the iteration and x^{n+1} is the updated value after the iteration. First an initial value of x is assumed, and the function value and its derivative are determined at this assumed value. The assumed value is updated by using Newton's formula, and again the function value and its derivative are determined at this new value of x (see Fig. 2.1). The value of x is again updated and the procedure is repeated till there is no change in the previous and updated values of x. By taking different starting (old) values, different roots can be obtained, if more than one real root occurs. Note that when the root is obtained, there is no change in the value of x. That is, $x^{n+1} = x^n$, which implies $f = 0$, which is the required condition, that function value should become zero at the root. Note that Newton's method works only if, at $f = 0$, the derivative of the function is not zero. In Fig. 2.1, the function value becomes zero at the root x_s. In this case the starting value is taken to be x_1.

The algorithm of Newton's method is:

(i) Take an initial value of x^n,

(ii) Calculate f and $f' = \dfrac{df}{dx}$ at the value of x^n,

(iii) Calculate the new value of x, using $x^{n+1} = x^n - \dfrac{f}{f'}$,

(iv) Check if $\left|x^{n+1} - x^n\right| < \varepsilon$; if yes, stop, else

(v) Make $x^n = x^{n+1}$ and go to Step (ii) and repeat the procedure till the condition stated in (iv) is satisfied. ε is the convergence criterion and may be of the order of 10^{-6}.

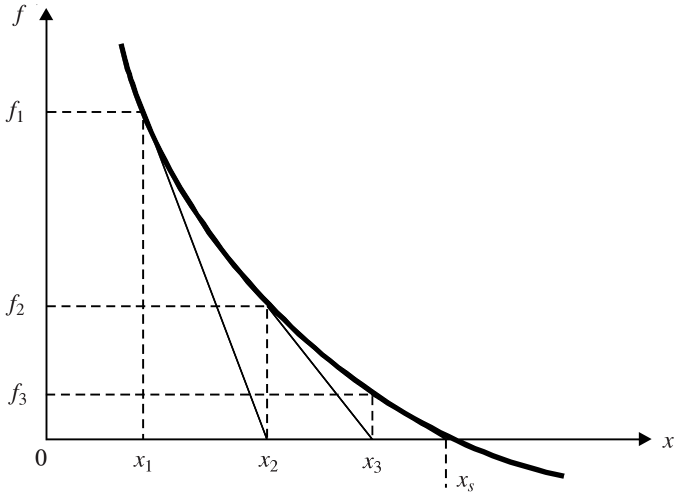

Fig. 2.1 Concept of Newton's method.

The derivation of Newton's formula is presented below. Let a nonlinear algebraic equation be represented as $f(x) = 0$. Let us start with an initial guess x^0 of the solution and let us assume that it is close to the actual solution x_s. We make a Taylor series to approximate $f(x)$ in the vicinity of x^0 as follows:

$$f(x) = f\left(x^0\right) + \left.\frac{df}{dx}\right|_{x^0} \left(x - x^0\right) + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x^0} \left(x - x^0\right)^2 + \cdots$$

At the solution, $f(x_S) = 0$ and the Taylor series yields

$$0 = f\left(x^0\right) + \left.\frac{df}{dx}\right|_{x^0} \left(x_S - x^0\right) + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x^0} \left(x_S - x^0\right)^2 + \cdots$$

If x^0 is sufficiently close to x_s, then

$$\left|x_S - x^0\right| \gg \left|x_S - x^0\right|^2 \gg \left|x_S - x^0\right|^3 \gg \cdots$$

In this case, as long as the first derivative is nonzero at x^0, we obtain a reasonable approximation of the solution, x^1, from the rule

$$0 = f\left(x^0\right) + \left.\frac{df}{dx}\right|_{x^0} \left(x^1 - x^0\right) \tag{2.2}$$

Successive application of this rule yields Newton's method for solving a single nonlinear algebraic equation in the form

$$x^{n+1} = x^n - \frac{f\left(x^n\right)}{f'\left(x^n\right)}$$

where f' denotes the derivative of the function with respect to x. The iterations are stopped when the previous and updated values of x are less than ε_{abs}, that is

$$\left| x^{n+1} - x^n \right| < \varepsilon_{\text{abs}} \tag{2.3}$$

or

$$\left| \frac{x^{n+1} - x^n}{x^{n+1}} \right| < \varepsilon_{\text{rel}} \tag{2.4}$$

Consider that the real roots of the equation $x^3 - 2x^2 - x + 2 = 0$ have to be determined. Different roots are obtained by taking different starting values of x. Newton's method discussed here determines only the real roots. For the above equation the starting values taken and the corresponding roots are listed in Table 2.1.

Table 2.1 Different roots obtained by taking different starting values in Newton's method

Starting value	*Real root of* $x^3 - 2x^2 - x + 2 = 0$ *by Newton's method*
4.0	2.0
1.5	–1.0
0.5	1.0
0.25	1.0
0.0	2.0
–1.0	–1.0
–2.0	–1.0
–4.0	–1.0
–100.0	–1.0
100.0	2.0

Thus the three roots on which the solution converges are (2, 1, –1). Various iterations in Newton's method to determine the real root of the equation $x^3 - 2x^2 - x + 2 = 0$ with starting value $x = 4$ are listed in Table 2.2.

Table 2.2 Various iterations in Newton's method for starting value of $x = 4$

Iteration number	*Starting point*	f	f'	$x^{n+1} = x^n - \dfrac{f}{f'}$
1	4.0	30.0	28.0	2.92857
2	2.92857	7.03533	13.01529	2.38803
3	2.38803	1.82478	6.55594	2.10969
4	2.10969	0.37852	3.91362	2.01297
5	2.01297	0.03959	3.10426	2.00022
6	2.00022	0.00066	3.00176	2.00000
7	2.00000	0.00000	3.00000	2.00000

In Table 2.2, $f = x^3 - 2x^2 - x + 2$, and $f' = 3x^2 - 4x - 1$.

EXAMPLE 2.1 Apply Newton's method to determine a real root of the equation

$$f(x) = x^3 - 5x + 1 = 0$$

Take the initial approximation as $x_0 = 0.5$.

Solution With an initial value of 0.5, it can be checked that the solution is 0.201640.

2.2 Pressure Drop in Pipe

The pressure drop in a pipe of length L is given by the relation

$$\Delta P = \frac{fL\bar{V}^2\rho}{2D} \tag{2.5}$$

where $\bar{V}$ is the average velocity in the pipe of internal diameter D and the fluid density is ρ. When the pressure drop is given by Eq. (2.5), the friction factor under laminar flow conditions is given by

$$f = \frac{64}{\text{Re}} \tag{2.6}$$

where $\text{Re} = \frac{\rho\bar{V}D}{\mu}$. For the entire nonlaminar range the friction factor is given by the Colebrook relation

$$\frac{1}{\sqrt{f}} = -2.0\log\left(\frac{\varepsilon/D}{3.7} + \frac{2.51}{\text{Re}\sqrt{f}}\right) \tag{2.7}$$

For the laminar conditions the friction factor can be easily determined. But for nonlaminar conditions the Colebrook equation has to be solved using Newton's method as described in the example below.

EXAMPLE 2.2 Air at 25°C and 1 atm flows through a 4 mm diameter tube with an average velocity of 50 m/s. The roughness is $\varepsilon = 0.0015$ mm. Calculate the friction factor using the Colebrook equation

$$\frac{1}{\sqrt{f}} = -2.0\log\left(\frac{\varepsilon/D}{3.7} + \frac{2.51}{\text{Re}\sqrt{f}}\right)$$

Determine the pressure drop in a 1 m section of the tube using the relation

$$\Delta P = \frac{fL\bar{V}^2\rho}{2D}$$

Density of air at 25°C and 1 atm is 1.23 kg/m^3 and viscosity is 1.79×10^{-5} kg/m-s.

Solution We have

$$\frac{\varepsilon}{D} = \frac{0.0015}{4} = 0.000375$$

$$\mathrm{Re} = \frac{\rho \bar{V} D}{\mu} = \frac{1.23 \times 50 \times 4 \times 10^{-3}}{1.79 \times 10^{-5}} = 13743$$

Thus

$$\frac{1}{\sqrt{f}} = -2.0 \log\left(\frac{0.000375}{3.7} + \frac{2.51}{13743\sqrt{f}}\right)$$

or

$$\frac{1}{\sqrt{f}} = -2.0 \log\left(1.01 \times 10^{-4} + \frac{1.83 \times 10^{-4}}{\sqrt{f}}\right)$$

Let us define a function, F, as

$$F = \frac{1}{\sqrt{f}} + 2.0 \log\left(1.01 \times 10^{-4} + \frac{1.83 \times 10^{-4}}{\sqrt{f}}\right)$$

The derivative of the function with respect to the friction factor is given by

$$F' = -0.5 f^{-1.5} + \frac{2.0 \times 1.83 \times 10^{-4} \times (-0.5) f^{-1.5}}{1.01 \times 10^{-4} + 1.83 \times 10^{-4} f^{-0.5}}$$

Using Newton's method, we get $f = 0.0291$. Under these conditions the pressure drop in a 1 m section of the pipe is given by

$$\Delta P = \frac{0.0291 \times 1 \times 50^2 \times 1.23}{2 \times 0.004} = 11185.3 \ \text{N/m}^2 = 11.19 \ \text{kPa}$$

Program 2.1 for calculating the pressure drop in a pipe under nonlaminar conditions is given in the Appendix.

2.3 Minimum Fluidization Velocity

Ergun proposed the following general equation applicable for low, medium and high Reynolds number for pressure drop across a packed bed:

$$\Delta P = \frac{150 \mu v \Delta L}{\phi_s^2 d_p^2} \frac{(1-\varepsilon)^2}{\varepsilon^3} + \frac{1.75 \rho v^2 \Delta L}{\phi_s d_p} \frac{(1-\varepsilon)}{\varepsilon^3} \tag{2.8}$$

where v is the superficial velocity of the fluid, d_p is the particle diameter, ϕ_s is the sphericity of the particle, ε is the voidage in the packed bed, and ΔP is the pressure drop across the packed bed of length $\Delta L \cdot \rho$ and μ are respectively the density and viscosity of the fluid. At the point of incipient fluidization the force obtained from the pressure drop across the fluidized bed ($\Delta P \times A$) is equal to the gravitational force exerted by the mass of the particles minus the buoyancy force. If L_{mf} is the height of the packed bed at the point of minimum fluidization and ε_{mf} is the voidage of the packed bed at minimum fluidization, then the total volume of the bed at minimum fluidization is $L_{\text{mf}} \times A$ and thus the volume of solids at minimum fluidization is $L_{\text{mf}} A(1 - \varepsilon_{\text{mf}})$. The gravitational force of the particles minus the buoyancy force is given by volume of the solid particles × $(\rho_p - \rho)g$. Thus at minimum fluidization conditions

$$\Delta P \times A = L_{\text{mf}} A\left(1 - \varepsilon_{\text{mf}}\right)\left(\rho_p - \rho\right) g \tag{2.9}$$

or

$$\frac{\Delta P}{L_{\text{mf}}} = \left(1 - \varepsilon_{\text{mf}}\right)\left(\rho_p - \rho\right) g \tag{2.10}$$

Substituting this value in the Ergun equation for packed bed, we get

$$\left[\frac{1.75\rho}{\phi_s d_p}\frac{\left(1 - \varepsilon_{\text{mf}}\right)}{\varepsilon_{\text{mf}}^3}\right] v_{\text{mf}}^2 + \left[\frac{150\mu}{\phi_s^2 d_p^2}\frac{\left(1 - \varepsilon_{\text{mf}}\right)^2}{\varepsilon_{\text{mf}}^3}\right] v_{\text{mf}} - \left(1 - \varepsilon_{\text{mf}}\right)\left(\rho_p - \rho\right) g = 0 \tag{2.11}$$

The real roots of the minimum fluidization velocity can be obtained using Newton's method.

EXAMPLE 2.3 Solid particles having a diameter of 0.12 mm, shape factor $\phi_s = 0.88$, and a density of 1000 kg/m^3 are to be fluidized using air at 2.0 atm and 25°C. The voidage at minimum fluidization is 0.42. The viscosity of air under these conditions is 1.845×10^{-5} kg/m-s. The molecular weight of air is 28.97.

Solution The density of air at 2.0 atm and 25°C is given by

$$\rho = \frac{PM}{RT} = \frac{2 \times 101325 \times 28.97 \times 10^{-3}}{8.314 \times 298.15} = 2.374 \text{ kg/m}^3$$

The diameter of the particle is $d_p = 1.2*10^{-4}$ m. The function is

$$f = \left[\frac{1.75\rho}{\phi_s d_p}\frac{\left(1 - \varepsilon_{\text{mf}}\right)}{\varepsilon_{\text{mf}}^3}\right] v_{\text{mf}}^2 + \left[\frac{150\mu}{\phi_s^2 d_p^2}\frac{\left(1 - \varepsilon_{\text{mf}}\right)^2}{\varepsilon_{\text{mf}}^3}\right] v_{\text{mf}} - \left(1 - \varepsilon_{\text{mf}}\right)\left(\rho_p - \rho\right) g$$

and the derivative of the function with respect to v_{mf} is

$$f' = 2\left[\frac{1.75\rho}{\phi_s d_p}\frac{\left(1 - \varepsilon_{\text{mf}}\right)}{\varepsilon_{\text{mf}}^3}\right] v_{\text{mf}} + \frac{150\mu}{\phi_s^2 d_p^2}\frac{\left(1 - \varepsilon_{\text{mf}}\right)^2}{\varepsilon_{\text{mf}}^3}$$

Starting with an initial value of $v_{\text{mf}} = 0.1$ m/s, the converged value is $v_{\text{mf}} = 0.0046$ m/s.

Program 2.2 for calculating the minimum fluidization velocity is given in the Appendix.

2.4 Terminal Velocity

Consider a particle of mass m kg falling at velocity of v m/s (see Fig. 2.2). The momentum balance equation is given by

$$m\frac{dv_p}{dt} = F_g - F_b - F_D \tag{2.12}$$

Gravitational force minus the buoyancy force on the particle is given by

$$F_g - F_b = V_p\left(\rho_p - \rho\right)g = \frac{m}{\rho_p}\left(\rho_p - \rho\right)g \tag{2.13}$$

where V_P is the volume of the particle and m is the mass of the particle.

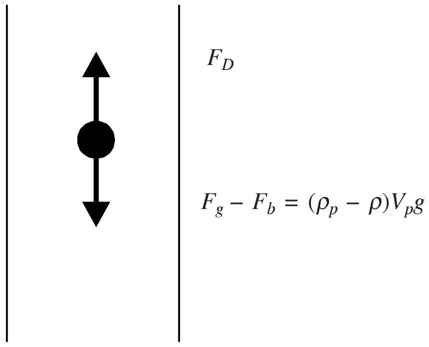

Fig. 2.2 Various forces acting on particle falling in stationary fluid.

The terminal velocity or free settling velocity is a constant velocity fall and is given when $\frac{dv_p}{dt} = 0$; thus

$$F_g - F_b = F_D \tag{2.14}$$

C_D is given by $C_D = \dfrac{F_D/A_p}{\frac{1}{2}\rho v_t^2}$. Thus Eq. (2.14) becomes

$$\frac{m}{\rho_p}\left(\rho_p - \rho\right)g = \frac{1}{2}\rho A_p C_D v_t^2 \tag{2.15}$$

where A_p is the projected area of the particle on a plane at right angles to the direction of motion and v_t is the terminal velocity of the falling particle. As the velocity of particle rises the drag force also increases till the drag force balances the (gravitational – buoyancy) force. Thus,

$$v_t = \sqrt{\frac{2g\left(\rho_p - \rho\right)m}{\rho_p A_p C_D \rho}}$$

For spherical particles,

$$m = \frac{4}{3}\pi r_p^3 \rho_p = \frac{\pi}{6} d_p^3 \rho_p$$

and the projected area is given by

$$A_p = \pi r_p^2 = \frac{\pi d_p^2}{4}$$

Thus for spherical particles the expression for terminal velocity becomes

$$v_t = \sqrt{\frac{4(\rho_p - \rho) g d_p}{3 C_D \rho}} \tag{2.16}$$

For laminar flow ($\mathrm{Re}_p < 1$), that is, in the Stokes law region

$$C_D = \frac{24}{\mathrm{Re}_p} \tag{2.17}$$

where Re_p is the particle Reynold's number and is given by $\mathrm{Re}_p = \frac{\rho v d_p}{\mu}$. We get the following expression for terminal settling velocity in the laminar flow regime

$$v_t = \frac{g d_p^2 (\rho_p - \rho)}{18\mu} \tag{2.18}$$

For turbulent flow, $C_D = 0.44$ ($\mathrm{Re}_p > 1000$ to 2×10^5). But for intermediate values of the particle Reynolds number, there are many correlations. The Schiller and Nauman correlation is applicable for $\mathrm{Re}_p < 800$ and is given by

$$C_D = \frac{24}{\mathrm{Re}_p}\left(1 + 0.15\,\mathrm{Re}_p^{0.687}\right) \tag{2.19}$$

The terminal velocity for the case of intermediate values of particle Reynolds number is determined using the following steps:

(i) A value of terminal velocity is assumed.

(ii) At the assumed value the particle Reynolds number is calculated and thereafter C_D is determined.

(iii) The terminal velocity is recalculated using $v_t = \sqrt{\frac{4(\rho_p - \rho) g d_p}{3 C_D \rho}}$.

If the assumed value and recalculated values are different, the new calculated value becomes the starting value for the next iteration. The procedure is repeated till the absolute value of the difference between the new value and the previous value of the terminal velocity in an iteration is negligible.

EXAMPLE 2.4 Oil droplets of diameter 2 mm are to be settled from air at 25°C and 1 atm. The density of oil is 900 kg/m^3. Calculate the terminal settling velocity of the particles. For air at these conditions, μ = 1.85 × 10^{-5} kg/m-s. C_D is given by

$$C_D = \frac{24}{\text{Re}_p}\left(1 + 0.15\text{Re}_p^{0.687}\right)$$

Solution The following data are given: $d_p = 2 \times 10^{-3}$ m, $\mu = 1.85 \times 10^{-5}$ kg/m-s. The density of air under the given conditions is given by

$$\rho = \frac{PM}{RT} = \frac{101325 \times 28.84 \times 10^{-3}}{8.314 \times 298.15} = 1.18 \text{ kg/m}^3$$

The particle Reynolds number is given by

$$\text{Re}_p = \frac{\rho_g v_t d_p}{\mu} = \frac{1.18 \times v_t \times 2 \times 10^{-3}}{1.85 \times 10^{-5}} = 127.57 v_t$$

The calculations are presented in Table 2.3.

Table 2.3 Calculations in Example 2.6

Assumed v_t	Re_p	C_D	v_t
0.03	3.83	8.63	1.5
1.5	191.35	0.82	4.9
4.9	625.0	0.52	6.2
6.2	790.0	0.47	6.47
6.47	825.38	0.47	6.52

The terminal velocity obtained is 6.5285 m/s.

Program 2.3 for calculating the terminal velocity is given in the Appendix.

2.5 System of Nonlinear Equations

We now extend Newton's method to solve a set of N simultaneous nonlinear algebraic equations for N unknowns.

$$\begin{gathered} f_1(x_1, x_2, x_3, \ldots, x_N) = 0 \\ f_2(x_1, x_2, x_3, \ldots, x_N) = 0 \\ f_3(x_1, x_2, x_3, \ldots, x_N) = 0 \\ \cdots \\ f_N(x_1, x_2, x_3, \ldots, x_N) = 0 \end{gathered}$$

We define the vector of unknowns

$$x = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots & x_N \end{bmatrix}^T$$

and write the system of equations as

$$f(x) = 0$$

We use a Taylor series expansion to obtain Newton's method, representing the *i*th function in the vicinity of the current estimate $\mathbf{x}^n$ as

$$f_i(x) = f_i\left(x^n\right) + \sum_{m=1}^{N} \frac{\partial f_i}{\partial x_m}\bigg|_{x^n} \left(x_m - x_m^n\right) + \frac{1}{2!}\sum_{m=1}^{N}\sum_{p=1}^{N}\left(x_m - x_m^n\right)\frac{\partial^2 f_i}{\partial x_m \partial x_p}\bigg|_{x^n}\left(x_p - x_p^n\right) + \cdots$$

Assuming that $\mathbf{x}^n$ is sufficiently close to the true solution x_S, we can drop the quadratic and higher order terms

$$0 \approx f_i\left(x^n\right) + \sum_{m=1}^{N} \frac{\partial f_i}{\partial x_m}\bigg|_{x^n}\left(x_{S,m} - x_m^n\right)$$

For convenience we collect the first partial derivatives into the $N \times N$ Jacobian matrix

$$J_{im} = \frac{\partial f_i}{\partial x_m}\bigg|_{x^n} \tag{2.20}$$

The truncated Taylor series expansion then becomes

$$0 \approx f_i\left(x^n\right) + \sum_{m=1}^{N} J_{im}^n \left(x_m^{n+1} - x_m^n\right)$$

or

$$\sum_{m=1}^{N} J_{im}^n \, \Delta x_m^{n+1} = -f_i\left(x^n\right) \tag{2.21}$$

where the update vector is given by

$$\Delta x^{n+1} = x^{n+1} - x^n \tag{2.22}$$

The terms on the left hand side of Eq. (2.21) are the *i*th component of a matrix–vector product. The linear system is

$$J^n \Delta x^{n+1} = -f\left(x^n\right) \tag{2.23}$$

Iterations are performed till there is no change in $x_1, x_2, x_3, \ldots, x_N$, that is

$$\left|\Delta x_1^{n+1}\right| < \varepsilon_{\text{abs}}, \left|\Delta x_2^{n+1}\right| < \varepsilon_{\text{abs}}, \left|\Delta x_3^{n+1}\right| < \varepsilon_{\text{abs}}, \ldots, \left|\Delta x_N^{n+1}\right| < \varepsilon_{\text{abs}} \tag{2.24}$$

Let us consider two nonlinear equations $f_1(x_1, x_2)$ and $f_2(x_1, x_2)$. To start the iteration, some initial values of x_1 and x_2 have to be assumed. The change in the values of x_1 and x_2 are determined using Eq. (2.23).

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} = -\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \tag{2.25}$$

Now we have to find the inverse of the Jacobian matrix. The inverse of a nonsingular 2×2 matrix $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ is given by $A^{-1} = \dfrac{1}{\det A}\begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$. Thus Eq. (2.25) can be written as

$$\begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} = -\frac{1}{D}\begin{bmatrix} \dfrac{\partial f_2}{\partial x_2} & -\dfrac{\partial f_1}{\partial x_2} \\ -\dfrac{\partial f_2}{\partial x_1} & \dfrac{\partial f_1}{\partial x_1} \end{bmatrix}\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \tag{2.26}$$

where

$$D = \frac{\partial f_1}{\partial x_1}\frac{\partial f_2}{\partial x_2} - \frac{\partial f_1}{\partial x_2}\frac{\partial f_2}{\partial x_1} \tag{2.27}$$

Thus

$$\Delta x_1 = \frac{f_2 \dfrac{\partial f_1}{\partial x_2} - f_1 \dfrac{\partial f_2}{\partial x_2}}{D} \tag{2.28}$$

and

$$\Delta x_2 = \frac{f_1 \dfrac{\partial f_2}{\partial x_1} - f_2 \dfrac{\partial f_1}{\partial x_1}}{D} \tag{2.29}$$

The algorithm for solution of two simultaneous nonlinear algebraic equations is given below:

(i) Assume x_1 and x_2,

(ii) Calculate f_1, f_2, $\dfrac{\partial f_1}{\partial x_1}$, $\dfrac{\partial f_1}{\partial x_2}$, $\dfrac{\partial f_2}{\partial x_1}$, and $\dfrac{\partial f_2}{\partial x_2}$,

(iii) Calculate Δx_1 and Δx_2, and

(iv) Calculate new values of x_1 and x_2.

Go to (ii) till $\left|x_1^{n+1} - x_1^n\right| < \varepsilon$ and $\left|x_2^{n+1} - x_2^n\right| < \varepsilon$.

EXAMPLE 2.5 Obtain the values of x and y that satisfy the following two nonlinear algebraic equations:

$$f(x, y) = e^x + xy - 1 = 0$$
$$g(x, y) = \sin xy + x + y - 1 = 0$$

Solution The partial derivatives of function f are given by

$$\frac{\partial f}{\partial x} = e^x + y$$
$$\frac{\partial f}{\partial y} = x$$

The partial derivatives of function g are given by

$$\frac{\partial g}{\partial x} = y\cos xy + 1$$

$$\frac{\partial g}{\partial y} = x\cos xy + 1$$

Let us assume $x = 0.1$ and $y = 0.5$.

$$f(x, y) = e^x + xy - 1 = 0.1552$$

$$g(x, y) = \sin xy + x + y - 1 = -0.3991$$

$$\frac{\partial f}{\partial x} = e^x + y = 1.6052$$

$$\frac{\partial f}{\partial y} = x = 0.1$$

$$\frac{\partial g}{\partial x} = y\cos xy + 1 = 1.5000$$

$$\frac{\partial g}{\partial y} = x\cos xy + 1 = 1.1000$$

$$D = \frac{\partial f}{\partial x}\frac{\partial g}{\partial y} - \frac{\partial f}{\partial y}\frac{\partial g}{\partial x} = 1.6157$$

$$\Delta x = \frac{g\dfrac{\partial f}{\partial y} - f\dfrac{\partial g}{\partial y}}{D} = \frac{-0.3991 \times 0.1 - 0.1552 \times 1.1}{1.6157} = -0.13036$$

$$\Delta y = \frac{f\dfrac{\partial g}{\partial x} - g\dfrac{\partial f}{\partial x}}{D} = \frac{0.1552 \times 1.5 + 0.3991 \times 1.6052}{1.6157} = 0.5406$$

New $x = 0.1 - 0.13036 = -0.03036$
New $y = 0.5 + 0.5406 = 1.0406$
The iterations are summarized in Table 2.4.

Table 2.4 Summary of iterations in Example 2.5

x	y	f	g	$\frac{\partial f}{\partial x}$	$\frac{\partial f}{\partial y}$	$\frac{\partial g}{\partial x}$	$\frac{\partial g}{\partial y}$	D	Δx	Δy
0.1	0.5	0.1552	−0.3991	1.6052	0.1	1.5	1.1	1.6157	−0.13036	0.5406
−0.03036	1.0406	−0.0615	0.0097	2.0107	−0.03036	2.0406	0.9696	2.0115	0.0295	−0.0721
−0.00086	0.9685	−0.0017	−0.0324	1.9676	−0.00086	1.9685	0.99914	1.9676	0.00088	0.0307
0	0.9992	0.0000	−0.0008	1.9992	0	1.9992	1	1.9992	0	0.0008
0	1	0	0	2	0	2	1	2	0	0

The solution of the given nonlinear algebraic equations is $x = 0$ and $y = 1$. Note that when $f = 0$ and $g = 0$ the solution is obtained.

Program 2.4 for the solution of the above two simultaneous nonlinear equations is given in the Appendix.

EXAMPLE 2.6 Modify Program 2.4 to solve the following system of two nonlinear algebraic equations:

$$f_1(x_1, x_2) = 3x_1^3 + 4x_2^2 - 145 = 0$$

$$f_2(x_1, x_2) = 4x_1^2 - x_2^3 + 28 = 0$$

Solution For the given nonlinear equations

$$\frac{\partial f_1}{\partial x_1} = 9x_1^2 \qquad \frac{\partial f_1}{\partial x_2} = 8x_2 \qquad \frac{\partial f_2}{\partial x_1} = 8x_1 \quad \text{and} \quad \frac{\partial f_2}{\partial x_2} = -3x_2^2$$

Program 2.4 can be modified to obtain the following solution: $x_1 = 3$ and $x_2 = 4$.

Exercises

2.1 Determine the root of the equation

$$15x^3 - 68x^2 + 95x - 47 = 0$$

which is close to 2.5.
(**Ans:** 2.5034)

2.2 Air at 25°C and 1 atm flows through a 4 mm diameter tube with an average velocity of 25 m/s. The roughness is $\varepsilon = 0.0015$ mm. The friction factor is given by

$$\frac{1}{\sqrt{f}} = -2.0 \log\left(\frac{\varepsilon/D}{3.7} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right)$$

Determine the pressure drop in a 1 m section of the tube using the relation

$$\Delta P = \frac{fL\bar{V}^2 \rho}{2D}$$

The density of air at 25°C and 1 atm is 1.23 kg/m^3 and the viscosity is 1.79×10^{-5} kg/m-s.
(**Ans:** $f = 0.03467$, $\Delta P = 3.33$ kPa)

2.3 Solid particles having a diameter of 0.05 mm, shape factor $\phi_s = 0.88$, and density of 1000 kg/m^3 are to be fluidized using air at 2.0 atm and 25°C. The voidage at minimum fluidization is 0.39. The viscosity of air under these conditions is 1.845×10^{-5} kg/m-s. The molecular weight of air is 28.97.
(**Ans:** 0.000611 m/s)

2.4 Solve Exercise 2.3 for solid particles having a diameter of 0.25 mm. The voidage at minimum fluidization is 0.48.
(**Ans:** 0.0327 m/s)

2.5 Oil droplets of diameter 0.2 mm are to be settled from air at 25°C and 1 atm. The density of oil is 900 kg/m^3. Calculate the terminal settling velocity of the particles. Viscosity of air under these conditions is 1.85×10^{-5} kg/m-s. C_D is given by

$$C_D = \frac{24}{\mathrm{Re}_p}\left(1 + 0.15\,\mathrm{Re}_p^{0.687}\right)$$

(**Ans:** 0.6462 m/s)

2.6 Solve Exercise 2.5 for oil droplets of diameter 0.02 mm.
(**Ans:** 0.0105 m/s)

Chapter 3

Chemical Engineering Thermodynamics

The calculation of molar volume using the van der Waals, Redlich–Kwong, and Peng–Robinson cubic equations of state at the given temperature and pressure is discussed first in this chapter. After this, bubble point, dew point, and flash calculations using Raoult's and modified Raoult's law are discussed. The determination of vapour pressure at the given temperature for a pure substance following a cubic equation of state is thereafter discussed. The determination of system pressure and vapour phase composition at the given temperature and liquid phase composition is discussed using the gamma–phi $\left(y_i P\hat{\phi}_i = x_i \gamma_i f_i\right)$ and phi–phi $\left(y_i P\hat{\phi}_i^V = x_i P\hat{\phi}_i^L\right)$ approaches. The solution of two simultaneous chemical reactions in equilibrium in the homogeneous phase and the calculation of adiabatic flame temperature are also discussed in this chapter.

3.1 Solution of Cubic Equations of State

The molar volume of both the saturated vapour and saturated liquid can be calculated using cubic equations of state. The cubic equations of state can have three real roots or one real root and two complex roots. When there is only one real root, then only one phase exists—liquid or vapour—and when three real roots exist, then there are two phases. The smallest root is the molar volume of saturated liquid and the largest root is the molar volume of saturated vapour. The intermediate root is of the no physical significance. To determine the molar volume of the liquid phase, the starting value taken is $V = b$, and to determine the molar volume of the vapour phase, the starting value taken is $V = \dfrac{RT}{P}$.

The van der Waals equation of state is

$$P = \frac{RT}{V-b} - \frac{a}{V^2} \tag{3.1}$$

The cubic form of the van der Waals cubic equation of state is given by

$$V^3 - \left(b + \frac{RT}{P}\right)V^2 + \frac{a}{P}V - \frac{ab}{P} = 0 \tag{3.2}$$

where $$a = \frac{27R^2T_c^2}{64P_c} \quad \text{and} \quad b = \frac{RT_c}{8P_c}$$

Let us define the function as $f = V^3 - \left(b + \frac{RT}{P}\right)V^2 + \frac{a}{P}V - \frac{ab}{P}$. At the given temperature and pressure and given critical properties of the substance, the only unknown in this equation is the molar volume V. The derivative of the function f with respect to the molar volume is given by

$$f' = 3V^2 - 2\left(b + \frac{RT}{P}\right)V + \frac{a}{P} \tag{3.3}$$

A value of molar volume is assumed. At the assumed molar volume the value of the function f and its derivative f' are determined and the new molar volume is determined using Newton's method [see Eq. (2.1)]

$$V^{n+1} = V^n - \frac{f}{f'} \tag{2.1}$$

Thereafter, the new molar volume becomes the old molar volume, and f and f' are determined again at this molar volume. The procedure is repeated till there is a very meagre change between the new and old molar volumes, that is, $\left|V^{n+1} - V^n\right| < 10^{-6}$.

The Redlich-Kwong equation of state is

$$P = \frac{RT}{V - b} - \frac{a}{T^{1/2}V(V + b)} \tag{3.4}$$

The cubic form of the Redlich-Kwong cubic equation of state is given by

$$V^3 - \frac{RT}{P}V^2 - \left(b^2 + \frac{bRT}{P} - \frac{a}{\sqrt{T}P}\right)V - \frac{ab}{\sqrt{T}P} = 0 \tag{3.5}$$

where $a = \frac{0.42748R^2T_c^{2.5}}{P_c}$ and $b = \frac{0.08664RT_c}{P_c}$.

Let us define the function as $f = V^3 - \frac{RT}{P}V^2 - \left(b^2 + \frac{bRT}{P} - \frac{a}{\sqrt{T}P}\right)V - \frac{ab}{\sqrt{T}P}$. At the given temperature and pressure and given the critical properties of the substance, the only unknown in this equation is the molar volume, V. The derivative of the function f with respect to the molar volume is given by

$$f' = 3V^2 - 2\frac{RT}{P}V - \left(b^2 + \frac{bRT}{P} - \frac{a}{\sqrt{T}P}\right) \tag{3.6}$$

The Peng–Robinson equation of state is

$$P = \frac{RT}{V - b} - \frac{a}{V^2 + 2bV - b^2} \tag{3.7}$$

The cubic form of the Peng–Robinson cubic equation of state is given by

$$V^3 + \left(b - \frac{RT}{P}\right)V^2 - \left(3b^2 + \frac{2RTb}{P} - \frac{a}{P}\right)V + b^3 + \frac{RT}{P}b^2 - \frac{ab}{P} = 0 \tag{3.8}$$

$$a = \frac{0.45724(RT_c)^2}{P_c}\alpha$$

$$\sqrt{\alpha} = 1 + m\left(1 - \sqrt{\frac{T}{T_c}}\right)$$

$$m = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

$$b = \frac{0.07780RT_c}{P_c}$$

Let us define the function as

$$f = V^3 + \left(b - \frac{RT}{P}\right)V^2 - \left(3b^2 + \frac{2RTb}{P} - \frac{a}{P}\right)V + b^3 + \frac{RT}{P}b^2 - \frac{ab}{P}$$

At the given temperature and pressure and given critical properties of the substance the only unknown in this equation is the molar volume V. The derivative of the function f with respect to the molar volume is given by

$$f' = 3V^2 + 2\left(b - \frac{RT}{P}\right)V - \left(3b^2 + \frac{2RTb}{P} - \frac{a}{P}\right) \tag{3.9}$$

EXAMPLE 3.1 Calculate the molar volume of saturated liquid water and saturated water vapor at 100°C and 101.325 kPa using van der Waals, Redlich–Kwong and Peng–Robinson cubic equations of state. For water: T_C = 647.1 K, P_C = 220.55 bar, and ω = 0.345.

Solution Program 3.1 for calculating the molar volume at the given temperature and pressure using various cubic equations of state is given in the Appendix. The result obtained from the program is given below.

Saturated liquid volume using Peng–Robinson equation of state = 2.25×10^{-5} m^3/mol
Saturated vapour volume using Peng–Robinson equation of state = 0.030352 m^3/mol
Saturated liquid volume using Redlich–Kwong equation of state = 2.64×10^{-5} m^3/mol
Saturated vapour volume using Redlich–Kwong equation of state = 0.030400 m^3/mol
Saturated liquid volume using van der Waals equation of state = 3.90×10^{-5} m^3/mol
Saturated vapour volume using van der Waals equation of state = 0.030469 m^3/mol.

3.2 Bubble Point and Dew Point Temperature Calculations Using Raoult's Law

3.2.1 Bubble Point Temperature Calculation

When the liquid phase composition is given, the governing equation is $P = x_1P_1^{\text{sat}} + x_2P_2^{\text{sat}}$. In this problem, along with the liquid phase composition the system pressure is given and the bubble point temperature and the vapour composition have to be determined. Newton's method is used to determine the temperature which satisfies the equation $P = x_1 P_1^{\text{sat}} + x_2 P_2^{\text{sat}}$. Let us formulate a function *f*.

$$f = P - x_1 P_1^{\text{sat}} - x_2 P_2^{\text{sat}} \tag{3.10}$$

Using Antoine equation

$$\ln P^{\text{sat}} = A - \frac{B}{T + C} \tag{3.11}$$

we get

$$f = P - x_1 \exp\left(A_1 - \frac{B_1}{T + C_1}\right) - x_2 \exp\left(A_2 - \frac{B_2}{T + C_2}\right) \tag{3.12}$$

In the above equation the Antoine parameters, system pressure and liquid composition are given. The only unknown is the temperature. The derivative of the function *f* with respect to temperature is given by

$$f' = -\frac{x_1 P_1^{\text{sat}} B_1}{(T + C_1)^2} - \frac{x_2 P_2^{\text{sat}} B_2}{(T + C_2)^2} \tag{3.13}$$

A value of temperature is assumed. At the assumed temperature the value of function *f* and its derivative f' are determined and the new temperature is determined using [see Eq. (2.1)]

$$T^{n+1} = T^n - \frac{f}{f'} \tag{2.1}$$

Thereafter the new temperature becomes the old temperature and again at this temperature, *f* and f' are determined. The procedure is repeated till there is a very meagre change between the new and old temperatures, that is, $\left|T^{n+1} - T^n\right| < 10^{-4}$. This equation can also be written as $\left|\frac{T^{n+1} - T^n}{T^{n+1}}\right| < 10^{-6}$.

The assumed temperature is calculated from the relation $T^n = \sum x_i T_i^{\text{sat}}$. The saturation temperatures T_1^{sat} and T_2^{sat} are calculated for the given pressure using the Antoine equation

$$T^{\text{sat}} = \frac{B}{A - \ln P} - C \tag{3.14}$$

Once the temperature that satisfies the equation $P = x_1 P_1^{\text{sat}} + x_2 P_2^{\text{sat}}$ is determined, the vapour phase composition can be determined using $y_1 = \frac{x_1 P_1^{\text{sat}}}{P}$ and $y_2 = \frac{x_2 P_2^{\text{sat}}}{P}$.

3.2.2 Dew Point Temperature Calculation

When the vapour phase composition is given, use is made of $\frac{1}{P} = \frac{y_1}{P_1^{\text{sat}}} + \frac{y_2}{P_2^{\text{sat}}}$. In this problem system pressure is given along with vapour phase composition and dew point temperature and liquid phase composition have to be determined. Newton's method is used to determine the temperature which satisfies the equation $\frac{1}{P} = \frac{y_1}{P_1^{\text{sat}}} + \frac{y_2}{P_2^{\text{sat}}}$. Let us formulate a function f.

$$f = \frac{1}{P} - \frac{y_1}{P_1^{\text{sat}}} - \frac{y_2}{P_2^{\text{sat}}} \tag{3.15}$$

Using the Antoine equation $\ln P^{\text{sat}} = A - \frac{B}{T + C}$, we get

$$f = \frac{1}{P} - y_1 \exp\left(-A_1 + \frac{B_1}{T + C_1}\right) - y_2 \exp\left(-A_2 + \frac{B_2}{T + C_2}\right) \tag{3.16}$$

Here in this equation the Antoine parameters, system pressure and vapour composition are given. The only unknown is the temperature. The derivative of the function f with respect to temperature is given by

$$f' = \frac{y_1 B_1}{P_1^{\text{sat}} (T + C_1)^2} + \frac{y_2 B_2}{P_2^{\text{sat}} (T + C_2)^2} \tag{3.17}$$

A value of temperature is assumed. At the assumed temperature the value of the function f and its derivative f' are determined and the new temperature is determined using

$$T^{n+1} = T^n - \frac{f}{f'}$$

Thereafter, the new temperature becomes the old temperature and f and f' are determined again at this temperature. The procedure is repeated till there is a very meagre change between the new and old temperatures, that is, $|T^{n+1} - T^n| < 10^{-4}$. This equation can also be written as $\left|\frac{T^{n+1} - T^n}{T^{n+1}}\right| < 10^{-6}$. The assumed temperature is calculated from the relation $T^n = \sum y_i T_i^{\text{sat}}$.

Once the temperature that satisfies the equation $\frac{1}{P} = \frac{y_1}{P_1^{\text{sat}}} + \frac{y_2}{P_2^{\text{sat}}}$ is determined, the liquid phase composition can be determined using $x_1 = \frac{y_1 P}{P_1^{\text{sat}}}$ and $x_2 = \frac{y_2 P}{P_2^{\text{sat}}}$.

EXAMPLE 3.2 Calculate the bubble point and dew point temperatures for the acetone (1) – water (2) system at 101.325 kPa for feed composition $z_1 = 0.5$. Assume the system to follow Raoult's law.

Solution Program 3.2 for calculating the bubble and dew point temperatures for a system following Raoult's law is given in the Appendix. The result obtained from the program is bubble point temperature = 71.81°C, dew point temperature = 87.08°C.

3.3 Flash Calculations Using Raoult's Law

The aim here is to calculate the compositions of the vapour and liquid phases at the given temperature and pressure under flash conditions, assuming Raoult's law to be true. For a mixture at the given pressure, if the temperature lies between the bubble point and dew point temperatures or at the given temperature, if the pressure lies between the dew point and bubble point pressure, both liquid and vapour exist. In this section we shall determine the equilibrium liquid and vapour phase compositions if the temperature, system pressure and feed composition are given. The overall composition is denoted by z_i and L and V denote the amount of moles in the liquid and vapour phases respectively. Let the initial total number of moles before flashing be 1. The distribution coefficient (K_i) for a species is defined as its composition in the vapour phase divided by its composition in the liquid phase. We can write for a particular species that

$$K_i = \frac{y_i}{x_i} \tag{3.18}$$

For a system following Raoult's law, $K_i = \frac{P_i^{\text{sat}}}{P}$; therefore, if the temperature and the pressure of the system are given, then the K values of all the components can be calculated. The composition of the vapour in terms of K_i and feed composition is given by

$$y_i = \frac{K_i z_i}{1 - V + VK_i} \tag{3.19}$$

and the composition of the liquid phase is given by

$$x_i = \frac{z_i}{1 - V + VK_i} \tag{3.20}$$

Finally we should have

$$\sum y_i = \sum \frac{K_i z_i}{1 - V + VK_i} = 1 \tag{3.21}$$

where the summation is over all the components, and also

$$\sum x_i = \sum \frac{z_i}{1 - V + VK_i} = 1 \qquad 3.22)$$

Therefore let us define a function

$$f = \sum y_i - \sum x_i = \sum \frac{(K_i - 1) z_i}{1 - V + VK_i} \tag{3.23}$$

The function has to be formulated in such a way that its required value is zero. In this equation the only unknown is V, which is the number of moles in the vapour phase per unit mol fed to the system. The derivative of the function with respect to V is given by

$$f' = -\sum \frac{(K_i - 1)^2 z_i}{(1 - V + VK_i)^2} \tag{3.24}$$

A value of V is assumed. At the assumed V the value of the function f and its derivative f' are determined and the new V is determined using

$$V^{n+1} = V^n - \frac{f}{f'}$$

Thereafter, the new V becomes the old V and again at this V the function f and its derivative f' are determined. The procedure is repeated till there is a very meagre change between the new and old values of V, that is, $\left|V^{n+1} - V^{n}\right| < 10^{-6}$. Once V is determined, the vapour and liquid phase composition can be determined.

EXAMPLE 3.3 Calculate the compositions of the liquid and vapour phases for the acetone (1)–acetonitrile (2)–nitromethane (3) system. The feed composition is $z_1 = 0.3$, $z_2 = 0.3$ and $z_3 = 0.4$. At the given temperature, $P_1^{\text{sat}} = 195.75$ kPa, $P_2^{\text{sat}} = 97.84$ kPa, and $P_3^{\text{sat}} = 50.32$ kPa. The pressure of the system is 100 kPa. Assume the system to follow Raoult's law.

Solution Program 3.3 for calculating the composition of the liquid and vapour phases under flash conditions for a system following Raoult's law is given in the Appendix. The result obtained from the program is given below: $x_1 = 0.25057$, $y_1 = 0.490491$, $x_2 = 0.301341$, $y_2 = 0.294832$, $x_3 = 0.44561$, $y_3 = 0.224231$. The number of moles in vapour phase is 0.206026.

3.4 Bubble Point and Dew Point Temperature Calculations Using Modified Raoult's Law

The modified Raoult's law is given by

$$y_1 P = x_1 \gamma_1 P_1^{\text{sat}} \tag{3.25}$$

$$y_2 P = x_2 \gamma_2 P_2^{\text{sat}} \tag{3.26}$$

The activity coefficients can be determined using various models. In the present case the Wilson model is used, because for a given system the activity coefficients can be determined as a function of the temperature and the liquid composition. The Wilson parameters are given by

$$\Lambda_{12} = \frac{V_2}{V_1} \exp\left(-\frac{a_{12}}{RT}\right) \tag{3.27}$$

$$\Lambda_{21} = \frac{V_1}{V_2} \exp\left(-\frac{a_{21}}{RT}\right) \tag{3.28}$$

The activity coefficients are given by

$$\ln \gamma_1 = -\ln(x_1 + x_2\Lambda_{12}) + x_2\left[\frac{\Lambda_{12}}{x_1 + x_2\Lambda_{12}} - \frac{\Lambda_{21}}{x_2 + x_1\Lambda_{21}}\right] \tag{3.29}$$

$$\ln \gamma_2 = -\ln(x_2 + x_1\Lambda_{21}) - x_1\left[\frac{\Lambda_{12}}{x_1 + x_2\Lambda_{12}} - \frac{\Lambda_{21}}{x_2 + x_1\Lambda_{21}}\right] \tag{3.30}$$

Calculation of bubble point pressure

(i) Enter the temperature and the liquid composition.

(ii) Calculate the vapour pressure of the components at the given temperature.

(iii) Calculate the activity coefficients at the given temperature and liquid composition.

(iv) Calculate the bubble point pressure using the relation $P = x_1\gamma_1 P_1^{\text{sat}} + x_2\gamma_2 P_2^{\text{sat}}$

Calculation of bubble point temperature

(i) Enter the pressure and the liquid composition

(ii) At the given pressure, calculate the saturation temperature of the components and the assumed temperature using $T^n = \Sigma x_i T_i^{\text{sat}}$.

(iii) At the assumed temperature, calculate the vapour pressure of the components and the activity coefficients.

(iv) Update the vapour pressure of Component 1 using the relation

$$P_1^{\text{sat}} = \frac{P}{x_1\gamma_1 + x_2\gamma_2 \dfrac{P_2^{\text{sat}}}{P_1^{\text{sat}}}}$$

(v) From the updated value of P_1^{sat}, calculate the temperature using

$$T = \frac{B_1}{A_1 - \ln P_1^{\text{sat}}} - C_1$$

(vi) Go to Step (iii) and repeat the procedure till convergence in temperature is obtained.

Calculation of dew point pressure

(i) Enter the temperature and the vapour composition.

(ii) Calculate the vapour pressure of the components at the given temperature.

(iii) Initially assume the activity coefficients to be one and calculate the system pressure using

$$P = \frac{1}{\dfrac{y_1}{\gamma_1 P_1^{\text{sat}}} + \dfrac{y_2}{\gamma_2 P_2^{\text{sat}}}}$$

(iv) Calculate the liquid composition using $x_1 = \dfrac{y_1 P}{\gamma_1 P_1^{\text{sat}}}$ and $x_2 = \dfrac{y_2 P}{\gamma_2 P_2^{\text{sat}}}$.

(v) Update the liquid composition using $x_1 = \dfrac{x_1}{x_1 + x_2}$ and $x_2 = 1 - x_1$.

(vi) At the liquid composition, calculate the activity coefficients.

(vii) Go to Step (iv) and repeat the procedure till convergence in activity coefficients is obtained.

(viii) Calculate the system pressure using

$$P = \frac{1}{\dfrac{y_1}{\gamma_1 P_1^{\text{sat}}} + \dfrac{y_2}{\gamma_2 P_2^{\text{sat}}}}$$

(ix) Go to Step (iv) and repeat the procedure till convergence in the pressure is obtained.

Calculation of dew point temperature

(i) Enter the pressure and the vapour composition.

(ii) At the given pressure, calculate the saturation temperature of the components and the assumed temperature using $T^n = \Sigma y_i T_i^{\text{sat}}$. Initially take $\gamma_1 = \gamma_2 = 1$.

(iii) At the assumed temperature, calculate the vapour pressure of the components.

(iv) Calculate the liquid composition using $x_1 = \dfrac{y_1 P}{\gamma_1 P_1^{\text{sat}}}$ and $x_2 = \dfrac{y_2 P}{\gamma_2 P_2^{\text{sat}}}$.

(v) Update the liquid composition using $x_1 = \dfrac{x_1}{x_1 + x_2}$ and $x_2 = 1 - x_1$.

(vi) At the liquid composition, calculate the activity coefficients.

(vii) Go to Step (iv) and repeat the procedure till convergence in activity coefficients is obtained.

(viii) Update the vapour pressure of Component 1 using the relation $P_1^{\text{sat}} = P\left(\dfrac{y_1}{\gamma_1} + \dfrac{y_2 P_1^{\text{sat}}}{\gamma_2 P_2^{\text{sat}}}\right)$

(ix) From the updated value of P_1^{sat}, calculate the temperature using $T = \dfrac{B_1}{A_1 - \ln P_1^{\text{sat}}} - C_1$

(x) Go to Step (iii) and repeat the procedure till convergence in temperature is obtained:

EXAMPLE 3.4 Consider a binary vapour–liquid equilibrium system. The Antoine equations of the components are given by

$$\ln P_1^{\text{sat}} = 16.678 - \frac{3640.2}{T + 219.61}$$

$$\ln P_2^{\text{sat}} = 16.2887 - \frac{3816.44}{T + 227.02}$$

where the temperature is in °C and the vapour pressure in kPa. The parameters in the Wilson equation are: a_{12} = 437.98 cal/mol and a_{21} = 1238 cal/mol. The molar volume of the components is V_1 = 76.92 cm^3/mol and V_2 = 18.07 cm^3/mol. Assume the system to follow the modified Raoult's law.

(i) Calculate the bubble point pressure at 100°C and x_1 = 0.5.

(ii) Calculate the bubble point temperature at 101.325 kPa and x_1 = 0.5.

(iii) Calculate the the dew point pressure at 100°C and $y_1 = 0.5$.

(iv) Calculate the dew point temperature at 101.325 kPa and $y_1 = 0.5$.

Solution Program 3.4 for the bubble point and dew point calculations for a system following the modified Raoult's law is given in the Appendix. The result obtained from the program is given below: (i) 204.264 kPa, (ii) 80.93°C, (iii) 184.10 kPa, and (iv) 83.82°C.

3.5 Flash Calculations Using Modified Raoult's Law

In flash the vapour and liquid phases coexist at the given temperature and pressure. The feed composition is given and the compositions of the liquid and vapour phases are to be determined using the modified Raoult's law. For the given temperature and feed composition, first the bubble point and dew point pressures are determined. Then a pressure is chosen between the bubble point and dew point pressures.

(i) Enter the temperature.

(ii) At the given temperature calculate the vapour pressure of components.

(iii) Calculate the activity coefficients by assuming the total feed as liquid.

(iv) Calculate the bubble point pressure using the relation $P = x_1\gamma_1 P_1^{\text{sat}} + x_2\gamma_2 P_2^{\text{sat}}$

(v) Record the bubble point pressure (P_{bubble}) and the activity coefficients (γ_{1b} and γ_{2b}).

(vi) For the calculation of the dew point pressure (total feed as vapour), first assume the activity coefficients to be1.

(vii) Calculate the pressure using $P = \dfrac{1}{\dfrac{y_1}{\gamma_1 P_1^{\text{sat}}} + \dfrac{y_2}{\gamma_2 P_2^{\text{sat}}}}$.

(viii) Calculate the liquid phase compositions using $x_1 = \dfrac{y_1 P}{\gamma_1 P_1^{\text{sat}}}$ and $x_2 = \dfrac{y_2 P}{\gamma_2 P_2^{\text{sat}}}$.

(ix) Update the liquid composition using $x_1 = \dfrac{x_1}{x_1 + x_2}$ and $x_2 = 1 - x_1$.

(x) At the liquid composition, calculate the activity coefficients.

(xi) Go to step (viii) and repeat the procedure till convergence in activity coefficients is obtained.

(xii) Calculate the system pressure using $P = \dfrac{1}{\dfrac{y_1}{\gamma_1 P_1^{\text{sat}}} + \dfrac{y_2}{\gamma_2 P_2^{\text{sat}}}}$.

(xiii) Go to step (viii) and repeat the procedure till convergence in pressure is obtained.

(xiv) Store the dew point pressure (P_{dew}) and the activity coefficients (γ_{1d} and γ_{2d}).

(xv) Enter the pressure between the bubble point and dew point pressures.

(xvi) The assumed number moles in vapour phase is calculated using $V = \dfrac{P_{\text{bubble}} - P}{P_{\text{bubble}} - P_{\text{dew}}}$.

(xvii) The assumed value of γ_1 is calculated using $\gamma_1 = \dfrac{(P - P_{\text{dew}})(\gamma_{1b} - \gamma_{1d})}{(P_{\text{bubble}} - P_{\text{dew}})} + \gamma_{1d}$.

(xviii) The assumed value of γ_2 is calculated using $\gamma_2 = \dfrac{(P - P_{\text{dew}})(\gamma_{2b} - \gamma_{2d})}{(P_{\text{bubble}} - P_{\text{dew}})} + \gamma_{2d}$.

(xix) Calculate $K_1 = \dfrac{\gamma_1 P_1^{\text{sat}}}{P}$ and $K_2 = \dfrac{\gamma_2 P_2^{\text{sat}}}{P}$.

(xx) Calculate $y_1 = \dfrac{K_1 z_1}{1 - V + VK_1}$ and $y_2 = \dfrac{K_2 z_2}{1 - V + VK_2}$.

(xxi) Calculate $x_1 = \dfrac{y_1}{K_1}$ and $x_2 = \dfrac{y_2}{K_2}$.

(xxii) Define a function $f = y_1 - x_1 + y_2 - x_2$.

(xxiii) $f' = -\sum \dfrac{(K_i - 1)^2 z_i}{(1 - V + VK_i)^2}$.

(xxiv) $V^{n+1} = V^n - \dfrac{f}{f'}$.

(xxv) Go to Step (xx) and repeat the procedure till convergence in V is obtained.

(xxvi) Calculate γ_1 and γ_2.

(xxvii) Go to Step (xix) and repeat the procedure till convergence in activity coefficients is obtained.

EXAMPLE 3.5 Calculate the composition of the liquid and vapour phases for the system acetone (1)–water (2) at 100°C and 200 kPa. The feed composition is $z_1 = 0.3$. The Antoine equations of the components are given by

$$\ln P_1^{\text{sat}} = 14.39155 - \frac{2795.817}{T + 230.002}$$

$$\ln P_2^{\text{sat}} = 16.26205 - \frac{3799.887}{T + 226.346}$$

where the temperature is in °C and the vapour pressure in kPa. The parameters in the Wilson equation are: $a_{12} = 292.66$ cal/mol and $a_{21} = 1445.26$ cal/mol. The molar volume of the components is $V_1 = 74.05$ cm^3/mol and $V_2 = 18.07$ cm^3/mol. Assume the system to follow the modified Raoult's law.

Solution Program 3.5 for calculating the composition of the liquid and vapour phases under flash conditions for a system following the modified Raoult's law is given in the Appendix. The result obtained from the program is: bubble point pressure = 310.47 kPa, dew point pressure = 142.80 kPa. The system pressure chosen is 200 kPa and after convergence the number of moles in the vapour phase is 0.546235. $x_1 = 0.045019$ and $y_1 = 0.511817$.

3.6 Vapour Pressure Using Cubic Equation of State

The cubic equations of state are applicable for both the liquid and vapour phases. At a given temperature, a cubic equation of state can be used to determine the vapour pressure of a pure substance. A pressure is assumed and the fugacities in the liquid and vapour phases are determined. If at the assumed pressure the fugacities are not identical, then another pressure is assumed and the pressure at which the fugacities are the same ($f^L = f^V$) is the vapour pressure. The algorithm for calculation of vapour pressure is given below.

(i) Assume a pressure.

(ii) At the given temperature and the assumed pressure, calculate V^V and V^L as described in Program 3.1.

(iii) Calculate f^L and f^V using cubic equation of state.

(iv) If $\left|\dfrac{f^L - f^V}{f^V}\right| < 0.00001$, stop.

(v) Calculate the new pressure using, $P_{\text{new}} = P_{\text{old}} \dfrac{f^L}{f^V}$, and go back to Step (ii) and repeat the procedure till Condition (iv) is satisfied.

For the Peng–Robinson cubic equation of state, the fugacity of a pure substance is given by

$$\ln \frac{f}{P} = Z - 1 - \ln\left(Z - \frac{Pb}{RT}\right) - \frac{a}{2\sqrt{2}bRT} \ln \frac{V + \left(1 + \sqrt{2}\right)b}{V + \left(1 - \sqrt{2}\right)b} \tag{3.31}$$

The fugacity of the liquid phase is given by

$$\ln \frac{f^L}{P} = Z^L - 1 - \ln\left(Z^L - \frac{Pb}{RT}\right) - \frac{a}{2\sqrt{2}bRT} \ln \frac{V^L + \left(1 + \sqrt{2}\right)b}{V^L + \left(1 - \sqrt{2}\right)b} \tag{3.31a}$$

where

$$Z^L = \frac{PV^L}{RT}$$

and the fugacity of the vapour phase is given by

$$\ln\frac{f^V}{P} = Z^V - 1 - \ln\left(Z^V - \frac{Pb}{RT}\right) - \frac{a}{2\sqrt{2}bRT}\ln\frac{V^V + \left(1+\sqrt{2}\right)b}{V^V + \left(1-\sqrt{2}\right)b} \tag{3.31b}$$

where

$$Z^V = \frac{PV^V}{RT}$$

EXAMPLE 3.6 Calculate the vapour pressure of water at 100°C using the Peng–Robinson cubic equation of state. For water: $T_C = 647.1$ K, $P_C = 220.55$ bar, and $\omega = 0.345$.

Solution Program 3.6 for calculating the vapour pressure using the cubic equation of state is given in the Appendix. The vapour pressure of water at 100°C as obtained from the program is 96071.375 Pa.

3.7 *P–x–y* Diagram Using Gamma–Phi Approach

In the Gamma–Phi approach, the vapour–liquid equilibrium is described using the equation

$$y_1 P\hat{\phi}_1^V = x_1\gamma_1 f_1 \tag{3.32}$$

$$y_2 P\hat{\phi}_2^V = x_2\gamma_2 f_2 \tag{3.33}$$

At the given temperature and liquid phase composition, the equilibrium pressure and the vapour composition are determined. Then again at the same temperature and at a different liquid phase composition, the equilibrium pressure and vapour composition are determined. This is used to generate the *P–x–y* diagram at the given temperature.

The algorithm is given below.

(i) Read T, x_1, T_{c1}, P_{c1}, T_{c2}, P_{c2}, ω_1, ω_2, Z_{C1}, Z_{C2}, P_1^{sat}, P_2^{sat}.

(ii) $x_2 = 1 - x_1$.

(iii) At the given temperature and liquid phase composition, calculate the activity coefficients γ_1 and γ_2.

(iv) At the given temperature, calculate B_{11}, B_{22}, B_{12} and δ_{12}.

(v) Calculate the initial value of the total pressure using $P = x_1\gamma_1 P_1^{\text{sat}} + x_2\gamma_2 P_2^{\text{sat}}$ (only to start the solution do we assume the modified Raoult's law to be true) and the composition in vapour phase using the relation $y_1 = \dfrac{x_1\gamma_1 P_1^{\text{sat}}}{P}$ and $y_2 = \dfrac{x_2\gamma_2 P_2^{\text{sat}}}{P}$.

(vi) At the total pressure, calculate the fugacity of the pure liquid species 1(f_1) and 2(f_2) at the given temperature and calculated pressure, using the relation

$$f_i = P_i^{\text{sat}}\exp\left(\frac{B_{ii}P_i^{\text{sat}}}{RT}\right)\exp\left[\frac{V_i^L\left(P - P_i^{\text{sat}}\right)}{RT}\right]$$

(vii) Calculate the fugacity coefficient of the species 1($\hat{\phi}_1$) and 2($\hat{\phi}_2$) in the vapour phase.

(viii) Calculate $K_1 = \dfrac{\gamma_1 f_1}{\hat{\phi}_1 P}$ and $K_2 = \dfrac{\gamma_2 f_2}{\hat{\phi}_2 P}$.

(ix) Calculate $S = K_1 \times x_1 + K_2 \times x_2$.

(x) Calculate $y_1 = \dfrac{K_1 \times x_1}{S}$ and $y_2 = \dfrac{K_2 \times x_2}{S}$. Go to Step (vii) and repeat the procedure till $\delta S < \varepsilon$. (This is because the composition of the vapour phase has changed and therefore the fugacity coefficients of the species in the vapour phase get changed.)

(xi) Calculate the new pressure using $P = \dfrac{x_1\gamma_1 f_1}{\hat{\phi}_1} + \dfrac{x_2\gamma_2 f_2}{\hat{\phi}_2}$ and calculate the new compositions in the vapour phase using $y_1 = \dfrac{x_1\gamma_1 f_1}{\hat{\phi}_1 P}$ and $y_2 = \dfrac{x_2\gamma_2 f_2}{\hat{\phi}_2 P}$. Go to Step (vi) and repeat the procedure till $\delta P < \varepsilon$.

EXAMPLE 3.7 Consider the methanol (1) – water (2) system in vapour–liquid equilibrium. The temperature of the system is 100°C and the liquid phase composition is $x_1 = 0.958$. Determine the system pressure and the vapour phase composition. Use the Gamma–Phi approach. The Antoine equations of the components are given by

$$\ln P_1^{\text{sat}} = 16.5938 - \frac{3644.3}{T + 239.76}$$

$$\ln P_2^{\text{sat}} = 16.2620 - \frac{3799.89}{T + 226.35}$$

where temperature is in °C and vapour pressure in kPa. The parameters in the Wilson equation are: $a_{12} = 107.38$ cal/mol and $a_{21} = 469.55$ cal/mol. The molar volume of the components is $V_1 = 40.73$ cm^3/mol and $V_2 = 18.07$ cm^3/mol. $T_{c1} = 512.6$ K, $P_{c1} = 80.97$ bar, $\omega_1 = 0.564$, $Z_{c1} = 0.224$, $T_{c2} = 647.1$ K, $P_{c2} = 220.55$ bar, $\omega_2 = 0.345$, $Z_{c2} = 0.229$.

Solution Program 3.7 for *P–x–y* calculations using the Gamma–Phi approach is given in the Appendix. The result obtained from the program is given below: pressure = 344930.59 Pa and $y_1 = 0.980694$.

3.8 *P-x-y* Diagram Using Cubic Equation of State

For the Peng–Robinson equation of state the fugacity coefficient of component 1 in the liquid phase is given by

$$\ln \hat{\phi}_1^L = \left(Z^L - 1\right)\frac{b_1}{b^L} - \ln\left(Z^L - \frac{Pb^L}{RT}\right)$$

$$-\frac{a^L}{2\sqrt{2}b^L RT}\left[\frac{2\left(x_1 a_{11}+x_2 a_{12}\right)}{a^L}-\frac{b_1}{b^L}\right]\ln\frac{Z^L+\left(1+\sqrt{2}\right)\frac{Pb^L}{RT}}{Z^L+\left(1-\sqrt{2}\right)\frac{Pb^L}{RT}} \tag{3.34}$$

and the fugacity coefficient of component 1 in the vapour phase is given by

$$\ln\hat{\phi}_1^V=\left(Z^V-1\right)\frac{b_1}{b^V}-\ln\left(Z^V-\frac{Pb^V}{RT}\right)$$

$$-\frac{a^V}{2\sqrt{2}b^V RT}\left[\frac{2\left(y_1 a_{11}+y_2 a_{12}\right)}{a^V}-\frac{b_1}{b^V}\right]\ln\frac{Z^V+\left(1+\sqrt{2}\right)\frac{Pb^V}{RT}}{Z^V+\left(1-\sqrt{2}\right)\frac{Pb^V}{RT}} \tag{3.35}$$

The fugacity coefficient of component 2 in the liquid phase is given by

$$\ln\hat{\phi}_2^L=\left(Z^L-1\right)\frac{b_2}{b^L}-\ln\left(Z^L-\frac{Pb^L}{RT}\right)$$

$$-\frac{a^L}{2\sqrt{2}b^L RT}\left[\frac{2\left(x_1 a_{12}+x_2 a_{22}\right)}{a^L}-\frac{b_2}{b^L}\right]\ln\frac{Z^L+\left(1+\sqrt{2}\right)\frac{Pb^L}{RT}}{Z^L+\left(1-\sqrt{2}\right)\frac{Pb^L}{RT}} \tag{3.36}$$

and the fugacity coefficient of component 2 in the vapour phase is given by

$$\ln\hat{\phi}_2^V=\left(Z^V-1\right)\frac{b_2}{b^V}-\ln\left(Z^V-\frac{Pb^V}{RT}\right)$$

$$-\frac{a^V}{2\sqrt{2}b^V RT}\left[\frac{2\left(y_1 a_{12}+y_2 a_{22}\right)}{a^V}-\frac{b_2}{b^V}\right]\ln\frac{Z^V+\left(1+\sqrt{2}\right)\frac{Pb^V}{RT}}{Z^V+\left(1-\sqrt{2}\right)\frac{Pb^V}{RT}} \tag{3.37}$$

where

$$a^L=x_1^2 a_{11}+x_2^2 a_{22}+2x_1 x_2 a_{12} \tag{3.38}$$

$$b^L=x_1 b_1+x_2 b_2 \tag{3.39}$$

$$a^V=y_1^2 a_{11}+y_2^2 a_{22}+2y_1 y_2 a_{12} \tag{3.40}$$

$$b^V=y_1 b_1+y_2 b_2 \tag{3.41}$$

$$Z^L=\frac{PV^L}{RT} \tag{3.42}$$

$$Z^V = \frac{PV^V}{RT} \tag{3.43}$$

For a binary VLE mixture the phase equilibrium equations are

$$y_1 P\, \hat{\phi}_1^V = x_1 P\, \hat{\phi}_1^L \tag{3.44}$$

$$y_2 P\, \hat{\phi}_2^V = x_2 P\, \hat{\phi}_2^L \tag{3.45}$$

and variables are T, P, x_1, and y_1. Thus, if any two variables (T or P, x_1 or y_1) are specified the other two can be determined.

Since the compositions of the liquid and vapour phases are different, a and b for each phase are different. Calculate a and b for the liquid phase and then Z^L and V^L (the smallest root), and a and b for the vapour phase and then Z^V and V^V (the largest root). The molar volume is calculated by solving the cubic form of the Peng–Robinson equation of state. The algorithm for the calculation of the bubble point pressure and the vapour phase composition at the given temperature and the liquid phase composition for a binary mixture using the cubic equations of state is given below.

(i) Read T, x_1, T_{c1}, P_{c1}, T_{c2}, P_{c2}, ω_1, ω_2

(ii) Calculate $x_2 = 1 - x_1$

(iii) Calculate a_{11}, a_{22}, $a_{12} = \sqrt{a_{11}a_{22}}$, b_1, b_2

(iv) Calculate for liquid phase: $a^L = x_1^2 a_{11} + x_2^2 a_{22} + 2x_1x_2a_{12}$ and $b^L = x_1b_1 + x_2b_2$.

(v) Assume some pressure (P) and composition in the vapour phase y_1 (assume y_1 greater than x_1 if component 1 is the more volatile component).

(vi) Using Newton's technique, calculate V^L using a^L, b^L, x_1, x_2. Take $V_{\text{old}} = b^L$ because the liquid phase molar volume is to be calculated. From V^L, calculate $Z^L = \dfrac{PV^L}{RT}$ (compressibility factor in the liquid phase).

(vii) Calculate the fugacity coefficient of the components $\hat{\phi}_1^L$ and $\hat{\phi}_2^L$ in the liquid mixture.

(viii) Calculate for the vapour phase: $a^V = y_1^2 a_{11} + y_2^2 a_{22} + 2y_1y_2a_{12}$ and $b^V = y_1b_1 + y_2b_2$.

(ix) Using Newton's technique, calculate V^V using a^V, b^V, y_1, y_2. Take $V_{\text{old}} = \dfrac{RT}{P}$ because the vapour phase molar volume is to be calculated. From V^V, calculate $Z^V = \dfrac{PV^V}{RT}$ (compressibility factor in the vapour phase).

(x) Calculate the fugacity coefficient of the components $\hat{\phi}_1^V$ and $\hat{\phi}_2^V$ in the vapour phase mixture.

(xi) Calculate $K_1 = \dfrac{\hat{\phi}_1^L}{\hat{\phi}_1^V}$ and $K_2 = \dfrac{\hat{\phi}_2^L}{\hat{\phi}_2^V}$.

(xii) Calculate $Sum = K_1 \times x_1 + K_2 \times x_2$.

(xiii) Calculate $y_1 = \dfrac{K_1 \times x_1}{Sum}$ and $y_2 = \dfrac{K_2 \times x_2}{Sum}$. Go to Step (viii) and repeat the procedure till $\delta(Sum) < \varepsilon$. This is because the composition of the vapour phase has changed; therefore a^V and b^V get changed.

(xiv) Calculate the new pressure using $P_{\text{new}} = P_{\text{old}} \times Sum$. Go to Step (vi) and repeat the procedure till $\delta P < \varepsilon$.

EXAMPLE 3.8 Consider the CO_2 (1) – *n*-pentane (2) system in vapour–liquid equilibrium. The temperature of the system is 377.65 K and the liquid phase composition is $x_1 = 0.5$. Determine the system pressure and the vapour phase composition using the Peng–Robinson cubic equation of state. $T_{c1} = 304.2$ K, $P_{c1} = 73.83$ bar, $\omega_1 = 0.224$, $T_{c2} = 469.7$ K, $P_{c2} = 33.70$ bar, and $\omega_2 = 0.252$.

Solution Program 3.8 for *P–x–y* calculations using the Peng–Robinson cubic equation of state is given in the Appendix. The result obtained from the program is given below: Pressure = 6524432 Pa and $y_1 = 0.81127$.

3.9 Chemical Reaction Equilibrium—Two Simultaneous Reactions

The solution of two simultaneous nonlinear algebraic equations is described in Section 2.5. The application in chemical reaction equilibrium in the homogeneous phase is described in the example below.

EXAMPLE 3.9 In the production of synthesis gas the following two independent reactions take place

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

$$CO + H_2O \rightarrow CO_2 + H_2$$

Starting with 5 moles of steam and 1 mole of methane, calculate the equilibrium composition of the resulting mixture at 600°C and 1 atm. At this temperature the equilibrium constants for the first and second reaction are 0.574 and 2.21 respectively. Assume the gas mixture to follow ideal gas behaviour.

Solution Let X_1 be the reaction coordinate for the first reaction and X_2 for the second. The number of moles of components at equilibrium is as follows:

CH_4: $1 - X_1$
H_2O: $5 - X_1 - X_2$
CO: $X_1 - X_2$
H_2: $3X_1 + X_2$
CO_2: X_2
Total: $6 + 2X_1$

Since the pressure is 1 atm, therefore $K = K_P K_y = K_y$.

$$\frac{(X_1 - X_2)(3X_1 + X_2)^3}{(1 - X_1)(5 - X_1 - X_2)(6 + 2X_1)^2} = 0.574$$

$$\frac{X_2(3X_1 + X_2)}{(X_1 - X_2)(5 - X_1 - X_2)} = 2.21$$

The two nonlinear algebraic equations are

$$f_1 = \frac{(X_1 - X_2)(3X_1 + X_2)^3}{(1 - X_1)(5 - X_1 - X_2)(6 + 2X_1)^2} - 0.574$$

$$f_2 = \frac{X_2(3X_1 + X_2)}{(X_1 - X_2)(5 - X_1 - X_2)} - 2.21$$

and their derivatives are

$$\frac{\partial f_1}{\partial X_1} = \frac{(12X_1 - 8X_2)(3X_1 + X_2)^2}{(1 - X_1)(5 - X_1 - X_2)(6 + 2X_1)^2} - \frac{(X_1 - X_2)(3X_1 + X_2)^3\left(8X_1^2 + 6X_1X_2 - 24X_1 + 2X_2 - 16\right)}{(1 - X_1)^2(5 - X_1 - X_2)^2(6 + 2X_1)^3}$$

$$\frac{\partial f_1}{\partial X_2} = \frac{3(X_1 - X_2)(3X_1 + X_2)^2 - (3X_1 + X_2)^3}{(1 - X_1)(5 - X_1 - X_2)(6 + 2X_1)^2} + \frac{(X_1 - X_2)(3X_1 + X_2)^3}{(1 - X_1)(5 - X_1 - X_2)^2(6 + 2X_1)^2}$$

$$\frac{\partial f_2}{\partial X_1} = \frac{3X_2}{(X_1 - X_2)(5 - X_1 - X_2)} - \frac{X_2(3X_1 + X_2)(5 - 2X_1)}{(X_1 - X_2)^2(5 - X_1 - X_2)^2}$$

$$\frac{\partial f_2}{\partial X_2} = \frac{3X_1 + 2X_2}{(X_1 - X_2)(5 - X_1 - X_2)} - \frac{X_2(3X_1 + X_2)(2X_2 - 5)}{(X_1 - X_2)^2(5 - X_1 - X_2)^2}$$

The algorithm is described in Section 2.5. Program 3.9 for solution of two chemical reaction equilibrium equations is given in the Appendix. The solution is $X_1 = 0.912$ and $X_2 = 0.633$. Thus at equilibrium: moles of $CH_4 = 0.09$ mol, moles of $H_2O = 3.465$ mol, moles of CO = 0.285 mol, moles of $H_2 = 3.355$ mol, moles of $CO_2 = 0.625$ mol, and total number of moles = 7.82 mol.

3.10 Adiabatic Flame Temperature

First the inlet species are laised from inlet temperature (T_1) to adiabatic flame temperature (T) and then the reaction at temperature T is carried out. The total enthalpy change is zero as there is no heat and work exchange with the surroundings. The algorithm for the calculation of adiabatic flame temperature is described below.

(i) Read the various constants of molar heat capacity at constant pressure for various species.

(ii) Read the various stoichiometric coefficients (ν_i) and moles of each species (n_i) entering.

(iii) Read the standard enthalpy of formation for various species and calculate the standard enthalpy change of reaction. Read the standard temperature (T_0) and inlet temperature (T_1).

(iv) Calculate *sa*, *sb*, *sc*, *sd* using the relations

$$sa = n_1a_1 + n_2a_2 + n_3a_3 + n_4a_4 \qquad sb = n_1b_1 + n_2b_2 + n_3b_3 + n_4b_4$$

$$sc = n_1c_1 + n_2c_2 + n_3c_3 + n_4c_4 \qquad sd = n_1d_1 + n_2d_2 + n_3d_3 + n_4d_4$$

(v) Calculate the heat required to raise the inlet species from the inlet temperature (T_1) to the adiabatic flame temperature (T) using

$$sa\left(T - T_1\right) + \frac{sb}{2}\left(T^2 - T_1^2\right) + \frac{sc}{3}\left(T^3 - T_1^3\right) + \frac{sd}{4}\left(T^4 - T_1^4\right)$$

Note that this formula is valid for the molar heat capacity given by the equation

$$C_P = a + bT + cT^2 + dT^3$$

(vi) Calculate

$$\Delta a = \nu_4a_4 + \nu_3a_3 + \nu_2a_2 + \nu_1a_1 \qquad \Delta b = \nu_4b_4 + \nu_3b_3 + \nu_2b_2 + \nu_1b_1$$

$$\Delta c = \nu_4c_4 + \nu_3c_3 + \nu_2c_2 + \nu_1c_1 \qquad \Delta d = \nu_4d_4 + \nu_3d_3 + \nu_2d_2 + \nu_1d_1$$

(vii) Calculate the standard enthalpy change of reaction at the adiabatic flame temperature (T) with respect to the standard enthalpy change of reaction at temperature (T_0)

$$\Delta H^0_{T_0} + \Delta a\left(T - T_0\right) + \frac{\Delta b}{2}\left(T^2 - T_0^2\right) + \frac{\Delta c}{3}\left(T^3 - T_0^3\right) + \frac{\Delta d}{4}\left(T^4 - T_0^4\right)$$

(viii) Assume an adiabatic flame temperature and at that temperature calculate the value of the function

$$f = sa\left(T - T_1\right) + \frac{sb}{2}\left(T^2 - T_1^2\right) + \frac{sc}{3}\left(T^3 - T_1^3\right) + \frac{sd}{4}\left(T^4 - T_1^4\right)$$

$$+\ \Delta H^0_{T_0} + \Delta a\left(T - T_0\right) + \frac{\Delta b}{2}\left(T^2 - T_0^2\right) + \frac{\Delta c}{3}\left(T^3 - T_0^3\right) + \frac{\Delta d}{4}\left(T^4 - T_0^4\right)$$

and its derivative

$$f' = sa + sb \times T + sc \times T^2 + sd \times T^3 + \Delta a + \Delta b \times T + \Delta c \times T^2 + \Delta d \times T^3$$

(ix) Calculate new temperature using Newton's formula $T^{n+1} = T^n - \dfrac{f}{f'}$, take this as the old temperature and go to Step (ν) and repeat the procedure till there is no significant change in temperature ($\delta T < \varepsilon$).

EXAMPLE 3.10 Calculate the adiabatic flame temperature of a gas initially at 25°C containing 1 mol C_2H_6 (1), 4 mol O_2 (2), 10 mol CO_2 (3) and 0 mol of H_2O (4). The ethane is completely burned. The standard heat capacity is given by $C_P^0 = a + bT + cT^2 + dT^3$, where T is in K and C_P^0 in cal/mol-K.

Species	a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$
C_2H_6	1.648	4.124	–1.530	1.740
O_2	6.085	0.3631	–0.1709	0.3133
CO_2	5.316	1.4285	–0.8362	1.784
$H_2O(g)$	7.700	0.04594	0.2521	–0.8587

The standard enthalpy of formation at 298.15 K is: $\Delta H^0_{f,\,CO_2} = -94.052$ kcal/mol, $\Delta H^0_{f,\,H_2O(g)} = -57.7979$ kcal/mol, $\Delta H^0_{f,C_2H_6} = -20.236$ kcal/mol.

Solution The reaction with stoichiometric amount of oxygen is

$$C_2H_6 + \frac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O$$

and the reaction with 4 mol of O_2 and 10 mol CO_2 is

$$C_2H_6 + 4O_2 + 10CO_2 \rightarrow 12CO_2 + 3H_2O + 0.5O_2$$

Program 3.10 for the calculation of adiabatic flame temperature (AFT) is given in the Appendix. The result obtained from the computer program is AFT = 2090.39 K.

Exercises

3.1 Calculate the molar volume of saturated liquid water and saturated water vapour at 180°C and 1.0 MPa using the van der Waals, Redlich–Kwong and Peng–Robinson cubic equations of state. For water: $T_C = 647.1$ K, $P_C = 220.55$ bar, and $\omega = 0.345$.

(**Ans:** V^L using the Peng–Robinson equation of state = 2.47×10^{-5} m^3/mol, V^V using the Peng–Robinson equation of state = 0.003570 m^3/mol, V^L using the Redlich–Kwong equation of state = 2.95×10^{-5} m^3/mol, V^V using the Redlich–Kwong equation of state = 0.003605 m^3/mol, V^L using the van der Waals equation of state = 4.31×10^{-5} m^3/mol, V^V using the van der Waals equation of state = 0.003647 m^3/mol)

3.2 Calculate the bubble point and dew point temperatures for the acetone (1)–water (2) system at 101.325 kPa for feed composition $z_1 = 0.9$. Assume the system to follow Raoult's law.
(**Ans:** Bubble point temperature = 58.58°C, dew point temperature = 66.93°C)

3.3 Calculate the composition of the liquid and vapour phases for the acetone (1)– acetonitrile (2)–nitromethane (3)–system. The feed composition is $z_1 = 0.25$, $z_2 = 0.5$ and $z_3 = 0.25$. At the given temperature: $P_1^{\text{sat}} = 195.75$ kPa, $P_2^{\text{sat}} = 97.84$ kPa, and $P_3^{\text{sat}} = 50.32$ kPa. The pressure of the system is 100 kPa. Assume the system to follow Raoult's law.
(**Ans:** $x_1 = 0.175384$, $y_1 = 0.343313$, $x_2 = 0.504845$, $y_2 = 0.493941$, $x_3 = 0.320819$, $y_3 = 0.161436$. The number of moles in the vapour phase is 0.444331.)

3.4 Consider a binary vapour–liquid equilibrium system. The Antoine equations of the components are given by

$$\ln P_1^{\text{sat}} = 16.678 - \frac{3640.2}{T + 219.61}$$

$$\ln P_2^{\text{sat}} = 16.2887 - \frac{3816.44}{T + 227.02}$$

where the temperature is in °C and the vapour pressure in kPa. The parameters in the Wilson equation are: a_{12} = 437.98 cal/mol and a_{21} = 1238 cal/mol. The molar volumes of the components are V_1 = 76.92 cm^3/mol and V_2 = 18.07 cm^3/mol. Assume the system to follow the modified Raoult's law.

(i) Calculate the bubble point pressure at 100°C and x_1 = 0.3.
(ii) Calculate the bubble point temperature at 101.325 kPa and x_1 = 0.3.
(iii) Calculate the dew point pressure at 100°C and y_1 = 0.3.
(iv) Calculate the dew point temperature at 101.325 kPa and y_1 = 0.3.

[**Ans:** (i) 193.78 kPa, (ii) 82.18°C, (iii) 140.78 kPa, and (iv) 91.00°C]

3.5 Calculate the composition of the liquid and vapour phases for the acetone (1)–water (2) system at 100°C and 200 kPa. The feed composition is z_1 = 0.5. The Antoine equations of the components are given by

$$\ln P_1^{\text{sat}} = 14.39155 - \frac{2795.817}{T + 230.002}$$

$$\ln P_2^{\text{sat}} = 16.26205 - \frac{3799.887}{T + 226.346}$$

where the temperature is in °C and the vapour pressure in kPa. The parameters in the Wilson equation are: a_{12} = 292.66 cal/mol and a_{21} = 1445.26 cal/mol. The molar volume of the components is V_1 = 74.05 cm^3/mol and V_2 = 18.07 cm^3/mol. Assume the system to follow the modified Raoult's law.

[**Ans:** Bubble point pressure = 334.97 kPa, dew point pressure = 195.68 kPa, number of moles in vapour phase = 0.974685, x_1 = 0.045018, y_1 = 0.511817]

3.6 Calculate the vapour pressure of water at 120°C using the Peng–Robinson cubic equation of state. For water: T_C = 647.1 K, P_C = 220.55 bar, and ω = 0.345.

(**Ans:** 191689.125 Pa)

3.7 Consider the methanol (1) – water (2) system in vapour–liquid equilibrium. The temperature of the system is 100°C and the liquid phase composition is x_1 = 0.5. Determine the system pressure and the vapour phase composition. Use the Gamma-Phi approach. The Antoine equations of the components are given by

$$\ln P_1^{\text{sat}} = 16.5938 - \frac{3644.3}{T + 239.76}$$

$$\ln P_2^{\text{sat}} = 16.2620 - \frac{3799.89}{T + 226.35}$$

where the temperature is in °C and the vapour pressure in kPa. The parameters in the Wilson equation are: a_{12} = 107.38 cal/mol and a_{21} = 469.55 cal/mol. The molar volumes of the components are V_1 = 40.73 cm^3/mol and V_2 = 18.07 cm^3/mol. T_{C1} = 512.6 K, P_{C1} = 80.97 bar, ω_1 = 0.564, Z_{C1} = 0.224, T_{C2} = 647.1 K, P_{C2} = 220.55 bar, ω_2 = 0.345, Z_{C2} = 0.229.

(**Ans:** Pressure = 253786 Pa, $y_1 = 0.757692$)

3.8 Consider the CO_2 (1) – *n*-pentane (2) system in vapour–liquid equilibrium. The temperature of the system is 377.65 K and the liquid phase composition is x_1 = 0.35. Determine the system pressure and the vapour phase composition using the Peng–Robinson cubic equation of state. T_{C1} = 304.2 K, P_{C1} = 73.83 bar, ω_1 = 0.224, T_{C2} = 469.7 K, P_{C2} = 33.70 bar, ω_2 = 0.252.

(**Ans:** Pressure = 4572206 Pa, $y_1 = 0.782462$)

3.9 Calculate the adiabatic flame temperature of a gas initially at 25°C containing 1 mol C_2H_6 (1), 5 mol O_2 (2), 10 mol CO_2 (3) and 0 mol of H_2O (4). The ethane is completely burned. The standard heat capacity is given by $C_P^0 = a + bT + cT^2 + dT^3$ where T is in K and C_P^0 in cal/mol-K.

Species	a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$
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CO_2	5.316	1.4285	−0.8362	1.784
$H_2O(g)$	7.700	0.04594	0.2521	−0.8587

The standard enthalpy of formation at 298.15 K is: $\Delta H^0_{f,\, CO_2}$ = –94.052 kcal/mol, $\Delta H^0_{f,\, H_2O(g)} = -57.7979$ kcal/mol, and $\Delta H^0_{f, C_2H_6} = -20.236$ kcal/mol.

(**Ans:** AFT = 2024.45 K)

Chapter 4

Initial Value Problems

Consider two simultaneous differential equations $\frac{dy}{dx} = z$ and $\frac{dz}{dx} = -y$. The analytical solution of the differential equations is $y = A \sin(x + \alpha)$ and $z = A \cos(x + \alpha)$. There are two constants of integration A and α. In general, a system of N first order equations has N constants of integration. If the values of the dependent variables y and z are specified for a value of x, then the problem of determining the values of y and z at some future x is called an *initial value problem*. Alternatively, the values of some of the dependent variables may be specified at a number of different values of x, then the problem is called a *boundary value problem*. The most common form is a two-point boundary value problem where the function values are given for two values of x. Boundary value problems are discussed in Chapters 5–10.

The examples discussed here include the calculation of temperature profile in a double pipe heat exchanger, of a single stirred tank with coil heater and also of a series of stirred tanks with coil heater. The velocity profile of a solid particle in a pneumatic conveyor, and the calculation of the concentration profile in the batch, stirred and plug flow reactors is also discussed in this chapter.

4.1 Solution of Single Ordinary Differential Equation

Consider an ordinary differential equation

$$\frac{dy}{dx} = f(x, y) \tag{4.1}$$

with the initial condition: at $x = x_0$, $y = y_0$. The ordinary differential equation has to be integrated to determine the value of y at some x. A step size, h, is chosen in the independent variable. At the initial condition both x and y are known and after a step size in independent variable, i.e. at $x = x_0 + h$ the value of y is computed. Then this becomes the starting point for the next value of independent variable, $x = x_0 + 2h$ at which the value of dependent variable is determined. This procedure is repeated till the value of x at which the y-value is to be determined is reached. For each problem there exists an optimum step size. The step size should not be high, otherwise the truncation errors will be high, and if the step size is very small, then round-off errors are high. At the optimum step size the total error (truncation error + round-off error) is the least, and thus the numerical results are accurate.

In the numerical formulation of the problem some terms are left out; those errors are called *truncation errors*. When the step size is small, these errors are less. If the step size is very low, then the truncation errors are less but the round-off errors are high. Consider a step size of 10^{-6} m; then to go from 1 to 10 m, the number of iterations required is 10^7, which is huge. Whenever the new concentration is computed, the number is not completely stored, it is stored up to some decimal places only, depending on the compiler used. So to avoid round-off errors the step size should not be very small and to avoid truncation errors it should not be very large. So there is an optimum step size and it varies with the problem. To determine the optimum step size, at a particular value of independent variable x the value of the dependent variable y is determined using various step sizes. When for two consecutive step sizes the value of y is the same, then the higher of the two is the optimum step size.

In the Runge–Kutta fourth order method the following are computed:

$$k_1 = h \times f\left(x_0, y_0\right) \tag{4.2}$$

$$k_2 = h \times f\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1\right) \tag{4.3}$$

$$k_3 = h \times f\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2\right) \tag{4.4}$$

$$k_4 = h \times f\left(x_0 + h, y_0 + k_3\right) \tag{4.5}$$

$$y_1 = y_0 + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{4.6}$$

From the initial condition (x_0, y_0) we have determined the value of y at $x_0 + h$. Now again the above calculations are carried out to determine the value of y at $x_0 + 2h$. But before carrying out the next calculation the following statements, due to which the value of y_1 becomes y_0 and $x_0 + h$ becomes x_0, are executed:

$$x_0 = x_0 + h \tag{4.7}$$

$$y_0 = y_1 \tag{4.8}$$

EXAMPLE 4.1 Integrate the ordinary differential equation

$$\frac{dy}{dx} = x + y$$

using the Runge–Kutta fourth order method. The initial condition is: at $x = 0$, $y = 0$. Determine the value of y at $x = 0.2$. The analytical solution is given by $y = e^x - x - 1$.

Solution Let us take step size of $h = \Delta x = 0.1$. The function is $f = \frac{dy}{dx} = x + y$. To compute y at $x = 0.1$ the starting point is $x_0 = 0$ and $y_0 = 0$. The calculations are given below.

$f(0,0) = 0$; therefore $k_1 = 0.1 \times f(0,0) = 0$;

$f(0.05,0) = 0.05$; therefore $k_2 = 0.1 \times 0.05 = 0.005$;

$f(0.05,0.0025) = 0.0525$; therefore $k_3 = 0.00525$;

$f(0.1,0.00525) = 0.10525$; therefore $k_4 = 0.010525$.

Thus

$$y_1 = y_0 + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) = 0.0051708 \qquad \text{at } x = 0.1$$

Now let us compute the value of y at $x = 0.2$. For this computation the starting point is $x_0 = 0.1$ and $y_0 = 0.0051708$. The calculations are given below.

$f(0.1, 0.0051708) = 0.1051708$; therefore $k_1 = 0.01051708$;

$f(0.15, 0.01042934) = 0.16042934$; therefore $k_2 = 0.0160429$;

$f(0.15, 0.01319225) = 0.16319225$; therefore $k_3 = 0.016319225$;

$f(0.2, 0.02149) = 0.22149$; therefore $k_4 = 0.022149$.

Thus

$$y = 0.0051708 + \frac{1}{6}\left(0.01051708 + 2 \times 0.0160429 + 2 \times 0.016319225 + 0.022149\right) = 0.0214025$$

Thus the value of y (at $x = 0.2$) = 0.0214025.
The analytical solution at $x = 0.2$ is $y = e^{0.2} - 0.2 - 1 = 0.0214028$, which is close to the numerical solution.

EXAMPLE 4.2 Solve the following ordinary differential equation:

$$\frac{dy}{dx} = -\frac{y}{1+x}$$

with the initial condition $y(0) = 2$. Determine y at $x = 2.5$ using the fourth-order Runge–Kutta method.

Solution The initial condition is: at $x = 0$: $y = 2$. We have to determine y at $x = 2.5$. The result from Program 4.1 (given in the Appendix) at step size of 0.01 is: at $x = 2.5$, $y = 0.57$.

4.2 Double Pipe Heat Exchanger

The schematic diagram of the inner pipe of the double pipe heat exchanger is shown in Fig. 4.1. The outer pipe contains steam at temperature T_S and the fluid in the inner pipe is heated.

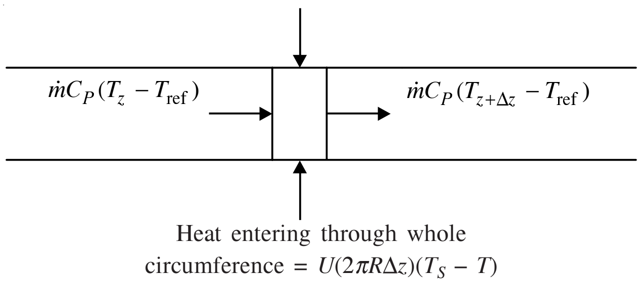


Fig. 4.1 Schematic diagram of double pipe heat exchanger.

Consider a differential section of the inner pipe. Through the circumference of the inner pipe heat enters from steam in the outer pipe. Under steady conditions (Input – Output = 0)

$$\dot{m}C_P\left(T_z - T_{\text{ref}}\right) - \dot{m}C_P\left(T_{z+\Delta z} - T_{\text{ref}}\right) + U\pi D\Delta z\left(T_S - T\right) = 0$$

Dividing by Δz, we get

$$-\dot{m}C_P\left(\frac{T_{z+\Delta z} - T_z}{\Delta z}\right) + U\pi D\left(T_S - T\right) = 0$$

As $\Delta z \to 0$, we get

$$-\dot{m}C_P\frac{dT}{dz} + U\pi D\left(T_S - T\right) = 0 \tag{4.9}$$

where T is the temperature of the fluid in the inner pipe and is a function of length, T_S is the temperature of steam in the outer pipe and is constant, and $\dot{m}$ is the mass flow rate of fluid in inner pipe. The analysis of the double pipe heat exchanger is described in the example below.

EXAMPLE 4.3 On one side of a double pipe heat exchanger is saturated steam and water is flowing in the inner tube. The temperature of entering water is 20°C and the velocity of water is 1 m/s. The inner diameter of the inner pipe is 2.4 cm. Under steady conditions, determine the temperature of water at the length of 5 and 10 m from the inlet. The total length of the heat exchanger is 10 m. Assume that the temperature does not change along the radius of the pipe. The density of water is 1000 kg/m^3 and the specific heat capacity is 4184 J/kg-K. The overall heat transfer coefficient based on the inside area of the inner pipe is 200 W/m^2-K and the temperature of saturated steam is 250°C.

Solution The mass flow rate of water is

$$\dot{m} = \rho vA = 1000 \times 1 \times \pi\left(\frac{1.2}{100}\right)^2 = 0.4524 \text{ kg/s}$$

Eq. (4.9) becomes

$$-0.4524 \times 4184\frac{dT}{dz} + 200 \times 3.1416 \times 0.024 \times \left(250 - T\right) = 0$$

$$\frac{dT}{dz} = 7.97 \times 10^{-3}\left(250 - T\right)$$

The initial condition is: at $z = 0$, $T = 20$. The temperature is to be determined at $z = 5$ and $z = 10$. The differential equation is integrated using the Runge–Kutta fourth order method. Program 4.1 can be modified, and with step size of 0.01 m, we get at $z = 5$ m, $T = 28.97$°C and at $z = 10$ m, $T = 37.60$°C.

Let us now check the answer. The exit temperature of water at $z = 10$ m is 37.60°C. The heat taken up by water is equal to $UA\Delta T_{\text{lmtd}}$, and from the energy balance equation we get

$$U\pi DL\Delta T_{\text{lmtd}} = \dot{m}C_P(T_2 - T_1)$$

where T_1 is the temperature of the inlet water, T_2 is the temperature of the exit water, and L = 10 m. The temperatures in the double pipe heat exchanger are shown in Fig. 4.2.

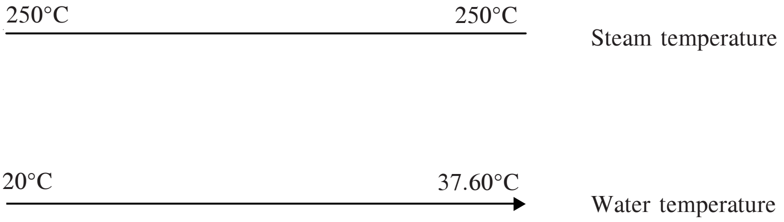


Fig. 4.2 Diagram for Example 4.3.

The log mean temperature difference is given by

$$\Delta T_{\text{lmtd}} = \frac{230 - 212.4}{\ln\left(\dfrac{230}{212.4}\right)} = 221.08$$

Substituting the values in the energy balance equation, we get

$$U = \frac{\dot{m} C_P (T_2 - T_1)}{\pi D L \Delta T_{\text{lmtd}}} = \frac{0.4524 \times 4184 \times 17.6}{\pi \times 0.024 \times 10 \times 221.08} = 199.86 \text{ W/m}^2\text{-K}$$

which is close to the given value. In this problem the overall heat transfer coefficient is given and temperature of water is determined. Usually in heat transfer laboratory experiments, the exit temperature of water is known and the overall heat transfer coefficient is determined.

4.3 Stirred Tank with Coil Heater

The schematic diagram of a stirred tank with coil heater is shown in Fig. 4.3.

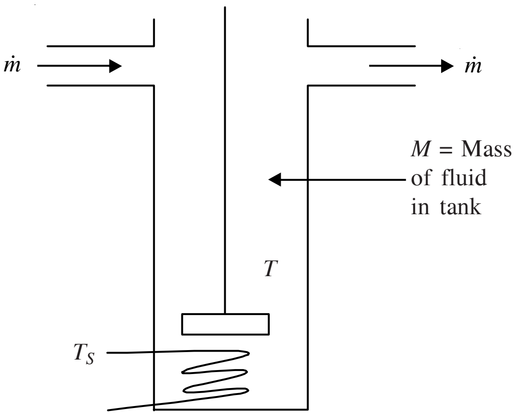


Fig. 4.3 Schematic diagram of stirred tank with coil heater.

The energy balance equation is given by Accumulation = Input – Output. The input is due to energy input by the entering stream and the heat input from the steam, and the output is energy carried away by the exit stream. From the energy balance equation, we get

$$MC_P \frac{dT}{dt} = \dot{m}C_P\left(T_1 - T\right) + \dot{Q} \tag{4.10}$$

where T_1 is the temperature of the entering stream and T is the temperature of exit stream and is equal to temperature of water in the stirred tank. The heat transfer between the steam in the coil and the fluid is given by $Q = UA\Delta T_{\text{lmtd}} = UA(T_S - T)$. The temperature throughout the coil is T_S as the steam is saturated, and outside the whole coil, that is inside the tank uniform temperature, T exists as the vessel is stirred; therefore $\Delta T_{\text{lmtd}} = T_S - T$. Note that though the temperature in the tank is uniform, it varies with time.

EXAMPLE 4.4 Consider a stirred tank heater. It is a square tank 0.5 m on its sides and 2 m high and is filled with water at 20°C. Water is fed to the tank at a flow rate of 1L/s and exits out at the same flow rate from the top of the tank. The temperature of inlet water is 20°C. At time $t = 0$ s, water in the tank is heated by a coil containing steam whose overall heat transfer coefficient based on the outside area of the coil is 200 W/m^2-K. The outside area of the coil through which heat exchange takes place is 1 m^2. The temperature of the steam is 250°C. The specific heat capacity of water is 4184 J/kg-K. After how much time is the temperature of exit water 28°C? What is the maximum temperature that can be reached in the tank?

Solution Volume of tank = 0.5 × 0.5 × 2 = 0.5 m^3. Since the density of water is 1000 kg/m^3, therefore the mass of water in the tank is 500 kg. Thus $M = 500$ kg, $C_P = 4184$ J/kg-K, $\dot{Q} = UA(T_S - T) = 200(T_S - T)$, and $\dot{m} = 1$ kg/s, and Eq. (4.10) becomes

$$500 \times 4184 \frac{dT}{dt} = 1 \times 4184 \times \left(20 - T\right) + 200 \times \left(250 - T\right)$$

Simplifying, we get

$$\frac{dT}{dt} = 0.064 - 0.0021T$$

The initial condition is: at $t = 0$, $T = 20$°C. We have to determine t at $T = 28$°C. Program 4.1 can be modified, and with step size of 0.1 we get $T = 28$°C at $t = 700$ s. The variation of temperature of the fluid in the tank with time is shown in Table 4.1.

Table 4.1 Variation of fluid temperature in tank with time in Example 4.4

Time (s)	Temperature (°C)
500	26.81
750	28.31
1000	29.19
3000	30.46
5000	30.48

The steady state temperature is obtained when in the differential equation $\frac{dT}{dt} = 0$; thus the steady state temperature is given by $0.064 - 0.0021\,T = 0$ or $T = 30.48°\text{C}$. The same is also obtained from the numerical solution. Note the temperature at 5000 s in Table 4.1.

EXAMPLE 4.5 Consider a stirred vessel which initially contains 760 kg of solvent at 25°C. 12 kg/min of solvent flows into the stirred vessel at 25°C and exits out also at the same rate. At $t = 0$ the flow of steam is started in a coil in the stirred vessel. The heat supplied by steam to the solvent is given by $\dot{Q} = UA(T_S - T)$, where UA is the overall heat transfer coefficient multiplied by coil area through which heat exchange takes place and T_S is the temperature of steam and is 150°C. UA = 11.5 kJ/min-K. The specific heat of the solvent is C_p = 2.3 kJ/kg-K. Show that

$$\frac{dT}{dt}\,(^{\text{o}}\text{C/s}) = 0.023 - 0.000373T$$

Determine the solvent temperature after 50 min. Also determine the maximum temperature that can be reached in the tank.

Solution From the energy balance equation we know: Accumulation = Input – Output. Here input energy is due to incoming fluid and steam and output is due to outgoing fluid. Substituting the values in Eq. (4.10), we get

$$760 \times 2.3\frac{dT}{dt} = \frac{12}{60} \times 2.3(25 - T) + \frac{11.5}{60}(150 - T)$$

Note that $\Delta T_{\text{lmtd}} = T_S - T$, where T is the temperature of the fluid in the stirred tank. In the coil throughout the temperature is T_S and the fluid temperature is T. Simplifying the above equation, we get

$$\frac{dT}{dt} = 0.023 - 0.000373T$$

The initial condition is: at $t = 0$, $T = 25°\text{C}$. We have to determine T at $t = 3000$ s. Program 4.1 can be modified, and with step size of 0.01 we get: at $t = 3000$ s, $T = 49.69°\text{C}$. The variation of temperature of the fluid in the tank with time is shown in Table 4.2.

Table 4.2 Variation of fluid temperature in tank with time in Example 4.5

Time (s)	Temperature (°C)
1000	36.41
2000	44.27
3000	49.69
5000	55.98
7500	59.43
10000	60.78
15000	61.53
20000	61.64
25000	61.66

The steady state temperature is obtained when in the differential equation, $\frac{dT}{dt} = 0$, thus the steady state temperature is given by $0.023 - 0.000373T = 0$ or $T = 61.66$°C. The same is also obtained from the numerical solution. Note the temperature at 25000 s in Table 4.2.

4.4 Pneumatic Conveying

Consider a pneumatic conveyor in which solids are inserted from the bottom along with the flowing gas. The forces acting on the particle are: drag force acting upwards, buoyancy force acting upwards and gravitational force acting downwards. The momentum balance equation becomes [see Eq. (2.15)]

$$\rho_p \frac{dv_p}{dt} = \frac{F_D + F_b - F_g}{V_p}$$

where ρ_p is the density of the particle, v_p is the upward velocity of the particle, F_D is the drag force acting on the particle, F_b is the buoyancy force acting on the particle, F_g is the gravitational force acting on the particle, and V_p is the volume of the particle. The drag force is given by

$$C_D = \frac{F_D/A_p}{\frac{1}{2}\rho_g \left(v_g - v_p\right)^2} \tag{4.11}$$

where ρ_g is the density of the gas, A_p is the projected area of the particle on a plane at right angles to the direction of motion, and $v_g - v_p$ is the relative velocity. The gravitational force minus the buoyancy force on the particle is given by [see Eq. (2.17)]

$$F_g - F_b = V_p\left(\rho_p - \rho_g\right)g$$

The various forces acting are shown in Figure 4.4.

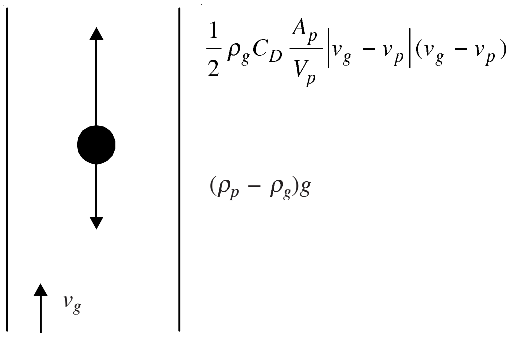


Fig. 4.4 Various forces (divided by volume of particle) acting on particle during pneumatic conveying.

Thus the momentum balance equation becomes

$$\rho_p \frac{dv_p}{dt} = \frac{1}{2} C_D \rho_g \frac{A_p}{V_p} \left(v_g - v_p\right)^2 + \left(\rho_g - \rho_p\right) g \tag{4.12}$$

Note that the terms have units of force acting on the particle divided by the volume of the particle. Dividing both sides of the equation by ρ_p, we get

$$\frac{dv_p}{dt} = \frac{1}{2} C_D \frac{\rho_g}{\rho_p} \frac{A_p}{V_p} \left(v_g - v_p\right)^2 + \left(\frac{\rho_g}{\rho_p} - 1\right) g$$

The derivative

$$\frac{dv_p}{dt} = v_p \frac{dv_p}{dz}$$

where z is the direction along the length of the pneumatic conveyor. Thus the momentum balance equation can be written as

$$v_p \frac{dv_p}{dz} = \frac{1}{2} C_D \frac{\rho_g}{\rho_p} \frac{A_p}{V_p} \left(v_g - v_p\right)^2 + \left(\frac{\rho_g}{\rho_p} - 1\right) g \tag{4.13}$$

Program 4.2 uses the Runge–Kutta fourth order method for integrating the above ordinary differential equation and is given in the Appendix.

EXAMPLE 4.6 Determine the velocity of the solid particles of diameter 3 × 10^{-4} m along the length of the pneumatic conveyor. The initial velocity of the particle is zero and superficial velocity of air is 12 m/s. The density of the particle is 900 kg/m^3. Air is fed at 25°C and 1 atm and the viscosity of air under these conditions is 1.8 × 10^{-5} kg/m-s. Neglect wall effects. Use the following relation to determine C_D:

$$C_D = \frac{24}{\text{Re}_p}\left(1 + 0.15\,\text{Re}_p^{0.687}\right)$$

where Re_p is the particle Reynolds number based on relative velocity and is given by

$$\text{Re}_p = \frac{\rho_g \left(v_g - v_p\right) d_p}{\mu}$$

Solution The following data are given:

d_p = 3 × 10^{-4} m

v_g = 12 m/s

μ = 1.8 × 10^{-5} kg/m-s.

The density of air under the given conditions is given by

$$\rho_g = \frac{PM}{RT} = \frac{101325 \times 28.84 \times 10^{-3}}{8.314 \times 298.15} = 1.1789\ \text{kg/m}^3$$

The projected area of the particle divided by the volume of the particle is given by

$$\frac{A_p}{V_p} = \frac{\pi r_p^2}{\frac{4}{3}\pi r_p^3} = \frac{0.75}{r_p} = \frac{1.5}{d_p} = \frac{1.5}{3 \times 10^{-4}} = 5000 \text{ m}^{-1}$$

The particle Reynolds number is

$$\text{Re}_p = \frac{\rho_g \left(v_g - v_p\right) d_p}{\mu} = \frac{1.1789 \times \left(12 - v_p\right) \times 3 \times 10^{-4}}{1.8 \times 10^{-5}} = 19.648\left(12 - v_p\right)$$

The momentum balance equation is

$$v_p \frac{dv_p}{dz} = \frac{1}{2} C_D \frac{\rho_g}{\rho_p} \frac{A_p}{V_p} \left(v_g - v_p\right)^2 + \left(\frac{\rho_g}{\rho_p} - 1\right) g$$

$$v_p \frac{dv_p}{dz} = \frac{5000}{2} C_D \frac{1.1789}{900} \left(12 - v_p\right)^2 + \left(\frac{1.1789}{900} - 1\right) 9.81$$

$$\frac{1}{2} \frac{dv_p^2}{dz} = 3.2747 C_D \left(12 - v_p\right)^2 - 9.797$$

Let $y = v_p^2$; thus

$$\frac{dy}{dz} = 6.55 C_D \left(12 - \sqrt{y}\right)^2 - 19.594$$

where $\text{Re}_p = 19.648\left(12 - \sqrt{y}\right)$ and $C_D = \frac{24}{\text{Re}_p}\left(1 + 0.15 \text{Re}_p^{0.687}\right)$. The initial condition is at $z = 0$, $y = 0$. The problem can be solved using the Runge–Kutta fourth order method. The velocity of the particle along the length of the pneumatic conveyor as obtained from Program 4.2 is presented in Table 4.3. The step size of 0.01 m is taken.

Table 4.3 Velocity of particle as obtained from Program 4.2

z (m)	v_p (m/s)
0.0	0.00
0.1	5.84
0.2	7.24
0.3	8.06
0.5	9.01
1.0	10.06
2.0	10.67
3.0	10.83
5.0	10.90
10.0	10.90

4.5 Solution of Simultaneous Ordinary Differential Equations

Consider a system of two ordinary differential equations

$$\frac{dy}{dx} = f_1(x, y, z) \tag{4.14}$$

$$\frac{dz}{dx} = f_2(x, y, z) \tag{4.15}$$

with the initial condition: at $x = x_0$, $y = y_0$ and $z = z_0$. The ordinary differential equations have to be integrated to determine the value of y and z at some x. A step size, h, is chosen in the independent variable and after a step size in independent variable, i.e., at $x = x_0 + h$ the value of y and z are to be computed. In the Runge–Kutta fourth order method the following are computed:

$$k_1 = h \times f_1(x_0, y_0, z_0) \tag{4.16}$$

$$l_1 = h \times f_2(x_0, y_0, z_0) \tag{4.17}$$

$$k_2 = h \times f_1\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right) \tag{4.18}$$

$$l_2 = h \times f_2\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1, z_0 + \frac{1}{2}l_1\right) \tag{4.19}$$

$$k_3 = h \times f_1\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2, z_0 + \frac{1}{2}l_2\right) \tag{4.20}$$

$$l_3 = h \times f_2\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2, z_0 + \frac{1}{2}l_2\right) \tag{4.21}$$

$$k_4 = h \times f_1(x_0 + h, y_0 + k_3, z_0 + l_3) \tag{4.22}$$

$$l_4 = h \times f_2(x_0 + h, y_0 + k_3, z_0 + l_3) \tag{4.23}$$

$$y_1 = y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{4.24}$$

$$z_1 = z_0 + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4) \tag{4.25}$$

From the initial condition (x_0, y_0, z_0), we have determined the value of y and z at $x_0 + h$. Now again, the above calculations are carried out to determine the value of y and z at $x_0 + 2h$. But before carrying out the next calculation the following statements are executed, due to which the value of y_1 becomes y_0, z_1 becomes z_0 and $x_0 + h$ becomes x_0:

$$x_0 = x_0 + h$$

$$y_0 = y_1$$

$$z_0 = z_1$$

EXAMPLE 4.7 Integrate the ordinary differential equations

$$\frac{dx}{dt} = x + 2y$$

$$\frac{dy}{dt} = 3x + 2y$$

using the Runge–Kutta fourth order method. The initial condition is: at $t = 0$, $x = 6$, $y = 4$. Determine the values of x and y at $t = 0.2$. The analytical solution is given by $x = 4e^{4t} + 2e^{-t}$ and $y = 6e^{4t} - 2e^{-t}$.

Solution Take step size of $h = \Delta t = 0.1$. The functions are $f_1 = \frac{dx}{dt} = x + 2y$ and $f_2 = \frac{dy}{dt} = 3x + 2y$. To compute the value at $t = 0.1$ the starting point is $t_0 = 0$, $x_0 = 6$ and $y_0 = 4$. The calculations are given below.

$f_1(0, 6, 4) = 14$; therefore $k_1 = 1.4$;

$f_2(0, 6, 4) = 26$; therefore $l_1 = 2.6$;

$f_1(0.05, 6.7, 5.3) = 17.3$; therefore $k_2 = 1.73$;

$f_2(0.05, 6.7, 5.3) = 30.7$; therefore $l_1 = 3.07$;

$f_1(0.05, 6.865, 5.535) = 17.935$; therefore $k_3 = 1.7935$;

$f_2(0.05, 6.865, 5.535) = 31.665$; therefore $l_3 = 3.1665$;

$f_1(0.1, 7.7935, 7.1665) = 22.1265$; therefore $k_4 = 2.21265$;

$f_2(0.1, 7.7935, 7.1665) = 37.7135$; therefore $l_4 = 3.77135$.

Thus

$$x_1 = x_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 7.7766 \qquad (\text{at } t = 0.1)$$

$$y_1 = y_0 + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4) = 7.140725 \qquad (\text{at } t = 0.1)$$

Now let us compute the value of y and z at $t = 0.2$. For this computation the starting point is $t_0 = 0.1$, $x_0 = 7.7766$, and $y_0 = 7.140725$. The calculations are given below.

$f_1(0.1, 7.7766, 7.140725) = 22.05805$; therefore $k_1 = 2.205805$;

$f_2(0.1, 7.7766, 7.140725) = 37.61125$; therefore $l_1 = 3.761125$;

$f_1(0.15, 8.8795, 9.0212875) = 26.922075$; therefore $k_2 = 2.6922075$;

$f_2(0.15, 8.8795, 9.0212875) = 44.681075$; therefore $l_2 = 4.4681075$;

$f_1(0.15, 9.12270375, 9.37477875) = 27.87226$; therefore $k_3 = 2.787226$;

$f_2(0.15, 9.12270375, 9.37477875) = 46.1176687$; therefore $l_3 = 4.61176687$;

$f_1(0.2, 10.563826, 11.75249187) = 34.06881$; therefore $k_4 = 3.406881$;

$f_2(0.2, 10.563826, 11.75249187) = 55.19646$; therefore $l_4 = 5.519646$.

Thus at $t = 0.2$

$$x_2 = 7.7766 + \frac{1}{6}\left(2.205805 + 2\times 2.6922075 + 2\times 2.787226 + 3.406881\right) = 10.5385$$

$$y_2 = 7.140725 + \frac{1}{6}\left(3.761125 + 2\times 4.4681075 + 2\times 4.61176687 + 5.519646\right) = 11.7141$$

From the analytical solution at $t = 0.2$: $x = 10.5396$, $y = 11.7158$, which is close to the numerical solution.

EXAMPLE 4.8 Solve the following ordinary differential equations:

$$\frac{dy}{dx} = z$$

$$\frac{dz}{dx} = -y$$

with the initial condition $y(0) = 2$, $z(0) = 1$. Determine the value of y and z at $x = 3$. Compare the numerical solution with the analytical solution. The analytical solution of the given differential equations is $y = A\sin(x + \alpha)$ and $z = A\cos(x + \alpha)$.

Solution The two simultaneous ordinary differential equations can be written as

$$f_1 = \frac{dy}{dx} = z$$

$$f_2 = \frac{dz}{dx} = -y$$

The initial condition is: at $x = 0$, $y = 2$, $z = 1$. We have to determine y and z at $x = 3$. The result from Program 4.3 at step size of 0.01 is: at $x = 3$: $y = -1.84$, $z = -1.27$. Now let us check the numerical result with the analytical solution. First let us determine the constants A and α. At $x = 0$: $y = 2$, $z = 1$, and thus

$$2 = A\sin(0 + \alpha)$$
$$1 = A\cos(0 + \alpha)$$

Thus $\tan\alpha = 2$ or $\alpha = 63.435°$ and thus $A = 2.236$. From the conversion of radians to degrees we know that 3.1416 radians = 180°. Thus $x = 3 = 171.887°$. At $x = 3$ the following is obtained:

$$y = 2.236\sin(171.887 + 63.435) = -1.84$$
$$z = 2.236\cos(171.887 + 63.435) = -1.27$$

which is the same as numerical solution.

EXAMPLE 4.9 Solve the following ordinary differential equation:

$$\frac{d^2y}{dx^2} = -yx$$

with the initial conditions $y(0) = 2$, $y'(0) = 1$. Determine the value of y at $x = 3$.

Solution Let us take

$$\frac{dy}{dx} = z$$

Then the given differential equation can be written as

$$\frac{dz}{dx} = -yx$$

The two simultaneous differential equations can be written as

$$f_1 = \frac{dy}{dx} = z$$

$$f_2 = \frac{dz}{dx} = -yx$$

The initial condition is at $x = 0$, $y = 2$, $z = 1$. We have to determine y at $x = 3$. Program 4.3 can be modified (only the functions func1 and func2 have to be changed) and with step size of 0.01 we get at $x = 3$: $y = -1.90$, $z = -1.15$.

4.6 Series of Stirred Tanks with Coil Heater

The schematic diagram of a series of stirred tanks with coil heater is shown in Fig. 4.5. The mass in each tank shall be assumed constant as the tank volume and density of oil are assumed constant. The energy balance of tank 1 (accumulation = Input – Output) gives

$$MC_P \frac{dT_1}{dt} = \dot{m}C_P\left(T_0 - T_1\right) + UA\left(T_S - T_1\right)$$

where M is the mass of oil in the tank and $\dot{m}$ is the flow rate of oil. T_0 is the inlet temperature

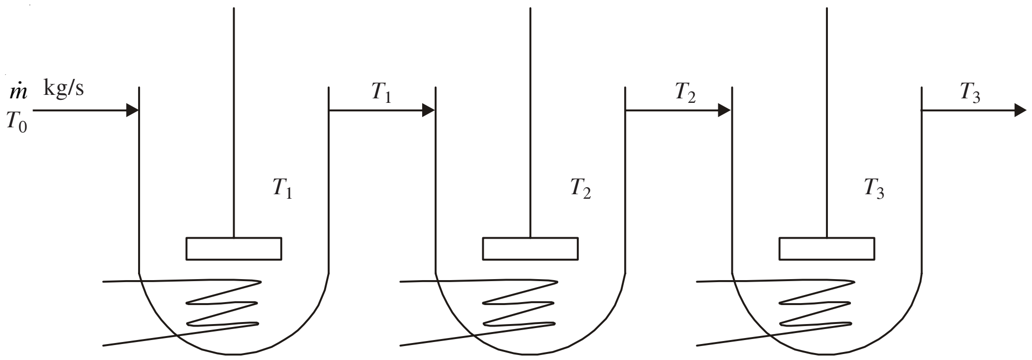


Fig. 4.5 Schematic diagram of series of stirred tanks with coil heater.

of the oil. T_1, T_2, and T_3 are the temperatures of the first, second and third tank respectively. T_S is the temperature of steam. The energy balance of tank 2 gives

$$MC_P \frac{dT_2}{dt} = \dot{m}C_P\left(T_1 - T_2\right) + UA\left(T_S - T_2\right)$$

The energy balance of tank 3 gives

$$MC_P \frac{dT_3}{dt} = \dot{m}C_P\left(T_2 - T_3\right) + UA\left(T_S - T_3\right)$$

The analysis is described in the example below.

EXAMPLE 4.10 Three tanks in series are used to heat oil (see Fig. 4.5). Each tank is initially filled with 1000 kg of oil at 20°C. Saturated steam at 250°C condenses within the coils immersed in each tank. Oil is fed into the first tank at a rate of 2 kg/s and overflows into the second and third tanks at the same flow rate. The temperature of the oil fed to the first tank is 20°C. The tanks are well mixed so that the temperature inside the tanks is uniform and the outlet stream temperature is the temperature within the tank. C_p of oil = 2000 J/kg-K. The rate of heat transferred to the oil from the steam is given by $\dot{Q} = UA(T_S - T)$, where A is the outside area of the coil in one tank, $A = 1$ m^2 and the overall heat transfer coefficient is based on the outside area of the coil, $U = 200$ W/m^2-K. Determine the steady state temperature in all the three tanks. What time interval is required for T_3 to reach 99% of this steady state value?

Solution $UA = 200$ W/K. From the first differential equation we get

$$1000 \times 2000 \frac{dT_1}{dt} = 2 \times 2000\left(20 - T_1\right) + 200\left(250 - T_1\right)$$

$$\frac{dT_1}{dt} = 0.065 - 0.0021 T_1$$

From the second differential equation we get

$$1000 \times 2000 \frac{dT_2}{dt} = 2 \times 2000\left(T_1 - T_2\right) + 200\left(250 - T_2\right)$$

$$\frac{dT_2}{dt} = 0.025 + 0.002 T_1 - 0.0021 T_2$$

From the third differential equation we get

$$1000 \times 2000 \frac{dT_3}{dt} = 2 \times 2000\left(T_2 - T_3\right) + 200\left(250 - T_3\right)$$

$$\frac{dT_3}{dt} = 0.025 + 0.002 T_2 - 0.0021 T_3$$

The initial condition is: at $t = 0$: $T_1 = T_2 = T_3 = 20$°C. Program 4.4 for the solution of above three ordinary differential equations by the Runge–Kutta fourth order method is given in the Appendix. The results at step size of 0.1 is shown in Table 4.4.

Table 4.4 Results in Example 4.10.

Time (s)	T_1 (°C)	T_2 (°C)	T_3 (°C)
1000	29.61	36.08	39.56
2500	30.89	40.98	49.87
7500	30.95	41.38	51.31
15000	30.95	41.38	51.31

The steady state temperature is obtained when in the differential equation $\frac{dT}{dt} = 0$; thus the steady state temperatures are given by

$$T_1 = \frac{0.065}{0.0021} = 30.95\ °\text{C}$$

$$T_2 = \frac{0.002 \times 30.95 + 0.025}{0.0021} = 41.38\ °\text{C}$$

$$T_3 = \frac{0.002 \times 41.38 + 0.025}{0.0021} = 51.31\ °\text{C}$$

The same steady state temperatures are also obtained from the numerical solution. Note the temperature at 7500 s in Table 4.4. We are required to determine the time required for temperature in tank 3 to reach 0.99 × 51.31 = 50.80°C. From Program 4.4 this time is 3150 s.

4.7 Initial Value Problems in Chemical Reaction Engineering

Batch and plug flow reactors are initial value problems. The initial conditions and ordinary differential equations for batch and plug flow reactors are shown in Table 4.5.

Table 4.5 Initial conditions and ODEs for batch and plug flow reactors

Initial Condition for Batch Reactor	ODE's for Batch Reactor	Initial Condition for Plug Flow Reactor	ODEs for Plug Flow Reactor
$A \xrightarrow{k_1} B$			
At $t = 0$: $C_A = 1$ $C_B = 0$	$\frac{dC_A}{dt} = -k_1 C_A$ $\frac{dC_B}{dt} = k_1 C_A$	At $x = 0$: $C_A = 1$ $C_B = 0$	$u\frac{dC_A}{dx} = -k_1 C_A$ $u\frac{dC_B}{dx} = k_1 C_A$

Table 4.5 (*Cont.*)

$A \xrightarrow{k_1} B \xrightarrow{k_2} C$			
At $t = 0$: $C_A = 1$ $C_B = C_C = 0$	$\frac{dC_A}{dt} = -k_1 C_A$ $\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$ $\frac{dC_C}{dt} = k_2 C_B$	At $x = 0$: $C_A = 1$ $C_B = C_C = 0$	$u\frac{dC_A}{dx} = -k_1 C_A$ $u\frac{dC_B}{dx} = k_1 C_A - k_2 C_B$ $u\frac{dC_C}{dx} = k_2 C_B$
$A + B \xrightarrow{k_1} C$ $B + C \xrightarrow{k_2} D$			
At $t = 0$: $C_A = C_B = 1$ $C_C = C_D = 0$	$\frac{dC_A}{dt} = -k_1 C_A C_B$ $\frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_B C_C$ $\frac{dC_C}{dt} = k_1 C_A C_B - k_2 C_B C_C$ $\frac{dC_D}{dt} = k_2 C_B C_C$	At $x = 0$: $C_A = C_B = 1$ $C_C = C_D = 0$	$u\frac{dC_A}{dx} = -k_1 C_A C_B$ $u\frac{dC_B}{dx} = -k_1 C_A C_B - k_2 C_B C_C$ $u\frac{dC_C}{dx} = k_1 C_A C_B - k_2 C_B C_C$ $u\frac{dC_D}{dx} = k_2 C_B C_C$

4.8 Batch and Stirred Tank Reactors

The solution of initial value problems in batch and stirred tank reactors is described with the examples given below.

EXAMPLE 4.11 Consider a reaction $A \rightarrow B$ carried out in a batch reactor. The differential equation for species A is

$$\frac{dC_A}{dt} = -kC_A$$

The initial condition is: at $t = 0$, $C_A = 1$ mol/m^3. The rate constant of the reaction is 1 s^{-1}. Using the Runge–Kutta fourth order method, determine the concentration of A at 3 s.

Solution The differential equation is written in the form $f = -kC_A$. Thereafter the following are computed:

$$k_1 = h \times f\left(t_0, C_0\right)$$

$$k_2 = h \times f\left(t_0 + \frac{1}{2}h, C_0 + \frac{1}{2}k_1\right)$$

$$k_3 = h \times f\left(t_0 + \frac{1}{2}h, C_0 + \frac{1}{2}k_2\right)$$

$$k_4 = h \times f\left(t_0 + h, C_0 + k_3\right)$$

$$C_1 = C_0 + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

$$t_0 = t_0 + h$$

$$C_0 = C_1$$

Program 4.1 can be modified and the results for step size of 0.01 s are presented in Table 4.6.

Table 4.6 Results in Example 4.11

t (s)	C_A (mol/m^3) Numerical solution	C_A (mol/m^3) = e^{-t} Analytical solution
0.0	1.000000	1.000000
1.0	0.367880	0.367879
2.0	0.135335	0.135335
3.0	0.049787	0.049787
5.0	0.006738	0.006738
10.0	0.000045	0.000045

EXAMPLE 4.12 A liquid phase reaction $A \rightarrow B$ is carried out in a stirred vessel reactor. Feed enters the reactor at a rate of $F = 1$ L/s and exits out also at the same flow rate. Both the reactant and product have the same density. The concentration of reactant in the feed is $C_{A0} = 1$ mol/m^3. The volume of the tank is $V = 10$ L and the concentration of A of the solution in the tank is 1 mol/m^3. The vessel may be considered perfectly mixed, so that the concentration of A in the product stream equals that inside the tank. The rate of consumption of A equals kC_A, where $k = 1$ s^{-1}. Determine the concentration of A at various time periods from 0 to 10 s.

Solution Mole balance on component A is given by

Accumulation = Input – Output – Consumption

Moles of A in the reactor = VC_A

$$\text{Accumulation} = \frac{d\left(VC_A\right)}{dt}$$

Input = FC_{A0}

Output = FC_A

Thus from the mole balance of component A, we get

$$\frac{d\left(VC_A\right)}{dt} = FC_{A0} - FC_A - kC_AV$$

Substituting the values we get

$$10\frac{d\left(C_A\right)}{dt} = 1 - C_A - 10C_A$$

$$\frac{dC_A}{dt} = 0.1 - 1.1C_A$$

The initial condition is: at $t = 0$, $C_A = 1$ mol/m^3. Program 4.1 can be modified and at step size of 0.01 the concentration of component *A* in the tank with time is shown in Table 4.7.

Table 4.7 Results in Example 4.12

Time (s)	C_A (mol/m^3)
0.10	0.9053
0.25	0.7891
0.50	0.6212
1.0	0.3969
2.0	0.1927
3.0	0.1248
5.0	0.0947
10.0	0.0909

At steady state, $\frac{dC_A}{dt} = 0$; thus $C_A = \frac{0.1}{1.1} = 0.0909$ mol/m^3. The same is also obtained from numerical solution. Note the concentration at 10 s in the Table 4.7.

***EXAMPLE* 4.13** Consider reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ carried out in a batch reactor. The differential equation for component *A* is

$$\frac{dC_A}{dt} = -k_1 C_A$$

for component *B*

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

for component *C*

$$\frac{dC_C}{dt} = k_2 C_B$$

The initial condition is: at $t = 0$, $C_A = 1$ mol/m^3, $C_B = 0$ mol/m^3, and $C_C = 0$ mol/m^3. The rate constants are $k_1 = 1$ s^{-1} and $k_2 = 1$ s^{-1}. Using the Runge–Kutta fourth order method, determine the concentration of *A, B,* and *C* up to 10 s.

Solution The differential equations are written in the form of functions

$$f_1 = -k_1 A$$
$$f_2 = k_1 A - k_2 B$$
$$f_3 = k_2 B$$

where *A*, *B* and *C* are the concentrations of the components *A*, *B*, and *C*, respectively. The initial condition is at time $t = t_0$, $A = A_0$, $B = B_0$, $C = C_0$. Thereafter the concentrations are computed at time $t = t_0 + h$.

$$k_1 = h \times f_1\left(t_0,\ A_0, B_0, C_0\right)$$

$$l_1 = h \times f_2\left(t_0, A_0, B_0, C_0\right)$$

$$m_1 = h \times f_3\left(t_0, A_0, B_0, C_0\right)$$

$$k_2 = h \times f_1\left(t_0 + \frac{1}{2}h, A_0 + \frac{1}{2}k_1, B_0 + \frac{1}{2}l_1, C_0 + \frac{1}{2}m_1\right)$$

$$l_2 = h \times f_2\left(t_0 + \frac{1}{2}h, A_0 + \frac{1}{2}k_1, B_0 + \frac{1}{2}l_1, C_0 + \frac{1}{2}m_1\right)$$

$$m_2 = h \times f_3\left(t_0 + \frac{1}{2}h, A_0 + \frac{1}{2}k_1, B_0 + \frac{1}{2}l_1, C_0 + \frac{1}{2}m_1\right)$$

$$k_3 = h \times f_1\left(t_0 + \frac{1}{2}h, A_0 + \frac{1}{2}k_2, B_0 + \frac{1}{2}l_2, C_0 + \frac{1}{2}m_2\right)$$

$$l_3 = h \times f_2\left(t_0 + \frac{1}{2}h, A_0 + \frac{1}{2}k_2, B_0 + \frac{1}{2}l_2, C_0 + \frac{1}{2}m_2\right)$$

$$m_3 = h \times f_3\left(t_0 + \frac{1}{2}h, A_0 + \frac{1}{2}k_2, B_0 + \frac{1}{2}l_2, C_0 + \frac{1}{2}m_2\right)$$

$$k_4 = h \times f_1\left(t_0 + h, A_0 + k_3, B_0 + l_3, C_0 + m_3\right)$$

$$l_4 = h \times f_2\left(t_0 + h, A_0 + k_3, B_0 + l_3, C_0 + m_3\right)$$

$$m_4 = h \times f_3\left(t_0 + h, A_0 + k_3, B_0 + l_3, C_0 + m_3\right)$$

$$A_1 = A_0 + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

$$B_1 = B_0 + \frac{1}{6}\left(l_1 + 2l_2 + 2l_3 + l_4\right)$$

$$C_1 = C_0 + \frac{1}{6}\left(m_1 + 2m_2 + 2m_3 + m_4\right)$$

$$t_0 = t_0 + h$$

$$A_0 = A_1$$

$$B_0 = B_1$$

$$C_0 = C_1$$

Program 4.5 for the solution of the above three simultaneous ordinary differential equations by the Runge–Kutta fourth order method is given in the Appendix. The results for step size of 0.01 s are presented in Table 4.8.

Table 4.8 Results in Example 4.13

t (s)	C_A (mol/m^3)	C_B (mol/m^3)	C_C (mol/m^3)
0.0	1.000000	0.000000	0.000000
1.0	0.367880	0.367879	0.264241
2.0	0.135335	0.270671	0.593994
3.0	0.049787	0.149361	0.800852
4.0	0.018316	0.073263	0.908422
5.0	0.006738	0.033690	0.959573
10.0	0.000045	0.000454	0.999503

EXAMPLE 4.14 Consider the following two reactions taking place in a batch reactor:

$$A + B \xrightarrow{k_1} C$$

$$B + C \xrightarrow{k_2} D$$

The concentration of various species with time are given by the following differential equations:

for component A

$$\frac{dC_A}{dt} = -k_1 C_A C_B$$

for component B

$$\frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_B C_C$$

for component C

$$\frac{dC_C}{dt} = k_1 C_A C_B - k_2 C_B C_C$$

for component D

$$\frac{dC_D}{dt} = k_2 C_B C_C$$

The initial conditions are: at $t = 0$, $C_A = 1$ mol/m^3, $C_B = 1$ mol/m^3, $C_C = 0$ mol/m^3, and $C_D = 0$ mol/m^3. The rate constant of the reactions are $k_1 = k_2 = 1$ m^3/mol-s. Using the Runge–Kutta fourth order method determine the concentration of species *A, B, C,* and *D* up to 10 s.

Solution Program 4.6 for solution of the above four simultaneous ordinary differential equations by the Runge–Kutta fourth order method is given in the Appendix. The results for step size of 0.01 s are presented in Table 4.9.

Table 4.9 Results in Example 4.14

t (s)	C_A (mol/m^3)	C_B (mol/m^3)	C_C (mol/m^3)	C_D (mol/m^3)
0.0	1.000000	1.000000	0.000000	0.000000
1.0	0.528875	0.394646	0.336895	0.134230
2.0	0.404510	0.175134	0.366113	0.229376
3.0	0.357692	0.083121	0.367737	0.274571
4.0	0.337090	0.040733	0.366553	0.296357
5.0	0.327357	0.020275	0.365561	0.307082
10.0	0.318152	0.000659	0.364356	0.317492

4.9 Plug Flow Reactor

The solution of initial value problems in plug flow reactor is described with examples given below.

EXAMPLE 4.15 Consider a reaction $A \rightarrow B$ carried out in a plug flow reactor. The differential equation for species A along the length of the plug flow reactor of length 10 m is

$$u\frac{dC_A}{dx} = -kC_A$$

The initial condition is: at $x = 0$ (inlet), $C_A = 1$ mol/m^3.

A fluid medium comprising initially only A flows through the reactor with a mean axial velocity $u = 1$ m/s. The rate constant of the reaction is 1 s^{-1}. Using the Runge–Kutta fourth order method, determine the concentration of A along the length of the plug flow reactor up to 10 m.

Solution Program 4.1 can be modified and the results for step size of 0.01 m are presented in Table 4.10.

Table 4.10 Results in Example 4.15

x (m)	C_A (mol/m^3)
0.0	1.000000
1.0	0.367880
2.0	0.135335
3.0	0.049787
5.0	0.006738
10.0	0.000045

EXAMPLE 4.16 Consider a reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ carried out in a plug flow reactor. The differential equation for component A is

$$u\frac{dC_A}{dx} = -k_1C_A$$

for component *B*

$$u\frac{dC_B}{dx} = k_1 C_A - k_2 C_B$$

for component *C*

$$u\frac{dC_C}{dx} = k_2 C_B$$

The initial condition is: at $x = 0$ (inlet), $C_A = 1$ mol/m^3, $C_B = 0$ mol/m^3, and $C_C = 0$ mol/m^3. A fluid medium comprising initially only *A* flows through the reactor with a mean axial velocity $u = 1$ m/s. The rate constants are: $k_1 = 1$ s^{-1} and $k_2 = 1$ s^{-1}. Using the Runge–Kutta fourth order method, determine the concentration of *A, B,* and *C* along the length of the plug flow reactor up to 10 m.

Solution Program 4.5 can be modified (time replaced by distance along the length of the tubular reactor) and the results for step size of 0.01 m are presented in Table 4.11.

Table 4.11 Results in Example 4.16

x (m)	C_A (mol/m^3)	C_B (mol/m^3)	C_C (mol/m^3)
0.0	1.000000	0.000000	0.000000
1.0	0.371577	0.367861	0.260562
2.0	0.136695	0.272024	0.591281
3.0	0.050287	0.150359	0.799353
4.0	0.018500	0.073814	0.907686
5.0	0.006806	0.033960	0.959234
10.0	0.000046	0.000458	0.999496

EXAMPLE 4.17 Consider the following two reactions taking place in a plug flow reactor:

$$A + B \xrightarrow{k_1} C$$

$$B + C \xrightarrow{k_2} D$$

The concentration of various species with the length of the reactor are given by the following differential equations:
for component *A*

$$u\frac{dC_A}{dx} = -k_1 C_A C_B$$

for component *B*

$$u\frac{dC_B}{dx} = -k_1 C_A C_B - k_2 C_B C_C$$

for component *C*

$$u\frac{dC_C}{dx} = k_1 C_A C_B - k_2 C_B C_C$$

for component *D*

$$u\frac{dC_D}{dx} = k_2 C_B C_C$$

The initial conditions are: at $x = 0$ (inlet), $C_A = 1$ mol/m^3, $C_B = 1$ mol/m^3, $C_C = 0$ mol/m^3, and $C_D = 0$ mol/m^3.

The length of the plug flow reactor is 10 m. A fluid medium comprising initially only A and B flows through the reactor with a mean axial velocity $u = 1$ m/s. The rate constant of the reactions are $k_1 = k_2 = 1$ m^3/mol-s. Using the Runge–Kutta fourth order method, determine the concentration of species A, B, C, and D along the length of the plug flow reactor up to 10 m.

Solution Substituting $k_1 = k_2 = 1$ m^3/mol-s and $u = 1$ m/s in the above ordinary differential equations, we get

$$\frac{dC_A}{dx} = -C_A C_B$$

$$\frac{dC_B}{dx} = -C_A C_B - C_B C_C$$

$$\frac{dC_C}{dx} = C_A C_B - C_B C_C$$

$$\frac{dC_D}{dx} = C_B C_C$$

Program 4.6 can be modified (time replaced by distance along the length of the tubular reactor) and the results for step size of 0.01 m are presented in Table 4.12.

Table 4.12 Results in Example 4.17

x (m)	C_A (mol/m^3)	C_B (mol/m^3)	C_C (mol/m^3)	C_D (mol/m^3)
0.0	1.000000	1.000000	0.000000	0.000000
1.0	0.528875	0.394646	0.336895	0.134230
2.0	0.404510	0.175134	0.366113	0.229376
3.0	0.357692	0.083121	0.367737	0.274571
4.0	0.337090	0.040733	0.366553	0.296357
5.0	0.327357	0.020275	0.365561	0.307082
10.0	0.318152	0.000659	0.364356	0.317492

4.10 Nonisothermal Plug Flow Reactor

EXAMPLE 4.18 Consider the reaction $A \rightarrow B$ carried out in a steam heated heat exchanger reactor. Reactant A is fed at the rate of 1.26 kg/s per tube. The feed consisting of pure A enters the reactor at a temperature of 21°C. It is desired to determine the height of reactor required for 90% conversion of A. The internal diameter of the reactor tubes may be taken as 2.54 cm. Steam at 388.71 K is available for heating purposes. The rate constant of the first order reaction is given by $k = 5.64x10^{13}\exp\left(-\frac{108847}{RT}\right)$, where T is in Kelvin. Take the following parameters: R = 8.314 J/mol-K, ρ = 980.9 kg/m^3, molecular weight of reacting stream, M = 200 g/mol, heat transfer coefficient based on inside area of reactor tube, U = 1900 W/m^2-K, C_p = 15.7 J/kg-K, ΔH^0_{rxn} = 92.9 kJ/mol. Assume the heat of reaction to be independent of temperature.

Solution Since the reaction is first order, $kC_A = \frac{kn_A}{F} = \frac{kn_A^0}{F}(1-X)$, where F is the volumetric flow rate of reactant A and n_A^0 is the inlet molar flow rate of A. The rate constant of the reaction can be written as

$$k = k_1 \exp\left[b\left(1-\frac{1}{\phi}\right)\right]$$

where $b = \frac{E}{RT_1}$, $\phi = \frac{T}{T_1}$ and $k_1 = 5.64 \times 10^{13}\exp(-b)$.

T_1 is a reference temperature and is taken to be the temperature of steam.

$$r_A = -\frac{dn_A}{dV} = n_A^0\frac{dX}{dV} = \frac{n_A^0}{A}\frac{dX}{dz}$$

$$\frac{dX}{dV} = \frac{r_A}{n_A^0} = \frac{k_1\exp\left[b\left(1-\frac{1}{\phi}\right)\right](1-X)}{F}$$

From energy balance on reactants we get

$$\dot{m}C_P\frac{dT}{dz} + r_A A\Delta H^0_{\text{rxn}} - q = 0$$

where $q = Ua(T_S - T)$ and a is the total area of heat transfer per unit length; thus $a = \pi D$ (for one tube). A is the cross-sectional area of the tube based on inside diameter. Thus the above equation becomes

$$-\dot{m}C_P\frac{dT}{dV} + \frac{4U}{D}(T_S - T) - r_A\Delta H^0_{\text{rxn}} = 0$$

$$F = 1.26\frac{\text{kg}}{\text{s}}\frac{1}{980.9}\frac{\text{m}^3}{\text{kg}} = 1.28 \times 10^{-3}\frac{\text{m}^3}{\text{s}}$$

$$b = \frac{E}{RT_1} = \frac{108847}{8.314 \times 388.71} = 33.68$$

$$k_1 = 5.64 \times 10^{13}\exp(-b) = 5.64 \times 10^{13}\exp(-33.68) = 0.133\ S^{-1}$$

$$\frac{dX}{dz}=\frac{Ak_1(1-X)\exp\left[33.68\left(1-\frac{1}{\phi}\right)\right]}{F}$$

$$\frac{Ak_1}{F}=\pi\left(\frac{1.27}{100}\right)^2\frac{0.133}{1.28\times10^{-3}}=0.0527\ \ \text{m}^{-1}$$

Thus

$$\frac{dX}{dz}=0.0527(1-X)\exp\left[33.68\left(1-\frac{T_1}{T}\right)\right]$$

$$\dot{m}C_P=1.26\frac{\text{kg}}{s}15.7\frac{J}{\text{kg}-K}=19.78\frac{W}{K}$$

a, *A* and *U* are all based on the internal diameter of tubes. The inlet molar flow rate of *A* is given by

$$n_A^0=1.26\frac{\text{kg}}{\text{s}}\frac{1\text{mol}}{0.2\text{kg}}=6.3\frac{\text{mol}}{\text{s}}$$

$$-\dot{m}C_P\frac{dT}{Adz}+\frac{4U}{D}(T_S-T)-r_A\Delta H^0_{\text{rxn}}=0$$

$$-\frac{19.78}{\pi(0.0127)^2}\frac{dT}{dz}+\frac{4\times1900}{0.0254}(T_S-T)-r_A\Delta H^0_{\text{rxn}}=0$$

$$r_A=\frac{k_1n_A^0\exp\left[b\left(1-\frac{1}{\phi}\right)\right](1-X)}{F}=\frac{0.133\times6.3\exp\left[33.68\left(1-\frac{T_1}{T}\right)\right](1-X)}{1.28\times10^{-3}}$$

$$r_A=654.61(1-X)\exp\left[33.68\left(1-\frac{T_1}{T}\right)\right]$$

$$r_A\Delta H^0_{\text{rxn}}=654.61\times92900(1-X)\exp\left[33.68\left(1-\frac{T_1}{T}\right)\right]$$

$$r_A\Delta H^0_{\text{rxn}}=6.08\times10^7(1-X)\exp\left[33.68\left(1-\frac{T_1}{T}\right)\right]$$

Thus the energy balance equation becomes

$$-39036\frac{dT}{dz}+299212.6(T_S-T)-6.08\times10^7(1-X)\exp\left[33.68\left(1-\frac{T_1}{T}\right)\right]=0$$

Thus the two simultaneous ordinary differential equations are

$$\frac{dX}{dz} = 0.0527(1 - X)\exp\left[33.68\left(1 - \frac{388.71}{T}\right)\right]$$

$$\frac{dT}{dz} = 7.665(388.71 - T) - 1557.5(1 - X)\exp\left[33.68\left(1 - \frac{388.71}{T}\right)\right]$$

The initial condition is: at $z = 0$, $X = 0$ and $T = 294.15$ K.

Program 4.7 for the solution of the above two simultaneous ordinary differential equations by Runge-Kutta fourth order method is given in the Appendix. The results for step size of 0.1 m are presented in Table 4.13.

Table 4.13 Results in Example 4.18

z (m)	X	T
0.1	0.000026	343.87
0.2	0.000363	359.29
0.3	0.00094	361.51
0.4	0.0015	362.69
0.5	0.0015	362.69
1.0	0.005	364.87
2.0	0.011	365.35
3.0	0.017	365.40
5.0	0.029	365.49
10	0.059	365.71
15	0.088	365.93
20	0.118	366.16
25	0.147	366.40
30	0.176	366.64
35	0.204	366.89
40	0.232	367.14
45	0.260	367.39
50	0.287	367.66
100	0.542	370.65
150	0.752	374.56
200	0.903	379.76
250	0.980	385.59
300	0.998	388.33
350	0.999	388.68

Thus 90% conversion is achieved at a height of 200 m.

Exercises

4.1 Integrate the following ODEs using the Runge–Kutta fourth order method:

$$\frac{dx}{dt} = -10x + 10y$$

$$\frac{dy}{dt} = 28x - y - xz$$

$$\frac{dz}{dt} = -2.666667z + xy$$

Initial condition at $t = 0$: $x = y = z = 5$. Determine $x(20)$, $y(20)$, $z(20)$.

(**Ans:** $x(20) = 6.76$, $y(20) = 12.61$, $z(20) = 10.96$)

4.2 Consider the second order ordinary differential equation

$$\frac{d^2x}{dt^2} + 4\frac{dx}{dt} + 5x = 0$$

with the initial conditions $x(0) = 3$ and $\frac{dx}{dt}(0) = -5$. Compute $x(5)$.

Hint: Take $\frac{dx}{dt} = y$ and thus the given ODE becomes $\frac{dy}{dt} = -5x - 4y$. The two simultaneous differential equations can be solved using the Runge-Kutta fourth order method by taking the following functions.

$$f_1 = \frac{dx}{dt} = y$$

$$f_2 = \frac{dy}{dt} = -5x - 4y$$

Initial condition at $t = 0$: $x = 3$ and $y = -5$. Note that since the ordinary differential equation is second order, therefore two conditions have to be given to completely define the problem.

(**Ans:** $x(5) = -4.9 \times 10^{-6}$)

4.3 Consider the second order ordinary differential equation

$$8\frac{d^2y}{dx^2} - x^2\frac{dy}{dx} + 2y^2 = 0$$

with the initial conditions $y(0) = 1$ and $\frac{dy}{dx}(0) = 0$. Compute $y(1)$.

Hint: Take $\frac{dy}{dx} = z$ and thus the given ODE becomes $\frac{dz}{dx} = \frac{x^2z - 2y^2}{8}$. The two simultaneous differential equations can be solved using the Runge–Kutta fourth order method by taking the following functions:

$$f_1 = \frac{dy}{dx} = z$$

$$f_2 = \frac{dz}{dx} = \frac{x^2 z - 2y^2}{8}$$

Initial condition at $x = 0$: $y = 1$ and $z = 0$.

(**Ans:** $y(1) = 0.8785$)

4.4 Determine the velocity of the solid particles of diameter 0.0003 m in a pneumatic conveyor at length of 10 m. The initial velocity of the particle is zero and superficial velocity of air is 10 m/s. The density of the particle is 900 kg/m^3. Air is fed at 25°C and 1 atm and the viscosity of air under these conditions is 1.8×10^{-5} kg/m-s. Neglect the wall effects. Use the following relation to determine C_D:

$$C_D = \frac{24}{\text{Re}_p}\left(1 + 0.15\,\text{Re}_p^{0.687}\right)$$

where Re_p is the particle Reynolds number based on relative velocity and is given by $\text{Re}_p = \dfrac{\rho_g \left(v_g - v_p\right) d_p}{\mu}$.

(**Ans:** 8.9044 m/s)

4.5 Consider a reaction $A \rightarrow B$ carried out in a batch reactor. The differential equation for species A is

$$\frac{dC_A}{dt} = -\,kC_A$$

The initial condition is: at $t = 0$, $C_A = 1$ mol/m^3. The rate constant of the reaction is 0.1 s^{-1}. Using the Runge–Kutta fourth order method, determine the concentration of A at 10 s.

(**Ans:** 0.36788 mol/m^3)

4.6 Solve Exercise 4.5 for rate constant of the reaction of 0.01 s^{-1}.

(**Ans:** 0.904838 mol/m^3)

4.7 Consider a reaction $A \rightarrow B$ carried out in a plug flow reactor. The differential equation for species A is

$$u\frac{dC_A}{dz} = -\,kC_A$$

The initial condition is: at $z = 0$, $C_A = 1$ mol/m^3. The rate constant of the reaction is 0.1 s^{-1}. Using Runge–Kutta fourth order method, determine the concentration of A at 5 m from entrance. Take $u = 1$ m/s.

(**Ans:** 0.606531 mol/m^3)

4.8 Solve Exercise 4.7 for rate constant of the reaction of 0.01 s^{-1}.

(**Ans:** 0.95123 mol/m^3)

4.9 Consider reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ carried out in a batch reactor. The differential equation for component *A* is

$$\frac{dC_A}{dt} = -k_1 C_A$$

for component *B*

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

for component *C*

$$\frac{dC_C}{dt} = k_2 C_B$$

The initial condition is: at $t = 0$, $C_A = 1$ mol/m^3, $C_B = 0$ mol/m^3, and $C_C = 0$ mol/m^3. The rate constants are: $k_1 = 1$ s^{-1} and $k_2 = 0.1$ s^{-1}. Using the Runge–Kutta fourth order method, determine the concentration of *A, B,* and *C* at 10 s.

(**Ans:** $C_A = 4.54 \times 10^{-5}$ mol/m^3, $C_B = 0.408704$ mol/m^3, $C_C = 0.59125$ mol/m^3)

4.10 Solve Exercise 4.9 for the following rate constants: $k_1 = 0.1$ s^{-1} and $k_2 = 1$ s^{-1}.

(**Ans:** $C_A = 0.3679$ mol/m^3, $C_B = 0.0409$ mol/m^3, $C_C = 0.5912$ mol/m^3)

4.11 Consider reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ carried out in a plug flow reactor. The differential equation for component *A* is

$$u\frac{dC_A}{dx} = -k_1 C_A$$

for component *B*

$$u\frac{dC_B}{dx} = k_1 C_A - k_2 C_B$$

for component *C*

$$u\frac{dC_C}{dx} = k_2 C_B$$

The initial condition is: at $x = 0$, $C_A = 1$ mol/m^3, $C_B = 0$ mol/m^3, and $C_C = 0$ mol/m^3. The rate constants are: $k_1 = 1$ s^{-1} and $k_2 = 0.1$ s^{-1}. Using the Runge–Kutta fourth order method, determine the concentration of *A, B,* and *C* at 5 m from entrance.

(**Ans:** $C_A = 0.006738$ mol/m^3, $C_B = 0.6664$ mol/m^3, $C_C = 0.3268$ mol/m^3)

4.12 Solve Exercise 4.11 for the following rate constants: $k_1 = 0.1$ s^{-1} and $k_2 = 1$ s^{-1}.

(**Ans:** $C_A = 0.6065$ mol/m^3, $C_B = 0.0666$ mol/m^3, $C_C = 0.3268$ mol/m^3)

4.13 Consider the following two reactions taking place in a batch reactor:

$$A + B \xrightarrow{k_1} C$$

$$B + C \xrightarrow{k_2} D$$

The concentration of various species with time are given by the following differential equations:

for component *A*

$$\frac{dC_A}{dt} = -k_1 C_A C_B$$

for component *B*

$$\frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_B C_C$$

for component *C*

$$\frac{dC_C}{dt} = k_1 C_A C_B - k_2 C_B C_C$$

for component *D*

$$\frac{dC_D}{dt} = k_2 C_B C_C$$

The initial conditions are: at $t = 0$, $C_A = 1$ mol/m^3, $C_B = 1$ mol/m^3, $C_C = 0$ mol/m^3, and $C_D = 0$ mol/m^3. The rate constant of the reactions are $k_1 = 1$ m^3/mol-s and $k_2 = 0.1$ m^3/mol-s. Using the Runge–Kutta fourth order method, determine the concentration of species *A*, *B*, *C*, and *D* at 10 s.

(**Ans:** $C_A = 0.1392$ mol/m^3, $C_B = 0.0361$ mol/m^3, $C_C = 0.7576$ mol/m^3, $C_D = 0.1032$ mol/m^3)

4.14 Solve Exercise 4.13 for the following rate constants: $k_1 = 0.1$ m^3/mol-s and $k_2 = 1$ m^3/mol-s.

(**Ans:** $C_A = 0.5899$ mol/m^3, $C_B = 0.2447$ mol/m^3, $C_C = 0.0650$ mol/m^3, $C_D = 0.3452$ mol/m^3)

4.15 Consider the following two reactions taking place in a plug flow reactor:

$$A + B \xrightarrow{k_1} C$$

$$B + C \xrightarrow{k_2} D$$

The concentration of various species are given by the following differential equations:

for component *A*

$$u\frac{dC_A}{dx} = -k_1 C_A C_B$$

for component *B*

$$u\frac{dC_B}{dx} = -k_1 C_A C_B - k_2 C_B C_C$$

for component *C*

$$u\frac{dC_C}{dx} = k_1 C_A C_B - k_2 C_B C_C$$

for component *D*

$$u\frac{dC_D}{dx} = k_2 C_B C_C$$

The initial conditions are: at $x = 0$ (inlet), $C_A = 1$ mol/m^3, $C_B = 1$ mol/m^3, $C_C = 0$ mol/m^3, and $C_D = 0$ mol/m^3. The rate constant of the reactions are $k_1 = 1$ m^3/mol-s and $k_2 = 0.1$ m^3/mol-s. Using the Runge–Kutta fourth order method, determine the concentration of species *A*, *B*, *C*, and *D* at 5 m from the entrance.

(**Ans:** $C_A = 0.1949$ mol/m^3, $C_B = 0.1168$ mol/m^3, $C_C = 0.7269$ mol/m^3, $C_D = 0.0781$ mol/m^3)

4.16 Solve Exercise 4.15 for the following rate constants: $k_1 = 0.1$ m^3/mol-s and $k_2 = 1$ m^3/mol-s.

(**Ans:** $C_A = 0.7009$ mol/m^3, $C_B = 0.4764$ mol/m^3, $C_C = 0.0747$ mol/m^3, $C_D = 0.2244$ mol/m^3)

Chapter 5

Boundary Value Problems

The application of finite difference method for the numerical solution of boundary value problems in ordinary differential equations is discussed in this chapter with various examples. One-dimensional steady heat conduction, steady heat conduction in a fin, and chemical reaction and diffusion in a pore are also discussed in this chapter. The discretization of the convection term is discussed in the next chapter.

5.1 Discretization in One-Dimensional Space

The basic idea of finite difference methods is that the derivatives in differential equations are written in terms of discrete quantities of dependent and independent variables, resulting in simultaneous algebraic equations with all unknowns prescribed at discrete nodal points. Consider a function $y(x)$ and its derivatives at point x. $y(x + \Delta x)$ can be expanded in Taylor series about $y(x)$ as follows:

$$y(x+\Delta x) = y(x) + \Delta x \left.\frac{dy}{dx}\right|_x + \frac{\Delta x^2}{2!}\left.\frac{d^2y}{dx^2}\right|_x + \frac{\Delta x^3}{3!}\left.\frac{d^3y}{dx^3}\right|_x + \cdots \tag{5.1}$$

Simplifying, we get

$$\frac{y(x+\Delta x) - y(x)}{\Delta x} = \left.\frac{dy}{dx}\right|_x + \frac{\Delta x}{2!}\left.\frac{d^2y}{dx^2}\right|_x + \cdots$$

Thus

$$\left.\frac{dy}{dx}\right|_x = \frac{y(x+\Delta x) - y(x)}{\Delta x} + O(\Delta x)$$

The derivative $\left.\frac{dy}{dx}\right|_x$ is of first order in Δx, indicating that the truncation error $O(\Delta x)$ goes to zero like the first power in Δx. That is why we write the derivative at point x as

$$\left.\frac{dy}{dx}\right|_x = \lim_{\Delta x \to 0} \frac{y(x+\Delta x) - y(x)}{\Delta x}$$

Consider a one-dimensional body as shown in Fig. 5.1.

Fig. 5.1 One-dimensional body.

We may write y in Taylor series at $i+1$ and $i-1$ as

$$y_{i+1} = y_i + \Delta x \left.\frac{dy}{dx}\right|_i + \frac{\Delta x^2}{2!}\left.\frac{d^2y}{dx^2}\right|_i + \frac{\Delta x^3}{3!}\left.\frac{d^3y}{dx^3}\right|_i + \frac{\Delta x^4}{4!}\left.\frac{d^4y}{dx^4}\right|_i + \cdots \tag{5.2a}$$

$$y_{i-1} = y_i - \Delta x \left.\frac{dy}{dx}\right|_i + \frac{\Delta x^2}{2!}\left.\frac{d^2y}{dx^2}\right|_i - \frac{\Delta x^3}{3!}\left.\frac{d^3y}{dx^3}\right|_i + \frac{\Delta x^4}{4!}\left.\frac{d^4y}{dx^4}\right|_i + \cdots \tag{5.2b}$$

From Eq. (5.2a), we get the *forward difference* approximation of $\frac{dy}{dx}$ at node i as

$$\left.\frac{dy}{dx}\right|_i = \frac{y_{i+1} - y_i}{\Delta x} + O(\Delta x) \tag{5.3}$$

and from Eq. (5.2b) we get the *backward difference* approximation of $\frac{dy}{dx}$ at node i as

$$\left.\frac{dy}{dx}\right|_i = \frac{y_i - y_{i-1}}{\Delta x} + O(\Delta x) \tag{5.4}$$

Subtracting Eq. (5.2b) from Eq. (5.2a), we get the *central difference* approximation of $\frac{dy}{dx}$ at node i as

$$\left.\frac{dy}{dx}\right|_i = \frac{y_{i+1} - y_{i-1}}{2\Delta x} + O(\Delta x^2) \tag{5.5}$$

It is seen that the truncation errors for the forward difference and backward differences are first order, whereas the central difference yields a second order truncation error. Adding the two equations, we get the central difference approximation of $\frac{d^2y}{dx^2}$ at node i

$$\left.\frac{d^2y}{dx^2}\right|_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} + O(\Delta x^2) \tag{5.6}$$

It should be noted that these finite difference approximations are only valid to some order of Δx. The error in the approximations is called the *truncation error*. It is possible to get approximations which are valid to higher order by using more grid points in the approximations. But for our purposes the approximations given above will be sufficient.

A numerical scheme is called *consistent* if the finite difference approximations have a truncation error that approaches zero in the limit that $\Delta x \to 0$, $\Delta t \to 0$.

Even if the numerical scheme is consistent, we are still not guaranteed that iterating the numerical scheme will give a good approximation to the true solution of the differential equation. A numerical scheme is called *convergent* if the solution of the discretized equations approaches the exact solution of the differential equation in the limit that $\Delta x \to 0$, $\Delta t \to 0$.

For linear equations the issue of convergence is intimately related to the issue of *stability* of the numerical scheme. A scheme is called *stable* if it does not magnify errors that arise in the course of the calculation.

As Δx and Δt are made smaller, the truncation error of approximating the derivatives by finite differences decreases. However, for smaller sizes, more computations need to be done to get solutions for the same domain and total time, which leads to increased *round-off errors*. The total error as a function of these sizes is shown in Fig. 5.2. Here it is assumed that the solution is calculated on the same domain and for the same total time.

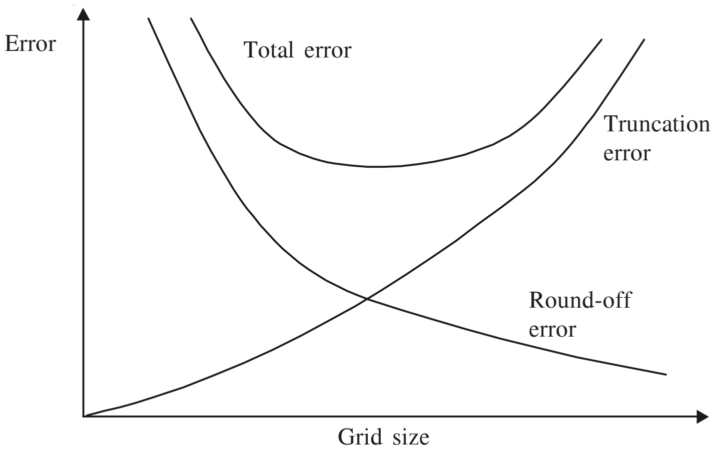


Fig. 5.2 Errors as function of grid size for finite difference calculation.

For a second order differential equation, two boundary conditions have to be specified and thus the problem is called the *two-point boundary value problem*. There are three types of boundary conditions: Dirichlet, Neumann and mixed. Dirichlet boundary condition is the one in which the variable is defined such as $y = 0$ and Neumann boundary condition is the one in which the gradient of the variable is defined perpendicular to the surface such as $\frac{dy}{dn} = 0$. Mixed boundary condition is the one which is a combination of Dirichlet and Neumann, such as $-k\frac{dT}{dx} = h\left(T - T_\infty\right)$. A well-posed problem is the one which has a unique solution.

EXAMPLE 5.1 Using finite difference method, solve the second order one dimensional linear differential equation

$$\frac{d^2y}{dx^2} - 2 = 0 \qquad (0 < x < 1)$$

with the Dirichlet boundary conditions

$$\text{at } x = 0: \; y = 0$$

$$\text{at } x = 1: \; y = 0$$

Compute the value of y at $x = 0.5$. Make two parts (see Fig. 5.3). The exact solution is $y = x^2 - x$.

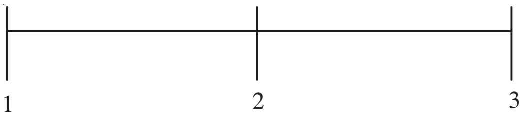


Fig. 5.3 Example 5.1.

Solution The central difference in space gives

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = 2$$

Substituting $i = 2$, we get

$$\frac{y_3 - 2y_2 + y_1}{\Delta x^2} = 2$$

Since two parts are made, therefore $\Delta x = 0.5$. It is given that $y_1 = 0$ and $y_3 = 0$ and we get $y_2 = -\frac{1}{4}$, which is the same as the exact solution.

EXAMPLE 5.2 Using the finite difference method, solve the second order one dimensional linear differential equation

$$\frac{d^2y}{dx^2} - 2 = 0 \qquad (0 < x < 1)$$

with the following boundary conditions:

At $x = 0$: $y = 0$ Dirichlet boundary condition

At $x = 1$: $\frac{dy}{dx} = 1$ Neumann boundary condition

Compute the value of y at $x = 0.5$. Make two parts (see Fig. 5.4).

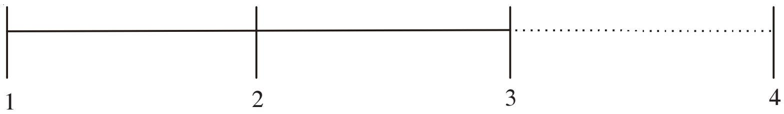


Fig. 5.4 Example 5.2.

Solution The central difference in space gives

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = 2$$

At node 2

$$\frac{y_3 - 2y_2 + y_1}{\Delta x^2} = 2$$

Since $y_1 = 0$, we get

$$y_3 - 2y_2 = 2\Delta x^2$$

At node 3

$$\frac{y_4 - 2y_3 + y_2}{\Delta x^2} = 2$$

where node 4 is a hypothetical node. From the boundary condition at node 3, we get

$$\frac{y_4 - y_2}{2\Delta x} = 1$$

thus $y_4 = y_2 + 2\Delta x$. Therefore

$$\frac{2\Delta x - 2y_3 + 2y_2}{\Delta x^2} = 2$$

Thus

$$\frac{\Delta x - y_3 + y_2}{\Delta x^2} = 1$$

Solving the equations for nodes 2 and 3, we get $y_2 = -\dfrac{1}{4}$ and $y_3 = 0$.

EXAMPLE 5.3 Using finite difference method, solve the differential equation with the source term $f(x)$

$$\frac{d^2y}{dx^2} - 2y = f(x) \qquad (0 < x < 1)$$

$$f(x) = 4x^2 - 2x - 4$$

with the Dirichlet boundary conditions

$$\text{At } x = 0\text{: } y = 0$$

$$\text{At } x = 1\text{: } y = -1$$

The total length is 1 m. Make 3 parts (see Fig. 5.5). The exact solution is $y = -2x^2 + x$.

Fig. 5.5 Example 5.3.

Solution The central difference in space gives

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} - 2y_i = f_i$$

At node 2

$$\frac{y_3 - 2y_2 + y_1}{\Delta x^2} - 2y_2 = f_2$$

$$\frac{y_3 - 2y_2 + 0}{\left(\frac{1}{3}\right)^2} - 2y_2 = -\frac{38}{9}$$

$$9\left(y_3 - 2y_2\right) - 2y_2 = -\frac{38}{9}$$

At node 3

$$\frac{y_4 - 2y_3 + y_2}{\left(\frac{1}{3}\right)^2} - 2y_3 = 4\left(\frac{2}{3}\right)^2 - 2\left(\frac{2}{3}\right) - 4 = -\frac{32}{9}$$

$$9\left(-1 - 2y_3 + y_2\right) - 2y_3 = -\frac{32}{9}$$

Solving the equations for nodes 2 and 3, we get $y_2 = 0.111$ and $y_3 = -0.222$.

EXAMPLE 5.4 Using finite difference method, solve the differential equation with the source term $f(x)$

$$\frac{d^2y}{dx^2} - 2y = f\left(x\right) \qquad (0 < x < 1)$$

$$f\left(x\right) = 4x^2 - 2x - 4$$

subject to the boundary conditions

At $x = 0$: $y = 0$

At $x = 1$: $\frac{dy}{dx} = -3$

The total length is 1 m. Make 3 parts (see Fig. 5.6). The exact solution is $y = -2x^2 + x$.

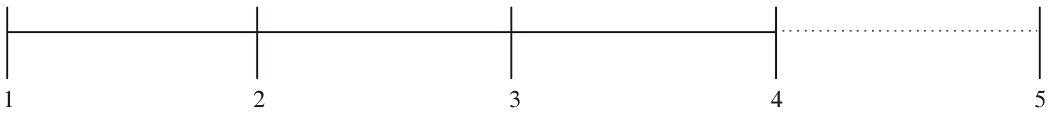


Fig. 5.6 Example 5.4.

Solution The central difference in space gives

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} - 2y_i = f_i$$

At node 2

$$\frac{y_3 - 2y_2 + y_1}{\Delta x^2} - 2y_2 = f_2$$

$$\frac{y_3 - 2y_2 + 0}{\left(\frac{1}{3}\right)^2} - 2y_2 = -\frac{38}{9}$$

$$9(y_3 - 2y_2) - 2y_2 = -\frac{38}{9}$$

At node 3

$$\frac{y_4 - 2y_3 + y_2}{\left(\frac{1}{3}\right)^2} - 2y_3 = 4\left(\frac{2}{3}\right)^2 - 2\left(\frac{2}{3}\right) - 4 = -\frac{32}{9}$$

$$9(y_4 - 2y_3 + y_2) - 2y_3 = -\frac{32}{9}$$

At node 4

$$\frac{y_3 - 2y_4 + y_5}{\left(\frac{1}{3}\right)^2} - 2y_4 = -2$$

$$9(y_3 - 2y_4 + y_5) - 2y_4 = -2$$

where node 5 is a hypothetical node. From the boundary condition at node 4, we get

$\frac{y_5 - y_3}{2\Delta x} = -3$, therefore $y_5 = y_3 - 2$ and the equation for node 4 becomes

$$9(2y_3 - 2y_4 - 2) - 2y_4 = -2$$

Thus the equation of node 2 is

$$-20y_2 + 9y_3 = -\frac{38}{9}$$

Thus the equation of node 3 is

$$9y_2 - 20y_3 + 9y_4 = -\frac{32}{9}$$

Thus the equation of node 4 is

$$18y_3 - 20y_4 = 16$$

The equation can be written as

$$\begin{bmatrix} -20 & 9 & 0 \\ 9 & -20 & 9 \\ 0 & 18 & -20 \end{bmatrix} \begin{bmatrix} y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} -38/9 \\ -32/9 \\ 16 \end{bmatrix}$$

Solving using TDMA, we get $y_2 = \frac{1}{9}$, $y_3 = -\frac{2}{9}$, $y_4 = -1$.

EXAMPLE 5.5 Solve the boundary value problem

$$\frac{d^2y}{dx^2} = y$$

$\frac{dy}{dx}(0) = 0$ and $y(1) = 1$. Take $\Delta x = 0.1$ m. Compare the results with the analytical solution

$$y = \frac{\cosh x}{\cosh 1}$$

Solution The schematic diagram is shown in Fig. 5.7.

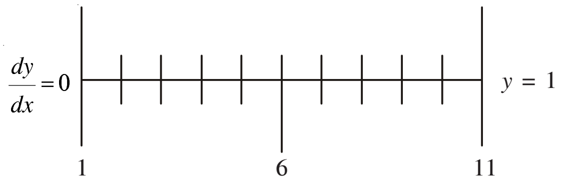


Fig. 5.7 Example 5.5.

Discretizing the given differential equation at node i using the central difference scheme, we get

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = y_i$$

$$y_{i-1} - \left(2 + \Delta x^2\right) y_i + y_{i+1} = 0$$

Since $\Delta x = 0.1$, therefore $\Delta x^2 = 0.01$ and the above equation becomes

$$y_{i-1} - 2.01 y_i + y_{i+1} = 0$$

At node 1

$$y_0 - 2.01 y_1 + y_2 = 0$$

Also at node 1, $\frac{dy}{dx} = 0$, thus $\frac{y_2 - y_0}{2\Delta x} = 0$, thus $y_0 = y_2$ and we get at node 1

$$-2.01 y_1 + 2y_2 = 0$$

At node 2

$$y_1 - 2.01 y_2 + y_3 = 0$$

At node 10

$$y_9 - 2.01 y_{10} + y_{11} = 0$$

Since $y_{11} = 1$, the above equation becomes

$$y_9 - 2.01 y_{10} = -1$$

Thus the unknowns are y_1 to y_{10}. The tridiagonal set of 10 equations becomes

$$\begin{bmatrix} -2.01 & 2 & & & \\ 1 & -2.01 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 1 & -2.01 & 1 \\ & & & 1 & -2.01 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_9 \\ y_{10} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -1 \end{bmatrix}$$

The solution can be obtained by modifying the parameters a_i (i = 2 to N), b_i (i = 1 to N) and c_i (i = 1 to N – 1) in Program 1.1 given in the Appendix. The numerical and analytical solution at nodes 1 to 10 are shown in Table 5.1.

Table 5.1 Numerical and analytical solutions at nodes 1 to 10 for Example 5.5

Node	x (m)	Numerical y	Analytical y
1	0.0	0.6482	0.6481
2	0.1	0.6515	0.6513
3	0.2	0.6612	0.6611
4	0.3	0.6776	0.6774
6	0.5	0.7309	0.7308
9	0.8	0.8668	0.8667
10	0.9	0.9287	0.9287

5.2 One-Dimensional Steady Heat Conduction

The steady heat conduction in one dimension is described with examples given below.

EXAMPLE 5.6 Consider 1-dimensional steady state conduction without heat generation taking place in a rectangular slab. The temperature of the left side of the slab is 100°C and of the right side is 200°C. The length of the slab is 10 cm and the thermal conductivity of the slab is 120 W/cm-K. Make nine uniform divisions. The governing equation is $k\dfrac{d^2T}{dx^2} = 0$

Solution Let us make nine uniform divisions as shown in Fig. 5.8.

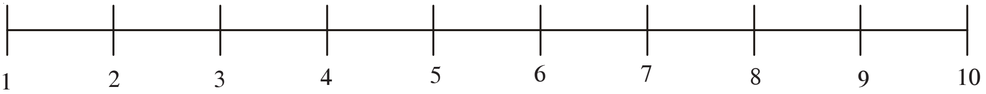


Fig. 5.8 Example 5.6.

Δx = 1.111, T_1 = 100°C, T_{10} = 200°C. Using the central difference scheme, we get

$$k\frac{T_{i+1} + T_{i-1} - 2T_i}{\Delta x^2} = 0$$

$$-T_{i-1} + 2T_i - T_{i+1} = 0$$

The equation for node 2 is

$$2T_2 - T_3 = 100$$

Similar equations can be written for all the nodes and the following set of eight linear algebraic equations is obtained. The equations can be written in tridiagonal form as

$$\begin{bmatrix} 2 & -1 & & & & & & \\ -1 & 2 & -1 & & & & & \\ & -1 & 2 & -1 & & & & \\ & & -1 & 2 & -1 & & & \\ & & & -1 & 2 & -1 & & \\ & & & & -1 & 2 & -1 & \\ & & & & & -1 & 2 & -1 \\ & & & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \end{bmatrix} = \begin{bmatrix} 100 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 200 \end{bmatrix}$$

The solution can be obtained by modifying the parameters a_i (i = 2 to N), b_i (i = 1 to N) and c_i (i = 1 to $N - 1$) in Program 1.1 given in the Appendix. Using TDMA the following solution is obtained:

$$\begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \end{bmatrix} = \begin{bmatrix} 111.11 \\ 122.22 \\ 133.33 \\ 144.44 \\ 155.55 \\ 166.66 \\ 177.77 \\ 188.88 \end{bmatrix}$$

EXAMPLE 5.7 A fin of diameter 0.02 m and length 0.05 m is attached to a wall. The temperature of the wall is 320°C. Determine the temperature of the fin at x = 0.0125, 0.025, 0.0375 and 0.05 m using the finite difference technique taking four parts. The thermal conductivity of the rod is 50 W/m-K and the convective heat transfer coefficient from the rod to the surroundings is 100 W/m^2-K. The temperature of the surroundings is 20°C. The governing differential equation is $-\dfrac{d^2\theta}{dx^2} + \dfrac{hP}{kA}\theta = 0$, where $\theta = T - T_{\text{surr}}$ and the boundary condition at x = 0.05 m is $\dfrac{d\theta}{dx} + \dfrac{h}{k}\theta = 0$.

Solution The schematic diagram of the fin is shown in Fig. 5.9.

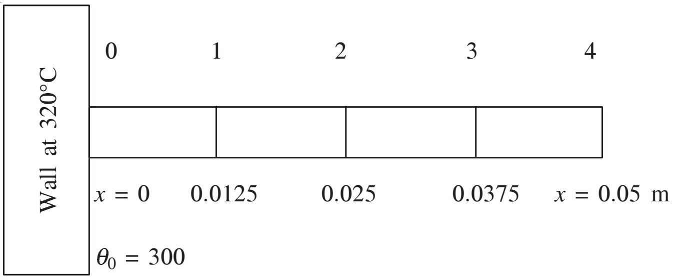


Fig. 5.9 Steady state heat transfer in fin.

Let $m = \sqrt{\frac{hP}{kA}}$.

From the discretization of the differential equation $-\frac{d^2\theta}{dx^2} + \frac{hP}{kA}\theta = 0$, we get

$$-\left(\frac{\theta_{i+1} - 2\theta_i + \theta_{i-1}}{\Delta x^2}\right) + m^2\theta_i = 0$$

Simplifying, we get

$$-\theta_{i-1} + \left[2 + (m\Delta x)^2\right]\theta_i - \theta_{i+1} = 0 \qquad \text{(for } i = 1, 2, 3, 4\text{)}$$

Let $D = 2 + (m\Delta x)^2$. Therefore the above equation becomes

$$-\theta_{i-1} + D\theta_i - \theta_{i+1} = 0$$

Applying the above equation to node 1, we get

$$-\theta_0 + D\theta_1 - \theta_2 = 0$$

Since $\theta_0 = 300$ the above equation becomes $D\theta_1 - \theta_2 = 300$.

Applying the above equation to node 2, we get

$$-\theta_1 + D\theta_2 - \theta_3 = 0$$

Applying the above equation to node 3, we get

$$-\theta_2 + D\theta_3 - \theta_4 = 0$$

Applying the above equation to node 4, we get

$$-\theta_3 + D\theta_4 - \theta_5 = 0$$

where θ_5 is a hypothetical node to the right of node 4.

At $x = L$ (node 4), the equation $\frac{d\theta}{dx} + \frac{h}{k}\theta = 0$ is applicable and the difference equation becomes

$$\frac{\theta_5 - \theta_3}{2\Delta x} + \frac{h}{k}\theta_4 = 0$$

From this expression we can determine θ_5 in terms of θ_3 and θ_4.

$$\theta_5 = \theta_3 - \frac{2h}{k}\theta_4\Delta x$$

Substituting this in the equation for node 4, we get

$$-2\theta_3 + \left(D + \frac{2h\Delta x}{k}\right)\theta_4 = 0$$

Thus the four difference equations are

$$D\theta_1 - \theta_2 = 300$$

$$-\theta_1 + D\theta_2 - \theta_3 = 0$$

$$-\theta_2 + D\theta_3 - \theta_4 = 0$$

$$-2\theta_3 + \left(D + \frac{2h\Delta x}{k}\right)\theta_4 = 0$$

$$m^2 = \frac{hP}{kA} = \frac{h(\pi d)}{k\left(\frac{\pi d^2}{4}\right)} = \frac{4h}{kd} = \frac{4 \times 100}{50 \times 0.02} = 400$$

$$D = 2 + (m\Delta x)^2 = 2 + 400 \times 0.0125 \times 0.0125 = 2.0625$$

Thus the four difference equations are

$$2.0625\theta_1 - \theta_2 = 300$$

$$-\theta_1 + 2.0625\theta_2 - \theta_3 = 0$$

$$-\theta_2 + 2.0625\theta_3 - \theta_4 = 0$$

$$-2\theta_3 + 2.1125\theta_4 = 0$$

The set of simultaneous linear algebraic equations can be written in tridiagonal form as

$$\begin{bmatrix} 2.0625 & -1 & & \\ -1 & 2.0625 & -1 & \\ & -1 & 2.0625 & -1 \\ & & -2 & 2.1125 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix} = \begin{bmatrix} 300 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The solution can be obtained by modifying the parameters a_i ($i = 2$ to N), b_i ($i = 1$ to N) and c_i ($i = 1$ to $N - 1$) in Program 1.1 given in the Appendix. The comparison of numerical and analytical results is presented in Table 5.2.

Table 5.2 Numerical and analytical results for Example 5.7

x (m)	θ (numerical solution for 4 parts)	θ (analytical solution)
0.0125	248.95	248.75
0.025	213.47	213.13
0.0375	191.32	190.90
0.05	181.13	180.66

Even when 4 parts are made the difference between the numerical and analytical solution is meagre. The numerical solution can exactly match with the analytical solution if a greater number of parts is made.

5.3 Chemical Reaction and Diffusion in Pore

The differential equation for diffusion and reaction in a pore is given by

$$\frac{d^2C}{dx^2} - \frac{k}{D}C = 0 \tag{5.7}$$

Let us define

$$m = \sqrt{\frac{k}{D}} \tag{5.8}$$

Thus the differential equation can be written as

$$\frac{d^2C}{dx^2} - m^2C = 0 \tag{5.9}$$

The boundary conditions are

at $x = 0$

$$C = C_S \tag{5.10a}$$

and at $x = L$

$$\frac{dC}{dx} = 0 \tag{5.10b}$$

where C_S is the concentration at the surface of the pore.

EXAMPLE 5.8 Diffusion and reaction take place in a pore of 1mm in length. The rate constant of the reaction, $k = 10^{-3}\text{s}^{-1}$ and effective diffusivity of species, $D = 10^{-9}$ m^2/s. Make 100 parts of the pore and determine the concentration at $x = 0.5$ mm. The concentration at the surface of the mouth of the pore is 1 mol/m^3.

Solution We have

$$m = \sqrt{\frac{k}{D}} = \sqrt{\frac{10^{-3}}{10^{-9}}} = 1000 \text{ m}^{-1}$$

The pore length is 1 mm = 10^{-3} m and 100 parts are made, thus $\Delta x = \frac{10^{-3}}{100} = 10^{-5}$ m. The schematic diagram of the pore is shown in Fig. 5.10. The first node is labelled 0 and therefore the last node is the 100th node as 100 parts are made.

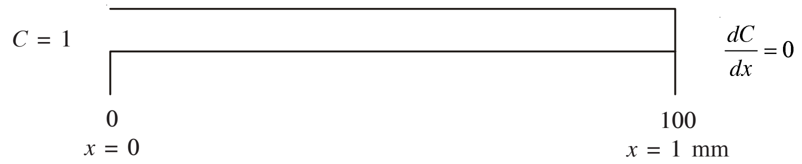


Fig. 5.10 Diffusion and reaction in pore.

The boundary conditions are

At $x = 0$: $C = 1$

At $x = 10^{-3}$ m: $\frac{dC}{dx} = 0$

Discretizing the differential equation at node *i*, we get

$$\frac{C_{i+1}+C_{i-1}-2C_i}{\Delta x^2}-10^6 C_i=0$$

At node 1

$$\frac{C_2+C_0-2C_1}{\Delta x^2}-10^6 C_1=0$$

It is given that $C_0 = 1$, therefore

$$\frac{C_2+1-2C_1}{\Delta x^2}-10^6 C_1=0$$

Substituting the value of $\Delta x = 10^{-5}$ m, we get

$$C_2+1-2C_1-10^6\times 10^{-10} C_1=0$$

Simplifying, we get

$$-2.0001C_1+C_2=-1$$

At node 2

$$\frac{C_3+C_1-2C_2}{\Delta x^2}-10^6 C_2=0$$

$$C_3 + C_1 - 2C_2 - 10^{-4}C_2 = 0$$

$$C_1 - 2.0001C_2 + C_3 = 0$$

At node 99

$$\frac{C_{100}+C_{98}-2C_{99}}{\Delta x^2}-10^6 C_{99}=0$$

$$C_{100} + C_{98} - 2C_{99} - 10^{-4}C_{99} = 0$$

$$C_{98} - 2.0001C_{99} + C_{100} = 0$$

At node 100

$$\frac{C_{101}+C_{99}-2C_{100}}{\Delta x^2}-10^6 C_{100}=0$$

$$C_{101}+C_{99}-2C_{100}-10^{-4} C_{100}=0$$

But $\frac{dC}{dx}=0$; thus $\frac{C_{101}-C_{99}}{2\Delta x}=0$ and therefore $C_{101} = C_{99}$.

Substituting $C_{101} = C_{99}$ in the previous equation, we get

$$2C_{99} - 2.0001C_{100} = 0$$

The 100 equations can be written in tridiagonal form as

$$\begin{bmatrix} -2.0001 & 1 & & & & & & & \\ 1 & -2.0001 & 1 & & & & & & \\ & 1 & -2.0001 & 1 & & & & & \\ & & \cdots & \cdots & \cdots & & & & \\ & & & \cdots & \cdots & \cdots & & & \\ & & & & \cdots & \cdots & \cdots & & \\ & & & & & 1 & -2.0001 & 1 & \\ & & & & & & 1 & -2.0001 & 1 \\ & & & & & & & 2 & -2.0001 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ \cdots \\ \cdots \\ \cdots \\ C_{98} \\ C_{99} \\ C_{100} \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \\ \cdots \\ \cdots \\ \cdots \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The solution can be obtained by modifying the parameters a_i (i = 2 to N), b_i (i = 1 to N) and c_i (i = 1 to N – 1) and d_i (i = 1 to N) in Program 1.1 given in the Appendix. From the results, we get C = 0.73 at x = 0.5 mm (50th node).

Exercises

5.1 Consider the two-point boundary value problem

$$\frac{d^2y}{dx^2} - y + 1 = 0$$

with the boundary conditions $y(0) = y(1) = 0$. List the tridiagonal set of equations and determine y at various values of x. Take $\Delta x = 0.1$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2.01 & 1 & & & \\ 1 & -2.01 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 1 & -2.01 & 1 \\ & & & 1 & -2.01 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_8 \\ y_9 \end{bmatrix} = \begin{bmatrix} -0.01 \\ -0.01 \\ \cdots \\ -0.01 \\ -0.01 \end{bmatrix}$$

$y_1 = y(0.1) = 0.041253$ $\quad y_2 = y(0.2) = 0.072919$ $\quad y_3 = y(0.3) = 0.095313$
$y_4 = y(0.4) = 0.108661$ $\quad y_5 = y(0.5) = 0.113096$ $\quad y_6 = y(0.6) = 0.108661$
$y_7 = y(0.7) = 0.095313$ $\quad y_8 = y(0.8) = 0.072919$ $\quad y_9 = y(0.9) = 0.041253$

5.2 Consider the two-point boundary value problem

$$8\frac{d^2y}{dx^2} - 2\frac{dy}{dx} - y + x = 0$$

with the boundary conditions $y(0) = 5$ and $y(20) = 8$. List the tridiagonal set of equations and determine y at $x = 10$. Take $\Delta x = 1$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -17 & 7 & & & & \\ 9 & -17 & 7 & & & \\ & \cdots & \cdots & \cdots & & \\ & & & 9 & -17 & 7 \\ & & & & 9 & -17 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_{18} \\ y_{19} \end{bmatrix} = \begin{bmatrix} -46 \\ -2 \\ \cdots \\ -18 \\ -75 \end{bmatrix}$$

$y_{10} = y(10) = 8.514381$.

5.3 Consider the ordinary differential equation

$$\frac{d^2y}{dx^2} = y$$

with the boundary conditions $y(1) = 1.175$ and $y(3) = 10.018$. Take $\Delta x = 0.5$. List the tridiagonal set of equations and determine y at various x.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2.25 & 1 & \\ 1 & -2.25 & 1 \\ & 1 & -2.25 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -1.175 \\ 0.0 \\ -10.018 \end{bmatrix}$$

$y_1 = y(1.5) = 2.146603 \quad y_2 = y(2.0) = 3.654857 \quad y_3 = y(2.5) = 6.076825$.

5.4 Consider the ordinary differential equation

$$\frac{d^2y}{dx^2} = y$$

with the boundary conditions: $\frac{dy}{dx}(1) = 1.175$ and $\frac{dy}{dx}(3) = 10.018$. Take $\Delta x = 0.5$. List the tridiagonal set of equations and determine y at various x.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2.25 & 2 & & & \\ 1 & -2.25 & 1 & & \\ & 1 & -2.25 & 1 & \\ & & 1 & -2.25 & 1 \\ & & & 2 & -2.25 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} 1.175 \\ 0 \\ 0 \\ 0 \\ -10.018 \end{bmatrix}$$

$y_1 = y(1.0) = 1.552429 \quad y_2 = y(1.5) = 2.333983 \quad y_3 = y(2.0) = 3.699032$
$y_4 = y(2.5) = 5.988840 \quad y_5 = y(3.0) = 9.775857$

5.5 Consider 1-D steady state conduction without heat generation taking place in a rectangular slab. The temperature of the left side of the slab is 100°C and of the right side is 50°C. The length of the slab is 1 m and the thermal conductivity of the slab is 120 W/cm-K. Take $\Delta x = 0.1$ m. Determine the temperature distribution in the slab and list the tridiagonal set of equations. The governing equation is $\dfrac{d^2T}{dx^2} = 0$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \cdots \\ T_8 \\ T_9 \end{bmatrix} = \begin{bmatrix} -100 \\ 0 \\ \cdots \\ 0 \\ -50 \end{bmatrix}$$

$T_1 = T(0.1) = 95.0$ $T_2 = T(0.2) = 90.0$ $T_3 = T(0.3) = 85.0$

$T_4 = T(0.4) = 80.0$ $T_5 = T(0.5) = 75.0$ $T_6 = T(0.6) = 70.0$

$T_7 = T(0.7) = 65.0$ $T_8 = T(0.8) = 60.0$ $T_9 = T(0.9) = 55.0$

5.6 A fin of diameter 0.02 m and length 0.08 m is attached to a wall (see Fig. 5.11). The temperature of the wall is 200°C. List the tridiagonal set of equations and determine the temperature of the fin at $x = 0.02$, 0.04, 0.06 and 0.08 m, using the finite difference technique taking four parts. The thermal conductivity of rod is 25 W/m-K and convective heat transfer coefficient from rod to surroundings is 40 W/m^2-K. The temperature of surroundings is 25°C. The governing differential equation is $-\dfrac{d^2\theta}{dx^2} + \dfrac{hP}{kA}\theta = 0$, where $\theta = T - T_{\text{surr}}$ and boundary condition at $x = 0.08$ m is $\dfrac{d\theta}{dx} + \dfrac{h}{k}\theta = 0$.

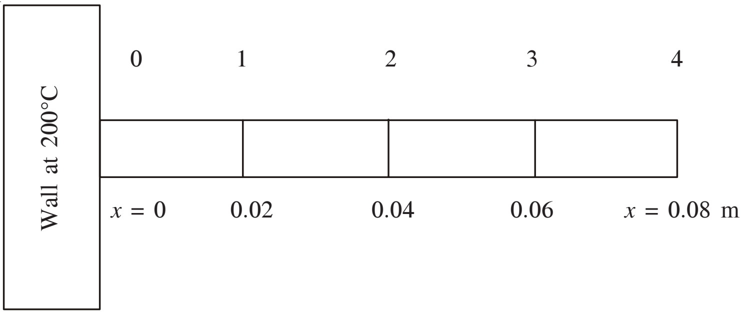


Fig. 5.11 Exercise 5.6.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} 2.128 & -1 & & \\ -1 & 2.128 & -1 & \\ & -1 & 2.128 & -1 \\ & & -2 & 2.192 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix} = \begin{bmatrix} 175 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$\theta_1 = \theta(0.02) = 128.49$ $\quad\theta_2 = \theta(0.04) = 98.44$ $\quad\theta_3 = \theta(0.06) = 80.98$

$\theta_4 = \theta(0.08) = 73.88$

5.7 Diffusion and reaction take place in a pore of 1mm in length. The rate constant of the reaction, $k = 2.5 \times 10^{-4}\text{s}^{-1}$ and effective diffusivity of species, $D = 10^{-9}$ m^2/s. Make 10 parts of the pore. List the tridiagonal set of equations and determine the concentration along x. The concentration at the surface of the mouth of the pore is 1 mol/m^3 and at pore end $\frac{dC}{dx} = 0$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2.0025 & 1 & & & \\ 1 & -2.0025 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 1 & -2.0025 & 1 \\ & & & 2 & -2.0025 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \cdots \\ C_9 \\ C_{10} \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

$C_1 = C(0.1) = 0.978139$ $\quad C_2 = C(0.2) = 0.958723$ $\quad C_3 = C(0.3) = 0.941703$

$C_4 = C(0.4) = 0.927039$ $\quad C_5 = C(0.5) = 0.914691$ $\quad C_6 = C(0.6) = 0.904631$

$C_7 = C(0.7) = 0.896832$ $\quad C_8 = C(0.8) = 0.891275$ $\quad C_9 = C(0.9) = 0.887947$

$C_{10} = C(1.0) = 0.886838$

Distance (in mm) is measured from the pore mouth.

5.8 Diffusion and reaction take place in a pore of 1 mm in length. The rate constant of the reaction, $k = 0.1$ s^{-1} and effective diffusivity of species, $D = 10^{-9}$ m^2/s. Make 10 parts of the pore. List the tridiagonal set of equations and determine the concentration along x. The concentration at the surface of the mouth of the pore is 1 mol/m^3 and at pore end $\frac{dC}{dx} = 0$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -3 & 1 & & & \\ 1 & -3 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 1 & -3 & 1 \\ & & & 2 & -3 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \cdots \\ C_9 \\ C_{10} \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

$C_1 = C(0.1) = 0.381966$ $C_2 = C(0.2) = 0.145898$ $C_3 = C(0.3) = 0.055728$

$C_4 = C(0.4) = 0.021286$ $C_5 = C(0.5) = 0.008131$ $C_6 = C(0.6) = 0.003107$

$C_7 = C(0.7) = 0.001190$ $C_8 = C(0.8) = 0.000463$ $C_9 = C(0.9) = 0.000198$

$C_{10} = C(1.0) = 0.000132$

Distance (in mm) is measured from the pore mouth.

5.9 Water flows between the two fixed parallel plates as shown in Fig. 5.12. Fluid moves in the *x*-direction parallel to the plates and there is no velocity in the *y* direction. The spacing between the plates is 0.02 m and pressure gradient is – 100 Pa/m. The viscosity of water under the flow conditions is 0.001 kg/m-s. Using the finite difference method, solve the velocity profile equation

$$-\frac{\partial p}{\partial x} + \mu \frac{\partial^2 u}{\partial y^2} = 0$$

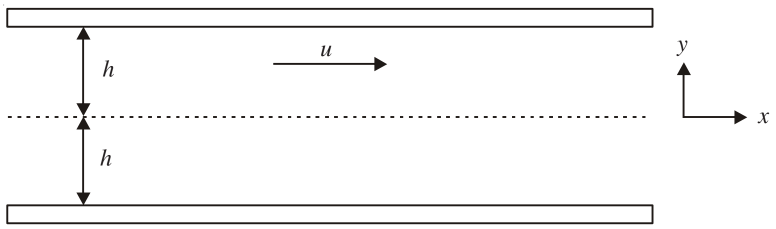


Fig. 5.12 Illustration for Exercise 5.9.

Determine the velocity at various nodes between the symmetry line and the wall. Make 10 parts. Compare the numerical solution with the analytical solution

$$u = \frac{1}{2\mu}\left(\frac{\partial p}{\partial x}\right)\left(y^2 - h^2\right).$$

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \cdots \\ u_9 \\ u_{10} \end{bmatrix} = \begin{bmatrix} -0.1 \\ -0.1 \\ \cdots \\ -0.1 \\ -0.1 \end{bmatrix}$$

and the results are presented in Table 5.3.

Table 5.3 Results in Exercise 5.9

x (m)	Node	u, Numerical (m/s)	u, Analytical (m/s)
0.000	1	5.00	5.00
0.001	2	4.95	4.95
0.002	3	4.80	4.80
0.003	4	4.55	4.55
0.004	5	4.20	4.20
0.005	6	3.75	3.75
0.006	7	3.20	3.20
0.007	8	2.55	2.55
0.008	9	1.80	1.80
0.009	10	0.95	0.95

Distance (in m) is measured from the symmetry line.

Chapter 6

Convection–Diffusion Problems

The convection-diffusion equation for the transport of a component of concentration C is given by

$$-u\frac{dC}{dx}+D\frac{d^2C}{dx^2}=0$$

In the above equation, $u\frac{dC}{dx}$ is the convection term and $D\frac{d^2C}{dx^2}$ is the diffusion term. The central difference scheme (CDS) or the upwind difference scheme (UDS) can be used for the discretization of the convection term, whereas CDS is used for the discretization of the diffusion term. The comparison of the central difference and upwind difference schemes for the discretization of convection term is also discussed here.

6.1 Upwind Schemes

The upwind scheme is used for the discretization of the convection term. The first order and second order upwind schemes are described below.

6.1.1 First Order Upwind Scheme

When the fluid is flowing from left to right properties at grid point i depend only on the properties at grid point $i - 1$ and when the fluid is flowing from right to left properties at grid point i depend only on the properties at grid point $i + 1$. This is nothing more than obeying the physics of the flow. For information propagated from left to right discretization of convection term at node i is given by

$$\frac{dC}{dx}=\frac{C_i-C_{i-1}}{\Delta x} \qquad (\rightarrow x,\ \rightarrow u) \tag{6.1}$$

and for information propagated from right to left discretization of convection term at node i is given by

$$\frac{dC}{dx}=\frac{C_{i+1}-C_i}{\Delta x} \qquad (\rightarrow x,\ \leftarrow u) \tag{6.2}$$

This is shown in Fig. 6.1.

6.1.2 Second Order Upwind Scheme

For information propagated from left to right, discretization of convection term at node i is given by

$$\frac{dC}{dx} = \frac{3C_i - 4C_{i-1} + C_{i-2}}{2\Delta x} \qquad (\rightarrow x, \rightarrow u) \tag{6.3}$$

and for information propagated from right to left, discretization of convection term at node i is given by

$$\frac{dC}{dx} = \frac{-3C_i + 4C_{i+1} - C_{i+2}}{2\Delta x} \qquad (\rightarrow x, \leftarrow u) \tag{6.4}$$

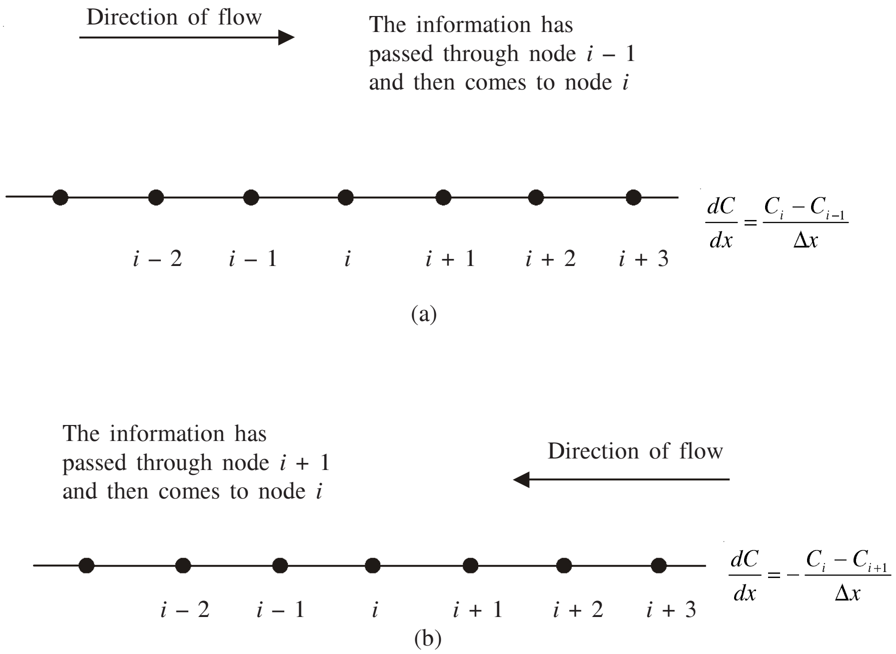


Fig. 6.1 Discretization of convection term using first order upwind method: (a) Direction of flow and space identical; (b) Direction of flow opposite to direction of space.

Let us now derive the formula for second order upwind scheme. Since upwind scheme is one-sided, we shall consider nodes near to a boundary (see Fig. 6.2). Assume that C can be expressed near the boundary by the polynomial

$$C = a + bx + cx^2$$

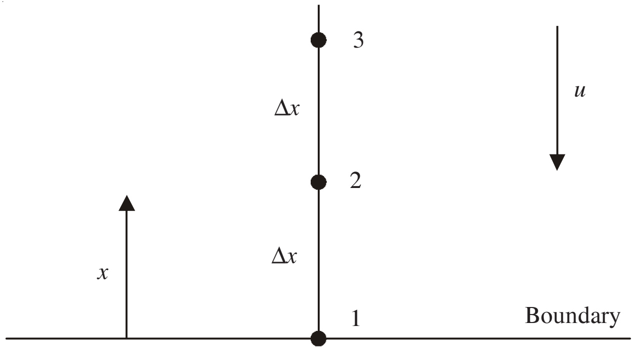


Fig. 6.2 Nodes near boundary.

At point 1 ($x = 0$)

$$C_1 = \mathrm{a}$$

At point 2 ($x = \Delta x$)

$$C_2 = a + b\Delta x + c\Delta x^2$$

At point 3 ($x = 2\Delta x$)

$$C_3 = a + 2b\Delta x + 4c\Delta x^2$$

Solving the above equations for b, we get

$$b = \frac{-3C_1 + 4C_2 - C_3}{2\Delta x}$$

We find b because it is equal to $\frac{dC}{dx}$ at the wall (at node 1). This is because $\frac{dC}{dx} = b + 2cx$ and at $x = 0$, $\frac{dC}{dx} = b$. Therefore at point 1

$$\frac{dC}{dx} = \frac{-3C_1 + 4C_2 - C_3}{2\Delta x}$$

This is a one-sided finite difference expression for the derivative at the boundary. This becomes the basis for second order upwind scheme

$$\left(\frac{\partial C}{\partial x}\right)_i = \frac{-3C_i + 4C_{i+1} - C_{i+2}}{2\Delta x}$$

Here information is propagated in the opposite direction as compared to the direction of x. If information is propagated in the direction of x, then

$$\left(\frac{\partial C}{\partial x}\right)_i = \frac{3C_i - 4C_{i-1} + C_{i-2}}{2\Delta x}$$

Oscillations do not take place when first order upwind scheme is used for discretization of convection term.

EXAMPLE 6.1 A component C is transported by means of convection and diffusion through a one-dimensional space shown in Fig. 6.3.

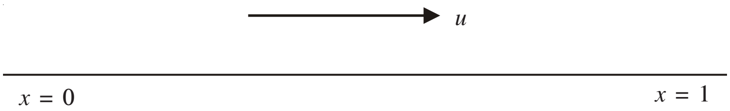


Fig. 6.3 One-dimensional space.

Discretize the convection–diffusion equation

$$-u\frac{dC}{dx}+D\frac{d^2C}{dx^2}=0$$

The boundary conditions are: at $x = 0$ m, $C = 0$ and at $x = 1$ m, $C = 1$. Discretize the equation using (i) central difference scheme for both diffusion and convection terms and (ii) central difference scheme for diffusion term and first order upwind scheme for convection term. Make 50 parts between $x = 0$ and $x = 1$ m. Calculate the distribution of C as a function of x for $x = 0.84$ to 1.0. Compare the numerical results with the analytical solution. For the boundary conditions, at $x = 0$: $C = C_0$ and at $x = L$: $C = C_L$, the analytical solution for $0 \le x \le L$ is

$$C(x)=C_0+\frac{e^{x(Pe)/L}-1}{e^{Pe}-1}(C_L-C_0)$$

where Pe is the Peclet number, the ratio of strength of convection by strength of diffusion, and is given by $Pe=\frac{uL}{D}$. Take $Pe=50$.

Solution We have

(i) *Central difference scheme for both diffusion and convection terms*

Using central difference scheme (CDS) at node i, we get

$$-u\left(\frac{C_{i+1}-C_{i-1}}{2\Delta x}\right)+D\left(\frac{C_{i+1}+C_{i-1}-2C_i}{\Delta x^2}\right)=0$$

Multiplying by $-2\frac{\Delta x^2}{D}$, we get

$$\frac{u\Delta x}{D}(C_{i+1}-C_{i-1})-2C_{i-1}-2C_{i+1}+4C_i=0$$

The local Peclet number is given by

$$Pe_{\text{loc}}=\frac{u\Delta x}{D}$$

Thus the discretized equation at node i becomes

$$-\left(Pe_{\text{loc}}+2\right)C_{i-1}+4C_i+\left(Pe_{\text{loc}}-2\right)C_{i+1}=0$$

Let $\alpha = Pe_{\text{loc}} - 2$ and $\beta = Pe_{\text{loc}} + 2$
Thus

$$-\beta C_{i-1}+4C_i+\alpha C_{i+1}=0$$

Let the total length be 1 m and let us make 50 parts of the length; therefore $\Delta x = 0.02$ m. The schematic diagram is shown in Fig. 6.4.

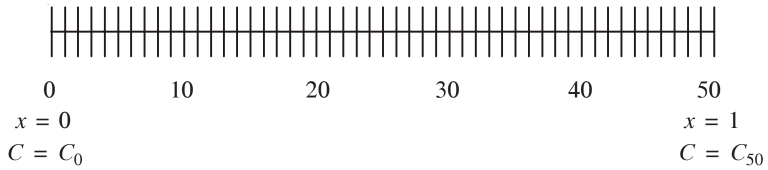


Fig. 6.4 Schematic diagram.

At node 0, $C = C_0$.
At node 1

$$-\beta C_0+4C_1+\alpha C_2=0$$

Since the value of C_0 is known; therefore the equation at node 1 becomes

$$4C_1+\alpha C_2=\beta C_0$$

At node 2

$$-\beta C_1+4C_2+\alpha C_3=0$$

At node 3

$$-\beta C_2+4C_3+\alpha C_4=0$$

At node 48

$$-\beta C_{47}+4C_{48}+\alpha C_{49}=0$$

At node 49

$$-\beta C_{48}+4C_{49}+\alpha C_{50}=0$$

At node 50 the value of C_{50} is known; therefore the equation for node 49 becomes

$$-\beta C_{48}+4C_{49}=-\alpha C_{50}$$

Thus the set of equations for value of C at node 1 to 49 using central difference scheme for both the diffusion and convection terms becomes

$$\begin{bmatrix} 4 & \alpha & & & & & & & & & & \\ -\beta & 4 & \alpha & & & & & & & & & \\ & -\beta & 4 & \alpha & & & & & & & & \\ & & -\beta & 4 & \alpha & & & & & & & \\ & & & -\beta & 4 & \alpha & & & & & & \\ & & & & -\beta & 4 & \alpha & & & & & \\ & & & & & \cdots & \cdots & \cdots & & & & \\ & & & & & & \cdots & \cdots & \cdots & & & \\ & & & & & & & \cdots & \cdots & \cdots & & \\ & & & & & & & & \cdots & \cdots & \cdots & \\ & & & & & & & & & -\beta & 4 & \alpha \\ & & & & & & & & & & -\beta & 4 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ C_{48} \\ C_{49} \end{bmatrix} = \begin{bmatrix} \beta C_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ 0 \\ -\alpha C_{50} \end{bmatrix}$$

For $Pe = 50$, $\frac{u}{D} = 50$ and the local Peclet number becomes $Pe_{\text{loc}} = \frac{u\Delta x}{D} = 50 \times 0.02 = 1.0$. Thus $\alpha = Pe_{\text{loc}} - 2 = -1$ and $\beta = Pe_{\text{loc}} + 2 = 3$. The solution can be obtained by modifying the parameters a_i ($i = 2$ to N), b_i ($i = 1$ to N) and c_i ($i = 1$ to $N - 1$) in Program 1.1 given in the Appendix. The numerical and analytical results are shown in Table 6.1.

(ii) *Central difference scheme for diffusion term and upwind difference scheme for convection term*

Using the upwind difference scheme (UDS) for the convection term and the central difference scheme for the diffusion term at node i, we get

$$-u\left(\frac{C_i - C_{i-1}}{\Delta x}\right) + D\left(\frac{C_{i+1} + C_{i-1} - 2C_i}{\Delta x^2}\right) = 0$$

On multiplying by $-\frac{\Delta x^2}{D}$, the discretized equation at node i becomes

$$-\left(Pe_{\text{loc}} + 1\right)C_{i-1} + \left(Pe_{\text{loc}} + 2\right)C_i - C_{i+1} = 0$$

Let $\beta = Pe_{\text{loc}} + 2$ and $\gamma = Pe_{\text{loc}} + 1$
Thus

$$-\gamma C_{i-1} + \beta C_i - C_{i+1} = 0$$

Let the total length be 1 m and let us make 50 parts of the length; therefore $\Delta x = 0.02$ m. At node 0, $C = C_0$.
At node 1

$$-\gamma C_0 + \beta C_1 - C_2 = 0$$

Since the value of C_0 is known, therefore the equation at node 1 becomes

$$\beta C_1 - C_2 = \gamma C_0$$

At node 2

$$-\gamma C_1 + \beta C_2 - C_3 = 0$$

At node 3

$$-\gamma C_2 + \beta C_3 - C_4 = 0$$

At node 48

$$-\gamma C_{47} + \beta C_{48} - C_{49} = 0$$

At node 49

$$-\gamma C_{48} + \beta C_{49} - C_{50} = 0$$

At node 50 the value of C_{50} is known; therefore the equation for node 49 becomes

$$-\gamma C_{48} + \beta C_{49} = C_{50}$$

Thus the set of equations for value of C at node 1 to 49 using the central difference scheme for the diffusion term and the first order upwind scheme for the convection term becomes

$$\begin{bmatrix} \beta & -1 & & & & & & & & & & \\ -\gamma & \beta & -1 & & & & & & & & & \\ & -\gamma & \beta & -1 & & & & & & & & \\ & & -\gamma & \beta & -1 & & & & & & & \\ & & & -\gamma & \beta & -1 & & & & & & \\ & & & & -\gamma & \beta & -1 & & & & & \\ & & & & & \cdots & \cdots & \cdots & & & & \\ & & & & & & \cdots & \cdots & \cdots & & & \\ & & & & & & & \cdots & \cdots & \cdots & & \\ & & & & & & & & \cdots & \cdots & \cdots & \\ & & & & & & & & & -\gamma & \beta & -1 \\ & & & & & & & & & & -\gamma & \beta \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ C_{48} \\ C_{49} \end{bmatrix} = \begin{bmatrix} \gamma C_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ 0 \\ C_{50} \end{bmatrix}$$

For $Pe = 50$, $\frac{u}{D} = 50$ and the local Peclet number becomes $Pe_{\text{loc}} = \frac{u\Delta x}{D} = 50 \times 0.02 = 1.0$. Thus $\beta = Pe_{\text{loc}} + 2 = 3$ and $\gamma = Pe_{\text{loc}} + 1 = 2$. The solution can be obtained by modifying the parameters a_i ($i = 2$ to N), b_i ($i = 1$ to N) and c_i ($i = 1$ to $N - 1$) in Program 1.1 given in the Appendix. The numerical and analytical results are shown in Table 6.1.

Table 6.1 Numerical and analytical results for Example 6.1

Node number	x (m)	C (CDS)	C (CDS/UDS)	$C = \frac{e^{50x} - 1}{e^{50} - 1}$ (Analytical)
42	0.84	0.000152	0.003906	0.000335
43	0.86	0.000457	0.007813	0.000912
44	0.88	0.001372	0.015625	0.002479
45	0.90	0.004115	0.031250	0.006738
46	0.92	0.012346	0.062500	0.018316
47	0.94	0.037037	0.125000	0.049787
48	0.96	0.111111	0.250000	0.135335
49	0.98	0.333333	0.500000	0.367879

The central difference scheme is a second order scheme and is therefore more accurate, whereas upwind scheme used is first order and is therefore less accurate. But if more parts are made, then more accurate results are obtained. The importance of first order upwind scheme is shown in the next example.

EXAMPLE 6.2 Solve the previous problem for $Pe = 500$.

Solution We have

(i) *Central difference scheme for both diffusion and convection terms*

For $Pe = 500$, $\frac{u}{D} = 500$ and the local Peclet number becomes $Pe_{\text{loc}} = \frac{u\Delta x}{D} = 500 \times 0.02 = 10$. Thus $\alpha = Pe_{\text{loc}} - 2 = 8$ and $\beta = Pe_{\text{loc}} + 2 = 12$. The solution can be obtained by modifying the parameters a_i ($i = 2$ to N), b_i ($i = 1$ to N) and c_i ($i =1$ to $N - 1$) in Program 1.1 given in the Appendix. The numerical results are shown in Table 6.2.

(ii) *Central difference scheme for diffusion term and upwind difference scheme for convection term*

For Pe = 500, $\frac{u}{D} = 500$ and the local Peclet number becomes $Pe_{\text{loc}} = \frac{u\Delta x}{D} = 500 \times 0.02 = 10.$ Thus $\beta = Pe_{\text{loc}} + 2 = 12$ and $\gamma = Pe_{\text{loc}} + 1 = 11$. The solution can be obtained by modifying the parameters a_i ($i = 2$ to N), b_i ($i = 1$ to N) and c_i ($i = 1$ to $N - 1$) in Program 1.1 given in the Appendix. The numerical results are shown in Table 6.2.

Table 6.2 Numerical results for Example 6.2

Node number	x (m)	C (CDS)	C (CDS/UDS)
42	0.84	0.039018	0.000000
43	0.86	–0.058528	0.000000
44	0.88	0.087791	0.000000
45	0.90	–0.131687	0.000006
46	0.92	0.197531	0.000060
47	0.94	–0.296296	0.000751
48	0.96	0.444444	0.008264
49	0.98	–0.666667	0.090909

When the local Peclet number is much below 1, then diffusion is dominant and when the local Peclet number is much above 1, then convection is dominant. When the central difference scheme is used for the discretization of both the diffusion and convection terms, then for all local Peclet number greater than zero, $\beta > 0$ but α changes sign at $Pe_{\text{loc}} = 2$. The subdiagonal elements are negative, diagonals are positive and superdiagonals are negative for $Pe_{\text{loc}} < 2$, whereas for $Pe_{\text{loc}} > 2$ the subdiagonals elements are negative, diagonals are positive and superdiagonals are positive. It is seen that when $Pe_{\text{loc}} > 2$, oscillations occur in the solution of CDS, whereas, when UDS is used for discretization of the convection term, then for all values of Pe_{loc} the subdiagonal elements are negative, diagonals are positive and superdiagonals are negative. When first order method (UDS) is used, oscillations do not occur. Note that the sign of subdiagonal, diagonal and superdiagonal elements in UDS match that of CDS for $Pe_{\text{loc}} < 2$. Thus if oscillations occur when CDS is used, then a larger number of parts can be made so that Δx becomes less and thus Pe_{loc} becomes less than 2, or UDS can be used to avoid oscillations.

6.2 Comparison of CDS and UDS

The upwind difference scheme at node *i* is given by [see Eq. (6.1)]

$$\left.\frac{dC}{dx}\right|^{\text{UDS}} = \frac{C_i - C_{i-1}}{\Delta x} \tag{6.1}$$

The right hand side can be written as

$$\frac{C_i - C_{i-1}}{\Delta x} = \frac{C_{i+1} - C_{i-1}}{2\Delta x} + \left(\frac{C_i - C_{i-1}}{\Delta x} - \frac{C_{i+1} - C_{i-1}}{2\Delta x}\right) \tag{6.5}$$

Thus

$$\left.\frac{dC}{dx}\right|^{\text{UDS}} = \left.\frac{dC}{dx}\right|^{\text{CDS}} + \left(\frac{C_i - C_{i-1}}{\Delta x} - \frac{C_{i+1} - C_{i-1}}{2\Delta x}\right) \tag{6.6}$$

$$\left.\frac{dC}{dx}\right|^{\text{UDS}} = \left.\frac{dC}{dx}\right|^{\text{CDS}} + \left(\frac{2C_i - 2C_{i-1}}{2\Delta x} - \frac{C_{i+1} - C_{i-1}}{2\Delta x}\right) \tag{6.7}$$

$$\left.\frac{dC}{dx}\right|^{\text{UDS}} = \left.\frac{dC}{dx}\right|^{\text{CDS}} + \left(\frac{2C_i - 2C_{i-1} - C_{i+1} + C_{i-1}}{2\Delta x}\right) \tag{6.8}$$

$$\left.\frac{dC}{dx}\right|^{\text{UDS}} = \left.\frac{dC}{dx}\right|^{\text{CDS}} - \left(\frac{-2C_i + C_{i-1} + C_{i+1}}{2\Delta x}\right) \tag{6.9}$$

$$\left.\frac{dC}{dx}\right|^{\text{UDS}} = \left.\frac{dC}{dx}\right|^{\text{CDS}} - \frac{\Delta x}{2}\left(\frac{-2C_i + C_{i-1} + C_{i+1}}{\Delta x^2}\right) \tag{6.10}$$

$$\left.\frac{dC}{dx}\right|^{\text{UDS}} = \left.\frac{dC}{dx}\right|^{\text{CDS}} - \frac{\Delta x}{2}\frac{d^2C}{dx^2} \tag{6.11}$$

Now consider the discretization of the convection–diffusion equation

$$-u\frac{dC}{dx} + D\frac{d^2C}{dx^2} = 0$$

Using the UDS for the discretization of the convection term, we get

$$-u\left.\frac{dC}{dx}\right|^{\text{UDS}} + D\frac{d^2C}{dx^2} = 0 \tag{6.12}$$

Substituting Eq. (6.11) in Eq. (6.12), we get

$$-u\left(\left.\frac{dC}{dx}\right|^{\text{CDS}}-\frac{\Delta x}{2}\frac{d^2C}{dx^2}\right)+D\frac{d^2C}{dx^2}=0$$

$$-u\left.\frac{dC}{dx}\right|^{\text{CDS}}+\frac{u\Delta x}{2}\frac{d^2C}{dx^2}+D\frac{d^2C}{dx^2}=0 \tag{6.13}$$

Thus UDS is equivalent to adding the additional numerical diffusion (or artificial diffusion) term to the CDS. The effective diffusion coefficient is

$$D_{\text{eff}}=D+\frac{u\Delta x}{2} \tag{6.14}$$

and the effective local Peclet number is

$$Pe_{\text{loc,eff}}=\frac{u\Delta x}{D_{\text{eff}}}=\frac{u\Delta x}{D+\dfrac{u\Delta x}{2}}=\frac{2}{\dfrac{2D}{u\Delta x}+1}=\frac{2}{1+\dfrac{2}{Pe_{\text{loc}}}} \tag{6.15}$$

Thus due to the addition of the numerical diffusion term, the effective local Peclet number is always less than 2, whatever the value of the local Peclet number and thus oscillations do not occur when first order UDS is used.

Exercises

6.1 A component of concentration C is transported by means of convection and diffusion through a one-dimensional space

$$-u\frac{dC}{dx}+D\frac{d^2C}{dx^2}=0$$

The boundary conditions are: at at $x = 0$ m, $C = 1$ and at $x = 1$ m, $C = 0$. Discretize the convection-diffusion equation using the central difference scheme for both diffusion and convection terms. Calculate the distribution of C as a function of x. Make 10 parts between $x = 0$ and $x = 1$ m. Take $\frac{u}{D}=10\ \text{m}^{-1}$. Compare the numerical result with the analytical solution $C(x)=1-\left(\frac{e^{10x}-1}{e^{10}-1}\right)$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2 & 0.5 & & & \\ 1.5 & -2 & 0.5 & & \\ & \cdots & \cdots & \cdots & \\ & & 1.5 & -2 & 0.5 \\ & & & 1.5 & -2 \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \\ \cdots \\ C_8 \\ C_9 \end{bmatrix}=\begin{bmatrix} -1.5 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

and the results are shown in Table 6.3.

Table 6.3 Results of Exercise 6.1

x (m)	C (numerical – CDS)	C (analytical)
0.1	0.999966	0.999922
0.2	0.999865	0.999710
0.3	0.999560	0.999133
0.4	0.998645	0.997567
0.5	0.995902	0.993307
0.6	0.987671	0.981729
0.7	0.962979	0.950256
0.8	0.888904	0.864704
0.9	0.666678	0.632149

6.2 A component of concentration C is transported by means of convection and diffusion through a one-dimensional space

$$-u\frac{dC}{dx}+D\frac{d^2C}{dx^2}=0$$

The boundary conditions are: At $x = 0$ m, $C = 1$ and at $x = 1$ m, $C = 0$. Discretize the convection-diffusion equation using the central difference scheme for the diffusion term and the first order upwind difference scheme for the convection term. Calculate the distribution of C as a function of x. Make 10 parts between $x = 0$ and $x = 1$ m. Take $\frac{u}{D}=10\text{ m}^{-1}$. Compare the numerical result with the analytical solution $C(x)=1-\left(\frac{e^{10x}-1}{e^{10}-1}\right)$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -3 & 1 & & & \\ 2 & -3 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 2 & -3 & 1 \\ & & & 2 & -3 \end{bmatrix}\begin{bmatrix} C_1 \\ C_2 \\ \cdots \\ C_8 \\ C_9 \end{bmatrix}=\begin{bmatrix} -2 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

and the results are shown in Table 6.4.

Table 6.4 Results of Exercise 6.2

x (m)	C (numerical – CDS/UDS)	C (analytical)
0.1	0.999023	0.999922
0.2	0.997068	0.999710
0.3	0.993157	0.999133
0.4	0.985337	0.997567
0.5	0.969697	0.993307
0.6	0.938417	0.981729
0.7	0.875855	0.950256
0.8	0.750733	0.864704
0.9	0.500489	0.632149

Since the first order upwind is used for the discretization of the convection term, therefore more parts are a must for a better answer as the first order method is $O(\Delta x)$.

6.3 Solve Exercise 6.1 for $\frac{u}{D} = 20\ \text{m}^{-1}$. Compare the numerical result with the analytical solution $C(x) = 1 - \left(\frac{e^{20x} - 1}{e^{20} - 1}\right)$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -1 & 0 & & & \\ 1 & -1 & 0 & & \\ & \cdots & \cdots & \cdots & \\ & & 1 & -1 & 0 \\ & & & 1 & -1 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \cdots \\ C_8 \\ C_9 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

and the results are shown in Table 6.5.

Table 6.5 Results of Exercise 6.3

x (m)	C (numerical – CDS)	C (analytical)
0.1	1.000000	0.999999
0.2	1.000000	0.999999
0.3	1.000000	0.999999
0.4	1.000000	0.999994
0.5	1.000000	0.999955
0.6	1.000000	0.999665
0.7	1.000000	0.997521
0.8	1.000000	0.981684
0.9	1.000000	0.864665

In this problem the local Peclet number is 2.0; therefore central difference gives a wrong answer.

6.4 Solve Exercise 6.2 for $\frac{u}{D} = 20\ \text{m}^{-1}$. Compare the numerical result with the analytical solution $C(x) = 1 - \left(\frac{e^{20x} - 1}{e^{20} - 1}\right)$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -2 & 0.5 & & & \\ 1.5 & -2 & 0.5 & & \\ & \cdots & \cdots & \cdots & \\ & & 1.5 & -2 & 0.5 \\ & & & 1.5 & -2 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \cdots \\ C_8 \\ C_9 \end{bmatrix} = \begin{bmatrix} -1.5 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

and the results are shown in Table 6.6.

Table 6.6 Results of Exercise 6.4

x (m)	C (numerical – CDS/UDS)	C (analytical)
0.1	0.999966	0.999999
0.2	0.999865	0.999999
0.3	0.999560	0.999999
0.4	0.998645	0.999994
0.5	0.995902	0.999955
0.6	0.987671	0.999665
0.7	0.962979	0.997521
0.8	0.888904	0.981684
0.9	0.666678	0.864665

Since the first order upwind method is used for the discretization of the convection term, therefore more parts are a must for a better answer as the first order method is $O(\Delta x)$.

6.5 Solve Exercise 6.1 for $\frac{u}{D} = 50\ \text{m}^{-1}$. Compare the numerical result with the analytical solution $C(x) = 1 - \left(\frac{e^{50x} - 1}{e^{50} - 1}\right)$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -0.4 & -0.3 & & & \\ 0.7 & -0.4 & -0.3 & & \\ & \cdots & \cdots & \cdots & \\ & & 0.7 & -0.4 & -0.3 \\ & & & 0.7 & -0.4 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \cdots \\ C_8 \\ C_9 \end{bmatrix} = \begin{bmatrix} -0.7 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

and the results are shown in Table 6.7.

Table 6.7 Results of Exercise 6.5

x (m)	C (numerical – CDS)	C (analytical)
0.1	1.000697	1.000000
0.2	0.999071	1.000000
0.3	1.002865	1.000000
0.4	0.994011	1.000000
0.5	1.014670	1.000000
0.6	0.966466	0.999999
0.7	1.078942	0.999999
0.8	0.816497	0.999955
0.9	1.428870	0.993262

In this problem the local Peclet number is greater than 2.0; therefore central difference gives oscillations.

6.6 Solve Exercise 6.2 for $\dfrac{u}{D} = 50\ \text{m}^{-1}$. Compare the numerical result with the analytical solution $C(x) = 1 - \left(\dfrac{e^{50x} - 1}{e^{50} - 1}\right)$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -1.4 & 0.2 & & & \\ 1.2 & -1.4 & 0.2 & & \\ & \dots & \dots & \dots & \\ & & 1.2 & -1.4 & 0.2 \\ & & & 1.2 & -1.4 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \dots \\ C_8 \\ C_9 \end{bmatrix} = \begin{bmatrix} -1.2 \\ 0 \\ \dots \\ 0 \\ 0 \end{bmatrix}$$

and the results are shown in Table 6.8.

Table 6.8 Results of Exercise 6.6

x (m)	C (numerical – CDS/UDS)	C (analytical)
0.1	1.000000	1.000000
0.2	1.000000	1.000000
0.3	0.999997	1.000000
0.4	0.999979	1.000000
0.5	0.999872	1.000000
0.6	0.999229	0.999999
0.7	0.995371	0.999999
0.8	0.972223	0.999955
0.9	0.833334	0.993262

Since the first order upwind method is used for the discretization of convection term, therefore more parts are a must for a better answer as the first order method is $O(\Delta x)$).

Chapter 7

Tubular Reactor with Axial Dispersion

Plug flow reactors were discussed in Chapter 4. When axial dispersion takes place in a tubular reactor, then the problem becomes a boundary value problem and the differential equation becomes second order due to the addition of a diffusion term. Thus two conditions are required to completely define the problem. Danckwerts boundary conditions are considered here. One boundary condition is specified at the inlet and one at the exit of the tubular reactor, for each species. The solution of various single, series and parallel reactions are discussed using the finite difference method in this chapter.

7.1 Boundary Value Problems in Chemical Reaction Engineering

In tubular reactor with axial dispersion the boundary conditions are specified. The boundary conditions and ordinary differential equations for the tubular reactor with axial dispersion are shown in Table 7.1.

Table 7.1 Boundary conditions and ODEs for tubular reactor with axial dispersion

Boundary condition at x = 0	*Boundary condition at x = L*	*ODEs for plug flow reactor*
$A \xrightarrow{k_1} B$		
$uC_{A,in} = uC_A - D\dfrac{dC_A}{dx}$	$\dfrac{dC_A}{dx} = 0$	$D\dfrac{d^2C_A}{dx^2} - u\dfrac{dC_A}{dx} - k_1C_A = 0$
$uC_{B,in} = uC_B - D\dfrac{dC_B}{dx}$	$\dfrac{dC_B}{dx} = 0$	$D\dfrac{d^2C_B}{dx^2} - u\dfrac{dC_B}{dx} + k_1C_A = 0$
$A \xrightarrow{k_1} B \xrightarrow{k_2} C$		
$uC_{A,in} = uC_A - D\dfrac{dC_A}{dx}$	$\dfrac{dC_A}{dx} = 0$	$D\dfrac{d^2C_A}{dx^2} - u\dfrac{dC_A}{dx} - k_1C_A = 0$
$uC_{B,in} = uC_B - D\dfrac{dC_B}{dx}$	$\dfrac{dC_B}{dx} = 0$	$D\dfrac{d^2C_B}{dx^2} - u\dfrac{dC_B}{dx} + k_1C_A - k_2C_B = 0$
$uC_{C,in} = uC_C - D\dfrac{dC_C}{dx}$	$\dfrac{dC_C}{dx} = 0$	$D\dfrac{d^2C_C}{dx^2} - u\dfrac{dC_C}{dx} + k_2C_B = 0$
$A + B \xrightarrow{k_1} C$ $B + C \xrightarrow{k_2} D$		

Table 7.1 (*Cont.*)

$uC_{A,\text{in}} = uC_A - D\dfrac{dC_A}{dx}$	$\dfrac{dC_A}{dx} = 0$	$D\dfrac{d^2C_A}{dx^2} - u\dfrac{dC_A}{dx} - k_1C_AC_B = 0$
$uC_{B,\text{in}} = uC_B - D\dfrac{dC_B}{dx}$	$\dfrac{dC_B}{dx} = 0$	$D\dfrac{d^2C_B}{dx^2} - u\dfrac{dC_B}{dx} - k_1C_AC_B - k_2C_BC_C = 0$
$uC_{C,\text{in}} = uC_C - D\dfrac{dC_C}{dx}$	$\dfrac{dC_C}{dx} = 0$	$D\dfrac{d^2C_C}{dx^2} - u\dfrac{dC_C}{dx} + k_1C_AC_B - k_2C_BC_C = 0$
$uC_{D,\text{in}} = uC_D - D\dfrac{dC_D}{dx}$	$\dfrac{dC_D}{dx} = 0$	$D\dfrac{d^2C_D}{dx^2} - u\dfrac{dC_D}{dx} + k_2C_BC_C = 0$

7.2 First Order Reaction

Consider a tubular vessel in which axial dispersion occurs along with convection. The velocity of the fluid is u, the axial dispersion coefficient is D, the concentration of species is C and A is the cross-sectional area. Consider a differential section in this vessel (see Fig. 7.1).

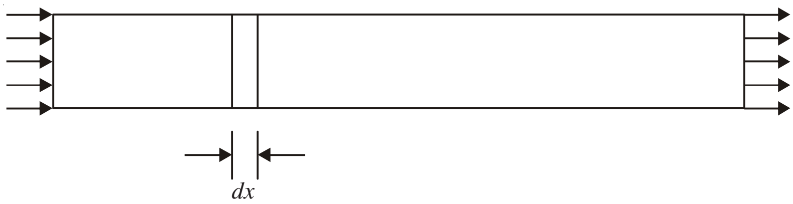


Fig. 7.1 Tubular reactor and differential section.

In this differential section the material entering through convection

$$= uCA \tag{7.1}$$

that entering through dispersion

$$= -D\frac{dC}{dx}A \tag{7.2}$$

that leaving through convection

$$= u\left(C + \frac{dC}{dx}.dx\right)A \tag{7.3}$$

and that leaving through dispersion

$$= -D\left[\frac{dC}{dx} + \frac{d}{dx}\left(\frac{dC}{dx}\right)dx\right]A \tag{7.4}$$

Accumulation

$$= \frac{dC}{dt}Adx \tag{7.5}$$

We know that Input – Output = Accumulation. Thus

$$\frac{dC}{dt}Adx = uCA - D\frac{dC}{dx}A - u\left(C + \frac{dC}{dx}\cdot dx\right)A + D\left[\frac{dC}{dx} + \frac{d}{dx}\left(\frac{dC}{dx}\right)dx\right]A \tag{7.6}$$

$$\frac{dC}{dt}dx = -u\frac{dC}{dx}dx + D\frac{d}{dx}\left(\frac{dC}{dx}\right)dx \tag{7.7}$$

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2} - u\frac{dC}{dx} \tag{7.8}$$

At steady state and if reaction also occurs in the tubular vessel, we get

$$D\frac{d^2C}{dx^2} - u\frac{dC}{dx} - (-r) = 0 \tag{7.9}$$

C now refers to the concentration of the reactant or product. $-r$ is a net positive quantity if C refers to a reactant and negative if C refers to a product.

Use of a dispersion model changes the reactor analysis from an initial value problem to a boundary value problem. The boundary conditions proposed by Danckwerts are

$$\text{At inlet:} \quad uC_{\text{in}} = uC - D\frac{dC}{dx} \tag{7.10}$$

$$\text{At exit:} \quad \frac{dC}{dx} = 0 \tag{7.11}$$

At the reactor inlet, the flux entering is uC_{in} but once inside the reactor and in the presence of dispersion, the flux is

$$uC - D\frac{dC}{dx}$$

Balancing these two fluxes at $x = 0$ yields the inlet boundary condition

$$uC_{\text{in}} = uC - D\frac{dC}{dx}$$

If the reaction stops once the stream leaves the reactor, the concentration profile becomes uniform, and the outlet boundary condition becomes $\frac{dC}{dx} = 0$.

EXAMPLE 7.1 Consider a reaction $A \to B$ carried out in a tubular reactor. The differential equation for species A along the length of the tubular reactor of length 10 m is

$$D\frac{d^2C_A}{dx^2} - u\frac{dC_A}{dx} - kC_A = 0$$

The boundary conditions are

$$\text{At } x = 0 \text{ (inlet):} \qquad uC_{A,\text{in}} = uC_A - D\frac{dC_A}{dx}$$

$$\text{At } x = 10 \text{ m (exit):} \qquad \frac{dC_A}{dx} = 0$$

A fluid medium comprising initially only A flows through the reactor with a mean axial velocity $u = 1$ m/s. The axial dispersion coefficient, $D = 10^{-4}$ m^2/s and rate constant of the reaction is 1 s^{-1}. The inlet concentration, $C_{A,\text{in}} = 1$ mol/m^3. Make 50, 20, and 10 parts of the reactor and determine the concentration of A at various nodes along the length of the tubular reactor.

Solution We have

Concentration profile for 50 parts

50 parts of the reactor are made as shown in Fig. 7.2.

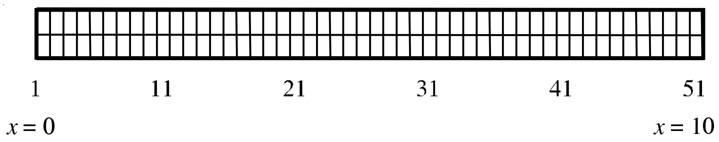


Fig. 7.2 Example 7.1.

$$\Delta x = \frac{10}{50} = 0.2 \text{ m}$$

We solve the differential equation using upwind difference scheme for convection term. Discretizing the differential equation at node i, we get

$$D\left(\frac{C_{Ai+1} + C_{Ai-1} - 2C_{Ai}}{\Delta x^2}\right) - u\left(\frac{C_{Ai} - C_{Ai-1}}{\Delta x}\right) - k_1 C_{Ai} = 0$$

At node 1

$$D\left(\frac{C_{A2} + C_{A0} - 2C_{A1}}{\Delta x^2}\right) - u\left(\frac{C_{A1} - C_{A0}}{\Delta x}\right) - k_1 C_{A1} = 0$$

$$C_{A1}\left(-\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1\right) + \frac{D}{\Delta x^2}C_{A2} + C_{A0}\left(\frac{D}{\Delta x^2} + \frac{u}{\Delta x}\right) = 0$$

From the boundary condition at node 1, we get

$$uC_{A,\text{in}} = uC_{A1} - D\left(\frac{C_{A2} - C_{A0}}{2\Delta x}\right)$$

Solving for C_{A0} we get

$$C_{A0} = \frac{2u\Delta x}{D}\left(C_{A,\text{in}} - C_{A1}\right) + C_{A2}$$

Substituting for C_{A0} in the equation for node 1, we get

$$C_{A1}\left(-\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1\right) + \frac{D}{\Delta x^2}C_{A2} + \left(\frac{D}{\Delta x^2} + \frac{u}{\Delta x}\right)\left[\frac{2u\Delta x}{D}\left(C_{A,\text{in}} - C_{A1}\right) + C_{A2}\right] = 0$$

$$\left(-\frac{2D}{\Delta x^2} - \frac{3u}{\Delta x} - k_1 - \frac{2u^2}{D}\right)C_{A1} + \left(\frac{2D}{\Delta x^2} + \frac{u}{\Delta x}\right)C_{A2} = -\left(\frac{2u^2}{D} + \frac{2u}{\Delta x}\right)C_{A,\text{in}}$$

At node 2

$$\left(\frac{D}{\Delta x^2} + \frac{u}{\Delta x}\right)C_{A1} + \left(-\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1\right)C_{A2} + \frac{D}{\Delta x^2}C_{A3} = 0$$

At node 3

$$\left(\frac{D}{\Delta x^2} + \frac{u}{\Delta x}\right)C_{A2} + \left(-\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1\right)C_{A3} + \frac{D}{\Delta x^2}C_{A4} = 0$$

At node 51

$$\left(\frac{D}{\Delta x^2} + \frac{u}{\Delta x}\right)C_{A50} + \left(-\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1\right)C_{A51} + \frac{D}{\Delta x^2}C_{A52} = 0$$

From the boundary condition at node 51, we get

$$\left(\frac{C_{A52} - C_{A50}}{2\Delta x}\right) = 0 \qquad \text{thus} \qquad C_{A52} = C_{A50}$$

Substituting for C_{A52} in the equation for node 51, we get

$$\left(\frac{2D}{\Delta x^2} + \frac{u}{\Delta x}\right)C_{A50} + \left(-\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1\right)C_{A51} = 0$$

The coefficients of equation 1 (at node 1) are

$$\text{Coefficient of } C_{A1} = -\frac{2D}{\Delta x^2} - \frac{3u}{\Delta x} - k_1 - \frac{2u^2}{D} = -\frac{2\times 10^{-4}}{0.2^2} - \frac{3}{0.2} - 1 - \frac{2}{10^{-4}} = -20016.005$$

$$\text{Coefficient of } C_{A2} = \frac{2D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{2\times 10^{-4}}{0.2^2} + \frac{1}{0.2} = 5.005$$

$$\text{Right hand side of equation 1} = -\left(\frac{2u^2}{D} + \frac{2u}{\Delta x}\right)C_{A,\text{in}} = -\frac{2}{0.2} - \frac{2}{10^{-4}} = -20010$$

The coefficients of equation 2 (at node 2) are

$$\text{Coefficient of } C_{A1} = \frac{D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{10^{-4}}{0.2^2} + \frac{1}{0.2} = 5.0025$$

$$\text{Coefficient of } C_{A2} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2 \times 10^{-4}}{0.2^2} - \frac{1}{0.2} - 1 = -6.005$$

$$\text{Coefficient of } C_{A3} = \frac{D}{\Delta x^2} = \frac{10^{-4}}{0.2^2} = 0.0025$$

Right hand side of equation 2 = 0.
The coefficients of equation 3 (at node 3) are

$$\text{Coefficient of } C_{A2} = \frac{D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{10^{-4}}{0.2^2} + \frac{1}{0.2} = 5.0025$$

$$\text{Coefficient of } C_{A3} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2 \times 10^{-4}}{0.2^2} - \frac{1}{0.2} - 1 = -6.005$$

$$\text{Coefficient of } C_{A4} = \frac{D}{\Delta x^2} = \frac{10^{-4}}{0.2^2} = 0.0025$$

Right hand side of equation 3 = 0.
The coefficients of equation 51 (at node 51) are

$$\text{Coefficient of } C_{A50} = \frac{2D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{2 \times 10^{-4}}{0.2^2} + \frac{1}{0.2} = 5.005$$

$$\text{Coefficient of } C_{A51} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2 \times 10^{-4}}{0.2^2} - \frac{1}{0.2} - 1 = -6.005$$

Right hand side of equation 51 = 0.

The above equations can be written in tridiagonal form as given below. The solution can be obtained by modifying the parameters a_i (i = 2 to N), b_i (i = 1 to N) and c_i (i = 1 to $N - 1$) in Program 1.1 given in the Appendix.

$$\begin{bmatrix} -20016.005 & 5.005 & & & \\ 5.0025 & -6.005 & 0.0025 & & \\ & \cdots & \cdots & \cdots & \\ & & 5.0025 & -6.005 & 0.0025 \\ & & & 5.005 & -6.005 \end{bmatrix} \begin{bmatrix} C_{A1} \\ C_{A2} \\ \cdots \\ C_{A50} \\ C_{A51} \end{bmatrix} = \begin{bmatrix} -20010 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

The solution using TDMA is presented in Table 7.2.

Table 7.2 Results for concentration profile for 50 parts

Node number	x (m)	C_A
1	0.0	0.999908
2	0.2	0.833268
3	0.4	0.694400
4	0.6	0.578675
5	0.8	0.482236
6	1.0	0.401869
7	1.2	0.334895
8	1.4	0.279083
9	1.6	0.232573
10	1.8	0.193813
11	2.0	0.161513
12	2.2	0.134596
13	2.4	0.112165
14	2.6	0.093472
15	2.8	0.077895
16	3.0	0.064913
17	3.2	0.054095
18	3.4	0.045080
19	3.6	0.037567
20	3.8	0.031306
21	4.0	0.026089
22	4.2	0.021741
23	4.4	0.018118
51	10.0	0.000110

More conversion would have occurred if the reactor is assumed to be ideal plug flow.

Concentration profile for 20 parts

If 20 parts of the reactor are made, then $\Delta x = \dfrac{10}{20} = 0.5$ m. The coefficients of the 21 equations at 21 nodes are as given below.

The coefficients of equation 1 (at node 1) are

$$\text{Coefficient of } C_{A1} = -\frac{2D}{\Delta x^2} - \frac{3u}{\Delta x} - k_1 - \frac{2u^2}{D}$$

$$= -\frac{2\times 10^{-4}}{0.5^2} - \frac{3}{0.5} - 1 - \frac{2}{10^{-4}} = -20006.9992$$

$$\text{Coefficient of } C_{A2} = \frac{2D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{2\times 10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0008$$

$$\text{Right hand side of equation 1} = -\left(\frac{2u^2}{D} + \frac{2u}{\Delta x}\right)C_{A,\text{in}} = -\frac{2}{0.5} - \frac{2}{10^{-4}} = -20004$$

The coefficients of equation 2 (at node 2) are

$$\text{Coefficient of } C_{A1} = \frac{D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0004$$

$$\text{Coefficient of } C_{A2} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2 \times 10^{-4}}{0.5^2} - \frac{1}{0.5} - 1 = -3.0008$$

$$\text{Coefficient of } C_{A3} = \frac{D}{\Delta x^2} = \frac{10^{-4}}{0.5^2} = 0.0004$$

Right hand side of equation 2 = 0.
The coefficients of equation 3 (at node 3) are

$$\text{Coefficient of } C_{A2} = \frac{D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0004$$

$$\text{Coefficient of } C_{A3} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2 \times 10^{-4}}{0.5^2} - \frac{1}{0.5} - 1 = -3.0008$$

$$\text{Coefficient of } C_{A4} = \frac{D}{\Delta x^2} = \frac{10^{-4}}{0.5^2} = 0.0004$$

Right hand side of equation 3 = 0.
The coefficients of equation 21 (at node 21) are

$$\text{Coefficient of } C_{A20} = \frac{2D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{2 \times 10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0008$$

$$\text{Coefficient of } C_{A21} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2 \times 10^{-4}}{0.5^2} - \frac{1}{0.5} - 1 = -3.0008$$

Right hand side of equation 21 = 0.
The above equations can be written in tridiagonal form as given below:

$$\begin{bmatrix} -20006.9992 & 2.0008 & & & \\ 2.0004 & -3.0008 & 0.0004 & & \\ & \cdots & \cdots & \cdots & \\ & & 2.0004 & -3.0008 & 0.0004 \\ & & & 2.0008 & -3.0008 \end{bmatrix} \begin{bmatrix} C_{A1} \\ C_{A2} \\ \cdots \\ C_{A20} \\ C_{A21} \end{bmatrix} = \begin{bmatrix} -20004 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

The solution can be obtained by modifying the parameters a_i (i = 2 to N), b_i (i = 1 to N) and c_i ($i = 1$ to $N - 1$) in Program 1.1 given in the Appendix. The results are presented in Table 7.3.

Table 7.3 Results for concentration profile for 20 parts

Node number	x (m)	C_A
1	0.0	0.999917
3	1.0	0.444400
5	2.0	0.197500
7	3.0	0.087800
9	4.0	0.039000
11	5.0	0.017300
13	6.0	0.007700
15	7.0	0.003400
17	8.0	0.001500
19	9.0	0.000677
21	10.0	0.000301

Concentration profile for 10 parts

If 10 parts of the reactor are made, then $\Delta x = \frac{10}{10} = 1.0$ m. The coefficients of the 11 equations at 11 nodes are as given below.

The coefficients of equation 1 (at node 1) are

Coefficient of $C_{A1} = -\frac{2D}{\Delta x^2} - \frac{3u}{\Delta x} - k_1 - \frac{2u^2}{D} = -\frac{2\times 10^{-4}}{1^2} - \frac{3}{1} - 1 - \frac{2}{10^{-4}} = -20004.0002$

Coefficient of $C_{A2} = \frac{2D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{2\times 10^{-4}}{1^2} + \frac{1}{1} = 1.0002$

Right hand side of equation 1 = $-\left(\frac{2u^2}{D} + \frac{2u}{\Delta x}\right)C_{A,\text{in}} = -\frac{2}{1} - \frac{2}{10^{-4}} = -20002$

The coefficients of equation 2 (at node 2) are

Coefficient of $C_{A1} = \frac{D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{10^{-4}}{1^2} + \frac{1}{1} = 1.0001$

Coefficient of $C_{A2} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2\times 10^{-4}}{1^2} - \frac{1}{1} - 1 = -2.0002$

Coefficient of $C_{A3} = \frac{D}{\Delta x^2} = \frac{10^{-4}}{1^2} = 0.0001$

Right hand side of equation 2 = 0.

The coefficients of equation 3 (at node 3) are

Coefficient of $C_{A2} = \frac{D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{10^{-4}}{1^2} + \frac{1}{1} = 1.0001$

$$\text{Coefficient of } C_{A3} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2\times 10^{-4}}{1^2} - \frac{1}{1} - 1 = -2.0002$$

$$\text{Coefficient of } C_{A4} = \frac{D}{\Delta x^2} = \frac{10^{-4}}{1^2} = 0.0001$$

Right hand side of equation 3 = 0.
The coefficients of equation 11 (at node 11) are

$$\text{Coefficient of } C_{A10} = \frac{2D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{2\times 10^{-4}}{1^2} + \frac{1}{1} = 1.0002$$

$$\text{Coefficient of } C_{A11} = -\frac{2D}{\Delta x^2} - \frac{u}{\Delta x} - k_1 = -\frac{2\times 10^{-4}}{1^2} - \frac{1}{1} - 1 = -2.0002$$

Right hand side of equation 11 = 0.
The above equations can be written in tridiagonal form as given below.

$$\begin{bmatrix} -20004.0002 & 1.0002 & & & \\ 1.0001 & -2.0002 & 0.0001 & & \\ & \cdots & \cdots & \cdots & \\ & & 1.0001 & -2.0002 & 0.0001 \\ & & & 1.0002 & -2.0002 \end{bmatrix} \begin{bmatrix} C_{A1} \\ C_{A2} \\ \cdots \\ C_{A10} \\ C_{A11} \end{bmatrix} = \begin{bmatrix} -20002 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

The solution can be obtained by modifying the parameters a_i (i = 2 to N), b_i (i = 1 to N) and c_i (i = 1 to N – 1) in Program 1.1 given in the Appendix. The results are presented in Table 7.4.

Table 7.4 Results for concentration profile for 10 parts

Node number	x (m)	C_A
1	0.0	0.999925
2	1.0	0.499975
3	2.0	0.249994
4	3.0	0.125000
5	4.0	0.062502
6	5.0	0.031252
7	6.0	0.015626
8	7.0	0.007813
9	8.0	0.003907
10	9.0	0.001953
11	10.0	0.000977

7.3 Second Order Reaction

Consider a tubular reactor with axial dispersion in which second order reaction takes place. The analysis is described with an example.

EXAMPLE 7.2 Consider a reaction $A \rightarrow B$ carried out in a tubular reactor. The differential equation for species A along the length of the tubular reactor of length 10 m is

$$D\frac{d^2C_A}{dx^2} - u\frac{dC_A}{dx} - kC_A^2 = 0$$

The boundary conditions are

$$\text{At } x = 0 \text{ (inlet):} \qquad uC_{A,\text{in}} = uC_A - D\frac{dC_A}{dx}$$

$$\text{At } x = 10 \text{ m (exit):} \qquad \frac{dC_A}{dx} = 0$$

A fluid medium comprising initially only A flows through the reactor with a mean axial velocity u = 1 m/s. The axial dispersion coefficient, $D = 10^{-4}$ m^2/s and rate constant of the reaction is 1 m^3/mol-s. The inlet concentration $C_{A,\text{in}}$ =1 mol/m^3. Make 20 parts of the reactor and determine the concentration of A at various nodes along the length of the tubular reactor.

Solution Since 20 parts of the reactor are made, $\Delta x = \frac{10}{20} = 0.5$ m. The coefficients of the 21 equations at 21 nodes are as given below.

The coefficients of equation 1 (at node 1) are

$$\text{Coefficient of } C_{A1} = -\frac{2D}{\Delta x^2} - \frac{3u}{\Delta x} - k_1 C_{A1} - \frac{2u^2}{D}$$

$$= -\frac{2\times 10^{-4}}{0.5^2} - \frac{3}{0.5} - C_{A1} - \frac{2}{10^{-4}} = -20005.9992 - C_{A1}$$

$$\text{Coefficient of } C_{A2} = \frac{2D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{2\times 10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0008$$

$$\text{Right hand side of equation 1} = -\left(\frac{2u^2}{D} + \frac{2u}{\Delta x}\right)C_{A,\text{in}} = -\frac{2}{0.5} - \frac{2}{10^{-4}} = -20004$$

The coefficients of equation 2 (at node 2) are

$$\text{Coefficient of } C_{A1} = \frac{D}{\Delta x^2} + \frac{u}{\Delta x} = \frac{10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0004$$

Coefficient of $C_{A2} = -\dfrac{2D}{\Delta x^2} - \dfrac{u}{\Delta x} - k_1 C_{A2} = -\dfrac{2\times 10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{A2} = -2.0008 - C_{A2}$

Coefficient of $C_{A3} = \dfrac{D}{\Delta x^2} = \dfrac{10^{-4}}{0.5^2} = 0.0004$

Right hand side of equation 2 = 0.
The coefficients of equation 3 (at node 3) are

Coefficient of $C_{A2} = \dfrac{D}{\Delta x^2} + \dfrac{u}{\Delta x} = \dfrac{10^{-4}}{0.5^2} + \dfrac{1}{0.5} = 2.0004$

Coefficient of $C_{A3} = -\dfrac{2D}{\Delta x^2} - \dfrac{u}{\Delta x} - k_1 C_{A3} = -\dfrac{2\times 10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{A3} = -2.0008 - C_{A3}$

Coefficient of $C_{A4} = \dfrac{D}{\Delta x^2} = \dfrac{10^{-4}}{0.5^2} = 0.0004$

Right hand side of equation 3 = 0.
The coefficients of equation 21 (at node 21) are

Coefficient of $C_{A20} = \dfrac{2D}{\Delta x^2} + \dfrac{u}{\Delta x} = \dfrac{2\times 10^{-4}}{0.5^2} + \dfrac{1}{0.5} = 2.0008$

Coefficient of $C_{A21} = -\dfrac{2D}{\Delta x^2} - \dfrac{u}{\Delta x} - k_1 C_{A21} = -\dfrac{2\times 10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{A21} = -2.0008 - C_{A21}$

Right hand side of equation 21 = 0.
The above equations can be written in tridiagonal form as given below.

$$\begin{bmatrix} -20005.9992 - C_{A1} & 2.0008 & & & \\ 2.0004 & -2.0008 - C_{A2} & 0.0004 & & \\ & \cdots & \cdots & \cdots & \\ & & 2.0004 & -2.0008 - C_{A20} & 0.0004 \\ & & & 2.0008 & -2.0008 - C_{A21} \end{bmatrix} \begin{bmatrix} C_{A1} \\ C_{A2} \\ \cdots \\ C_{A20} \\ C_{A21} \end{bmatrix} = \begin{bmatrix} -20004 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

Program 7.1 for the solution of the above problem is given in the Appendix. In the program the initial values of concentration of A at nodes 1 to 21 is assumed and then the TDMA is used to determine new values of concentration of A at nodes 1 to 21. Again, these values are used to determine the coefficients in the matrix, and after the coefficients are determined the TDMA is used to determine new values of concentration of A at nodes 1 to 21. The procedure is repeated till there is no change in the concentration at each node. The results are presented in Table 7.5.

Table 7.5 Results in Example 7.2

Node number	x (m)	C_A
1	0.0	0.999923
3	1.0	0.569732
5	2.0	0.387587
7	3.0	0.290241
9	4.0	0.230588
11	5.0	0.190624
13	6.0	0.162124
15	7.0	0.140841
17	8.0	0.124379
19	9.0	0.111286
21	10.0	0.100638

7.4 Multiple Reactions

Consider a tubular reactor with axial dispersion in which multiple reactions takes place. The analysis is described with an example.

EXAMPLE 7.3 Consider the following two reactions taking place in a tubular reactor with axial dispersion:

$$A + B \xrightarrow{k_1} C$$

$$B + C \xrightarrow{k_2} D$$

Assuming the axial dispersion coefficient to be the same for all the species, the concentration of various species along the length of the reactor are given by the following differential equations:
for component A

$$D\frac{d^2C_A}{dx^2} - u\frac{dC_A}{dx} - k_1C_AC_B = 0$$

for component B

$$D\frac{d^2C_B}{dx^2} - u\frac{dC_B}{dx} - k_1C_AC_B - k_2C_BC_C = 0$$

for component C

$$D\frac{d^2C_C}{dx^2} - u\frac{dC_C}{dx} + k_1C_AC_B - k_2C_BC_C = 0$$

for component D

$$D\frac{d^2C_D}{dx^2} - u\frac{dC_D}{dx} + k_2C_BC_C = 0$$

The boundary conditions are

At inlet:

$$uC_{A,\text{in}} = uC_A - D\frac{dC_A}{dx}$$

$$uC_{B,\text{in}} = uC_B - D\frac{dC_B}{dx}$$

$$uC_{C,\text{in}} = uC_C - D\frac{dC_C}{dx}$$

$$uC_{D,\text{in}} = uC_D - D\frac{dC_D}{dx}$$

At exit: $\frac{dC_A}{dx} = 0 \qquad \frac{dC_B}{dx} = 0 \qquad \frac{dC_C}{dx} = 0$ and $\frac{dC_D}{dx} = 0$

Make 20 parts of the reactor of length 10 m. A fluid medium comprising initially only *A* and *B* flows through the reactor with a mean axial velocity u = 1 m/s. The axial dispersion coefficient is the same for all the species, $D = 10^{-4}$ m^2/s, and the rate constants of the reactions are $k_1 = k_2 = 1$ m^3/mol-s. The inlet concentrations of *A* and *B* are $C_{A,\text{in}} = C_{B,\text{in}} = 1$ mol/m^3. Compute the concentration of various species along the length of the reactor.

Solution We have

$$\Delta x = \frac{10}{20} = 0.5 \text{ m}$$

We solve the differential equation using the upwind difference scheme for the convection term. Discretizing the differential equation at node *i*, we get for species *A*

$$D\left(\frac{C_{Ai+1} + C_{Ai-1} - 2C_{Ai}}{\Delta x^2}\right) - u\left(\frac{C_{Ai} - C_{Ai-1}}{\Delta x}\right) - k_1 C_{Ai} C_{Bi} = 0$$

for species *B*

$$D\left(\frac{C_{Bi+1} + C_{Bi-1} - 2C_{Bi}}{\Delta x^2}\right) - u\left(\frac{C_{Bi} - C_{Bi-1}}{\Delta x}\right) - k_1 C_{Ai} C_{Bi} - k_2 C_{Bi} C_{Ci} = 0$$

for species *C*

$$D\left(\frac{C_{Ci+1} + C_{Ci-1} - 2C_{Ci}}{\Delta x^2}\right) - u\left(\frac{C_{Ci} - C_{Ci-1}}{\Delta x}\right) + k_1 C_{Ai} C_{Bi} - k_2 C_{Bi} C_{Ci} = 0$$

for species *D*

$$D\left(\frac{C_{Di+1} + C_{Di-1} - 2C_{Di}}{\Delta x^2}\right) - u\left(\frac{C_{Di} - C_{Di-1}}{\Delta x}\right) + k_2 C_{Bi} C_{Ci} = 0$$

At node 1 the discretized equation for the component A is

$$D\left(\frac{C_{A2}+C_{A0}-2C_{A1}}{\Delta x^2}\right)-u\left(\frac{C_{A1}-C_{A0}}{\Delta x}\right)-k_1C_{A1}C_{B1}=0$$

$$C_{A1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{B1}\right)+\frac{D}{\Delta x^2}C_{A2}+C_{A0}\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)=0$$

From the boundary condition at node 1, we get

$$uC_{A,\text{in}}=uC_{A1}-D\left(\frac{C_{A2}-C_{A0}}{2\Delta x}\right)$$

Solving for C_{A0}, we get

$$C_{A0}=\frac{2u\Delta x}{D}\left(C_{A,\text{in}}-C_{A1}\right)+C_{A2}$$

Substituting for C_{A0} in the equation for node 1, we get

$$C_{A1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{B1}\right)+\frac{D}{\Delta x^2}C_{A2}+\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)\left[\frac{2u\Delta x}{D}\left(C_{A,\text{in}}-C_{A1}\right)+C_{A2}\right]=0$$

$$\left(-\frac{2D}{\Delta x^2}-\frac{3u}{\Delta x}-k_1C_{B1}-\frac{2u^2}{D}\right)C_{A1}+\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{A2}=-\left(\frac{2u^2}{D}+\frac{2u}{\Delta x}\right)C_{A,\text{in}}$$

At node 1 the discretized equation for component B is

$$D\left(\frac{C_{B2}+C_{B0}-2C_{B1}}{\Delta x^2}\right)-u\left(\frac{C_{B1}-C_{B0}}{\Delta x}\right)-k_1C_{A1}C_{B1}-k_2C_{B1}C_{C1}=0$$

$$C_{B1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{A1}-k_2C_{C1}\right)+\frac{D}{\Delta x^2}C_{B2}+C_{B0}\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)=0$$

From the boundary condition at node 1, we get

$$uC_{B,\text{in}}=uC_{B1}-D\left(\frac{C_{B2}-C_{B0}}{2\Delta x}\right)$$

Solving for C_{B0}, we get

$$C_{B0}=\frac{2u\Delta x}{D}\left(C_{B,\text{in}}-C_{B1}\right)+C_{B2}$$

Substituting for C_{B0} in the equation for node 1, we get

$$C_{B1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{A1}-k_2C_{C1}\right)+\frac{D}{\Delta x^2}C_{B2}+\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)\left[\frac{2u\Delta x}{D}\left(C_{B,\text{in}}-C_{B1}\right)+C_{B2}\right]=0$$

$$\left(-\frac{2D}{\Delta x^2}-\frac{3u}{\Delta x}-k_1C_{A1}-k_2C_{C1}-\frac{2u^2}{D}\right)C_{B1}+\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{B2}=-\left(\frac{2u^2}{D}+\frac{2u}{\Delta x}\right)C_{B,\text{in}}$$

At node 1 the discretized equation for component C is

$$D\left(\frac{C_{C2}+C_{C0}-2C_{C1}}{\Delta x^2}\right)-u\left(\frac{C_{C1}-C_{C0}}{\Delta x}\right)+k_1C_{A1}C_{B1}-k_2C_{B1}C_{C1}=0$$

$$C_{C1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_2C_{B1}\right)+\frac{D}{\Delta x^2}C_{C2}+C_{C0}\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)=-k_1C_{A1}C_{B1}$$

From the boundary condition at node 1, we get

$$0=uC_{C1}-D\left(\frac{C_{C2}-C_{C0}}{2\Delta x}\right)$$

Solving for C_{C0}, we get

$$C_{C0}=-\frac{2u\Delta xC_{C1}}{D}+C_{C2}$$

Substituting for C_{C0}, in the equation for node 1, we get

$$C_{C1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_2C_{B1}\right)+\frac{D}{\Delta x^2}C_{C2}+\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)\left(-\frac{2u\Delta xC_{C1}}{D}+C_{C2}\right)=-k_1C_{A1}C_{B1}$$

$$\left(-\frac{2D}{\Delta x^2}-\frac{3u}{\Delta x}-k_2C_{B1}-\frac{2u^2}{D}\right)C_{C1}+\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{C2}=-k_1C_{A1}C_{B1}$$

At node 1 the discretized equation for component D is

$$D\left(\frac{C_{D2}+C_{D0}-2C_{D1}}{\Delta x^2}\right)-u\left(\frac{C_{D1}-C_{D0}}{\Delta x}\right)+k_2C_{B1}C_{C1}=0$$

$$C_{D1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}\right)+\frac{D}{\Delta x^2}C_{D2}+C_{D0}\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)=-k_2C_{B1}C_{C1}$$

From the boundary condition at node 1, we get

$$0=uC_{D1}-D\left(\frac{C_{D2}-C_{D0}}{2\Delta x}\right)$$

Solving for C_{D0}, we get

$$C_{D0}=-\frac{2u\Delta xC_{D1}}{D}+C_{D2}$$

Substituting for C_{D0}, in the equation for node 1, we get

$$C_{D1}\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}\right)+\frac{D}{\Delta x^2}C_{D2}+\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)\left(-\frac{2u\Delta xC_{D1}}{D}+C_{D2}\right)=-k_2C_{B1}C_{C1}$$

$$\left(-\frac{2D}{\Delta x^2}-\frac{3u}{\Delta x}-\frac{2u^2}{D}\right)C_{D1}+\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{D2}=-k_2C_{B1}C_{C1}$$

At node 2 the discretized equations for various components are

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{A1}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{B2}\right)C_{A2}+\frac{D}{\Delta x^2}C_{A3}=0$$

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{B1}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{A2}-k_2C_{C2}\right)C_{B2}+\frac{D}{\Delta x^2}C_{B3}=0$$

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{C1}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_2C_{B2}\right)C_{C2}+\frac{D}{\Delta x^2}C_{C3}=-k_1C_{A2}C_{B2}$$

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{D1}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}\right)C_{D2}+\frac{D}{\Delta x^2}C_{D3}=-k_2C_{B2}C_{C2}$$

At node 21 the discretized equation for component A is

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{A20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{B21}\right)C_{A21}+\frac{D}{\Delta x^2}C_{A22}=0$$

From the boundary condition at node 21, we get

$$\left(\frac{C_{A22}-C_{A20}}{2\Delta x}\right)=0 \qquad \text{thus } C_{A22}=C_{A20}$$

Substituting for C_{A22} in the equation for node 21, we get

$$\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{A20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{B21}\right)C_{A21}=0$$

At node 21 the discretized equation for component B is

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{B20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{A21}-k_2C_{C21}\right)C_{B21}+\frac{D}{\Delta x^2}C_{B22}=0$$

From the boundary condition at node 21, we get

$$\left(\frac{C_{B22}-C_{B20}}{2\Delta x}\right)=0 \qquad \text{thus } C_{B22}=C_{B20}$$

Substituting for C_{B22} in the equation for node 21, we get

$$\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{B20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_1C_{A21}-k_2C_{C21}\right)C_{B21}=0$$

At node 21 the discretized equation for component C is

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{C20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_2C_{B21}\right)C_{C21}+\frac{D}{\Delta x^2}C_{C22}=-k_1C_{A21}C_{B21}$$

From the boundary condition at node 21, we get

$$\left(\frac{C_{C22}-C_{C20}}{2\Delta x}\right)=0 \qquad \text{thus } C_{C22}=C_{C20}$$

Substituting for C_{C22} in the equation for node 21, we get

$$\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{C20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}-k_2C_{B21}\right)C_{C21}=-k_1C_{A21}C_{B21}$$

At node 21 the discretized equation for component D is

$$\left(\frac{D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{D20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}\right)C_{D21}+\frac{D}{\Delta x^2}C_{D22}=-k_2C_{B21}C_{C21}$$

From the boundary condition at node 21, we get

$$\left(\frac{C_{D22}-C_{D20}}{2\Delta x}\right)=0 \qquad \text{thus } C_{D22} = C_{D20}$$

Substituting for C_{D22} in the equation for node 21, we get

$$\left(\frac{2D}{\Delta x^2}+\frac{u}{\Delta x}\right)C_{D20}+\left(-\frac{2D}{\Delta x^2}-\frac{u}{\Delta x}\right)C_{D21}=-k_2C_{B21}C_{C21}$$

The coefficients of equation 1 (node 1, species A) are

Coefficient of $C_{A1}=-\frac{2\times10^{-4}}{0.5^2}-\frac{3}{0.5}-C_{B1}-\frac{2}{10^{-4}}=-20005.9992-C_{B1}$

Coefficient of C_{B1} = 0
Coefficient of C_{C1} = 0
Coefficient of C_{D1} = 0

Coefficient of $C_{A2}=\frac{2\times10^{-4}}{0.5^2}+\frac{1}{0.5}=2.0008$

Coefficient of C_{B2} = 0
Coefficient of C_{C2} = 0
Coefficient of C_{D2} = 0

Right hand side of equation 1 = $-\left(\frac{2u^2}{D}+\frac{2u}{\Delta x}\right)C_{A,\text{in}}=-\frac{2}{0.5}-\frac{2}{10^{-4}}=-20004$

The coefficients of equation 2 (node 1, species B) are
Coefficient of C_{A1} = 0

Coefficient of C_{B1} = $-\frac{2\times10^{-4}}{0.5^2}-\frac{3}{0.5}-C_{A1}-C_{C1}-\frac{2}{10^{-4}}=-20005.9992-C_{A1}-C_{C1}$

Coefficient of C_{C1} = 0
Coefficient of C_{D1} = 0
Coefficient of C_{A2} = 0

Coefficient of $C_{B2} = \frac{2 \times 10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0008$

Coefficient of $C_{C2} = 0$
Coefficient of $C_{D2} = 0$

Right hand side of equation 2 = $-\left(\frac{2u^2}{D} + \frac{2u}{\Delta x}\right)C_{B,\text{in}} = -\frac{2}{0.5} - \frac{2}{10^{-4}} = -20004$

The coefficients of equation 3 (node 1, species *C*) are:
Coefficient of $C_{A1} = 0$
Coefficient of $C_{B1} = 0$

Coefficient of $C_{C1} = -\frac{2 \times 10^{-4}}{0.5^2} - \frac{3}{0.5} - C_{B1} - \frac{2}{10^{-4}} = -20005.9992 - C_{B1}$

Coefficient of $C_{D1} = 0$
Coefficient of $C_{A2} = 0$
Coefficient of $C_{B2} = 0$

Coefficient of $C_{C2} = \frac{2 \times 10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0008$

Coefficient of $C_{D2} = 0$
Right hand side of equation 3 = $-C_{A1}C_{B1}$.

The coefficients of equation 4 (node 1, species *D*) are:
Coefficient of $C_{A1} = 0$
Coefficient of $C_{B1} = 0$
Coefficient of $C_{C1} = 0$

Coefficient of $C_{D1} = -\frac{2 \times 10^{-4}}{0.5^2} - \frac{3}{0.5} - \frac{2}{10^{-4}} = -20005.9992$

Coefficient of $C_{A2} = 0$
Coefficient of $C_{B2} = 0$
Coefficient of $C_{C2} = 0$

Coefficient of $C_{D2} = \frac{2 \times 10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0008$

Right hand side of equation 4 = $-C_{B1}C_{C1}$.

The coefficients of equation 5 (node 2, species *A*) are:

Coefficient of $C_{A1} = \frac{10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0004$

Coefficient of C_{B1} = 0
Coefficient of C_{C1} = 0
Coefficient of C_{D1} = 0

Coefficient of $C_{A2} = -\dfrac{2 \times 10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{B2} = -2.0008 - C_{B2}$

Coefficient of C_{B2} = 0
Coefficient of C_{C2} = 0
Coefficient of C_{D2} = 0

Coefficient of $C_{A3} = \dfrac{10^{-4}}{0.5^2} = 0.0004$

Coefficient of C_{B3} = 0
Coefficient of C_{C3} = 0
Coefficient of C_{D3} = 0
Right hand side of equation 5 = 0.

The coefficients of equation 6 (node 2, species *B*) are:
Coefficient of C_{A1} = 0

Coefficient of $C_{B1} = \dfrac{10^{-4}}{0.5^2} + \dfrac{1}{0.5} = 2.0004$

Coefficient of C_{C1} = 0
Coefficient of C_{D1} = 0
Coefficient of C_{A2} = 0

Coefficient of $C_{B2} = -\dfrac{2 \times 10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{A2} - C_{C2} = -2.0008 - C_{A2} - C_{C2}$

Coefficient of C_{C2} = 0
Coefficient of C_{D2} = 0
Coefficient of C_{A3} = 0

Coefficient of $C_{B3} = \dfrac{10^{-4}}{0.5^2} = 0.0004$

Coefficient of C_{C3} = 0
Coefficient of C_{D3} = 0
Right hand side of equation 6 = 0.

The coefficients of equation 7 (node 2, species *C*) are:
Coefficient of C_{A1} = 0
Coefficient of C_{B1} = 0

Coefficient of $C_{C1} = \dfrac{10^{-4}}{0.5^2} + \dfrac{1}{0.5} = 2.0004$

Coefficient of $C_{D1} = 0$
Coefficient of $C_{A2} = 0$
Coefficient of $C_{B2} = 0$

$$\text{Coefficient of } C_{C2} = -\frac{2\times10^{-4}}{0.5^2} - \frac{1}{0.5} - C_{B2} = -2.0008 - C_{B2}$$

Coefficient of $C_{D2} = 0$
Coefficient of $C_{A3} = 0$
Coefficient of $C_{B3} = 0$

$$\text{Coefficient of } C_{C3} = \frac{10^{-4}}{0.5^2} = 0.0004$$

Coefficient of $C_{D3} = 0$
Right hand side of equation 7 = $-C_{A2}C_{B2}$

The coefficients of equation 8 (node 2, species *D*) are:
Coefficient of $C_{A1} = 0$
Coefficient of $C_{B1} = 0$
Coefficient of $C_{C1} = 0$

$$\text{Coefficient of } C_{D1} = \frac{10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0004$$

Coefficient of $C_{A2} = 0$
Coefficient of $C_{B2} = 0$
Coefficient of $C_{C2} = 0$

$$\text{Coefficient of } C_{D2} = -\frac{2\times10^{-4}}{0.5^2} - \frac{1}{0.5} = -2.0008$$

Coefficient of $C_{A3} = 0$
Coefficient of $C_{B3} = 0$
Coefficient of $C_{C3} = 0$

$$\text{Coefficient of } C_{D3} = \frac{10^{-4}}{0.5^2} = 0.0004$$

Right hand side of equation 8 = $-C_{B2}C_{C2}$.

The coefficients of equation 81 (node 21, species *A*) are:

$$\text{Coefficient of } C_{A20} = \frac{2\times10^{-4}}{0.5^2} + \frac{1}{0.5} = 2.0008$$

Coefficient of $C_{B20} = 0$
Coefficient of $C_{C20} = 0$
Coefficient of $C_{D20} = 0$

Coefficient of $C_{A21} = -\dfrac{2\times10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{B21} = -2.0008 - C_{B21}$
Coefficient of $C_{B21} = 0$
Coefficient of $C_{C21} = 0$
Coefficient of $C_{D21} = 0$
Right hand side of equation 81 = 0.

The coefficients of equation 82 (node 21, species *B*) are:
Coefficient of $C_{A20} = 0$
Coefficient of $C_{B20} = \dfrac{2\times10^{-4}}{0.5^2} + \dfrac{1}{0.5} = 2.0008$
Coefficient of $C_{C20} = 0$
Coefficient of $C_{D20} = 0$
Coefficient of $C_{A21} = 0$
Coefficient of $C_{B21} = -\dfrac{2\times10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{A21} - C_{C21} = -2.0008 - C_{A21} - C_{C21}$
Coefficient of $C_{C21} = 0$
Coefficient of $C_{D21} = 0$
Right hand side of equation 82 = 0.

The coefficients of equation 83 (node 21, species *C*) are:
Coefficient of $C_{A20} = 0$
Coefficient of $C_{B20} = 0$
Coefficient of $C_{C20} = \dfrac{2\times10^{-4}}{0.5^2} + \dfrac{1}{0.5} = 2.0008$
Coefficient of $C_{D20} = 0$
Coefficient of $C_{A21} = 0$
Coefficient of $C_{B21} = 0$
Coefficient of $C_{C21} = -\dfrac{2\times10^{-4}}{0.5^2} - \dfrac{1}{0.5} - C_{B21} = -2.0008 - C_{B21}$
Coefficient of $C_{D21} = 0$
Right hand side of equation 83 = $-C_{A21}C_{B21}$.

The coefficients of equation 84 (node 21, species *D*) are:
Coefficient of $C_{A20} = 0$
Coefficient of $C_{B20} = 0$
Coefficient of $C_{C20} = 0$

Coefficient of $C_{D20} = \dfrac{2 \times 10^{-4}}{0.5^2} + \dfrac{1}{0.5} = 2.0008$

Coefficient of $C_{A21} = 0$
Coefficient of $C_{B21} = 0$
Coefficient of $C_{C21} = 0$

Coefficient of $C_{D21} = -\dfrac{2 \times 10^{-4}}{0.5^2} - \dfrac{1}{0.5} = -2.0008$

Right hand side of equation 84 = $-C_{B21}C_{C21}$.

Thus the set of equations for concentration of species A, B, C, and D at nodes 1 to 21 can be written in the block tridiagonal form as

$$\begin{bmatrix} B_1 & C_1 & & & & & & & & & & \\ A_2 & B_2 & C_2 & & & & & & & & & \\ & A_3 & B_3 & C_3 & & & & & & & & \\ & & A_4 & B_4 & C_4 & & & & & & & \\ & & & A_5 & B_5 & C_5 & & & & & & \\ & & & & A_6 & B_6 & C_6 & & & & & \\ & & & & & \cdots & \cdots & \cdots & & & & \\ & & & & & & \cdots & \cdots & \cdots & & & \\ & & & & & & & \cdots & \cdots & \cdots & & \\ & & & & & & & & \cdots & \cdots & \cdots & \\ & & & & & & & & & A_{20} & B_{20} & C_{20} \\ & & & & & & & & & & A_{21} & B_{21} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ X_{20} \\ X_{21} \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \\ D_6 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ D_{20} \\ D_{21} \end{bmatrix}$$

where

$$X_1 = \begin{bmatrix} C_{A1} \\ C_{B1} \\ C_{C1} \\ C_{D1} \end{bmatrix} \qquad X_2 = \begin{bmatrix} C_{A2} \\ C_{B2} \\ C_{C2} \\ C_{D2} \end{bmatrix} \qquad X_{21} = \begin{bmatrix} C_{A21} \\ C_{B21} \\ C_{C21} \\ C_{D21} \end{bmatrix}$$

For node 1

$$B_1 = \begin{bmatrix} -20005.9992 - C_{B1} & 0 & 0 & 0 \\ 0 & -20005.9992 - C_{A1} - C_{C1} & 0 & 0 \\ 0 & 0 & -20005.9992 - C_{B1} & 0 \\ 0 & 0 & 0 & -20005.9992 \end{bmatrix}$$

$$C_1 = \begin{bmatrix} 2.0008 & 0 & 0 & 0 \\ 0 & 2.0008 & 0 & 0 \\ 0 & 0 & 2.0008 & 0 \\ 0 & 0 & 0 & 2.0008 \end{bmatrix}$$

$$D_1 = \begin{bmatrix} -20004 \\ -20004 \\ -C_{A1}C_{B1} \\ -C_{B1}C_{C1} \end{bmatrix}$$

For node 2

$$A_2 = \begin{bmatrix} 2.0004 & 0 & 0 & 0 \\ 0 & 2.0004 & 0 & 0 \\ 0 & 0 & 2.0004 & 0 \\ 0 & 0 & 0 & 2.0004 \end{bmatrix}$$

$$B_2 = \begin{bmatrix} -2.0008 - C_{B2} & 0 & 0 & 0 \\ 0 & -2.0008 - C_{A2} - C_{C2} & 0 & 0 \\ 0 & 0 & -2.0008 - C_{B2} & 0 \\ 0 & 0 & 0 & -2.0008 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} 0.0004 & 0 & 0 & 0 \\ 0 & 0.0004 & 0 & 0 \\ 0 & 0 & 0.0004 & 0 \\ 0 & 0 & 0 & 0.0004 \end{bmatrix}$$

$$D_2 = \begin{bmatrix} 0 \\ 0 \\ -C_{A2}C_{B2} \\ -C_{B2}C_{C2} \end{bmatrix}$$

For node 3

$$A_3 = \begin{bmatrix} 2.0004 & 0 & 0 & 0 \\ 0 & 2.0004 & 0 & 0 \\ 0 & 0 & 2.0004 & 0 \\ 0 & 0 & 0 & 2.0004 \end{bmatrix}$$

$$B_3 = \begin{bmatrix} -2.0008 - C_{B3} & 0 & 0 & 0 \\ 0 & -2.0008 - C_{A3} - C_{C3} & 0 & 0 \\ 0 & 0 & -2.0008 - C_{B3} & 0 \\ 0 & 0 & 0 & -2.0008 \end{bmatrix}$$

$$C_3 = \begin{bmatrix} 0.0004 & 0 & 0 & 0 \\ 0 & 0.0004 & 0 & 0 \\ 0 & 0 & 0.0004 & 0 \\ 0 & 0 & 0 & 0.0004 \end{bmatrix}$$

$$D_3 = \begin{bmatrix} 0 \\ 0 \\ -C_{A3}C_{B3} \\ -C_{B3}C_{C3} \end{bmatrix}$$

For node 21

$$A_{21} = \begin{bmatrix} 2.0008 & 0 & 0 & 0 \\ 0 & 2.0008 & 0 & 0 \\ 0 & 0 & 2.0008 & 0 \\ 0 & 0 & 0 & 2.0008 \end{bmatrix}$$

$$B_{21} = \begin{bmatrix} -2.0008 - C_{B21} & 0 & 0 & 0 \\ 0 & -2.0008 - C_{A21} - C_{C21} & 0 & 0 \\ 0 & 0 & -2.0008 - C_{B21} & 0 \\ 0 & 0 & 0 & -2.0008 \end{bmatrix}$$

$$D_{21} = \begin{bmatrix} 0 \\ 0 \\ -C_{A21}C_{B21} \\ -C_{B21}C_{C21} \end{bmatrix}$$

The 84 linear algebraic equations can be written in the form $Ax = d$, where A is a 84 × 84 matrix, x is the vector of size 84 × 1 containing the variables to be determined, and d is also a vector of size 84 × 1. The variables can be written as

$$x = \begin{bmatrix} C_{A1} & C_{B1} & C_{C1} & C_{D1} & \cdots & \cdots & \cdots & \cdots & C_{A21} & C_{B21} & C_{C21} & C_{D21} \end{bmatrix}^T$$

The Gauss elimination method can be used to solve these 84 linear algebraic equations. The non-zero elements of the matrix A are

$A(1,1) = -20005.9992 - C_{B1}$, $A(1,5) = 2.0008$, $A(2,2) = -20005.9992 - C_{A1} - C_{C1}$, $A(2,6) = 2.0008$ $A(3,3) = -20005.9992 - C_{B1}$, $A(3,7) = 2.0008$, $A(4,4) = -20005.9992$, $A(4,8) = 2.0008$, $A(5,1) = 2.0004$, $A(5,5) = -2.0008 - C_{B2}$, $A(5,9) = 0.0004$, $A(6,2) = 2.0004$, $A(6,6) = -2.0008 - C_{A2} - C_{C2}$, $A(6,10) = 0.0004$, $A(7,3) = 2.0004$, $A(7,7) = -2.0008 - C_{B2}$, $A(7,11) = 0.0004$, $A(8,4) = 2.0004$, $A(8,8) = -2.0008$, $A(8,12) = 0.0004$, $A(9,5) = 2.0004$, $A(9,9) = -2.0008 - C_{B3}$, $A(9,13) = 0.0004$, $A(10,6) = 2.0004$, $A(10,10) = -2.0008 - CA_3 - C_{C3}$, $A(10,14) = 0.0004$, $A(11,7) = 2.0004$, $A(11,11) = -2.0008 - C_{B3}$, $A(11,15) = 0.0004$, $A(12,8) = 2.0004$, $A(12,12) = -2.0008$, $A(12,16) = 0.0004$, $A(13,9) = 2.0004$, $A(13,13) = -2.0008 - C_{B4}$, $A(13,17) = 0.0004$, $A(14,10) = 2.0004$, $A(14,14) = -2.0008 - CA_4 - C_{C4}$, $A(14,18) = 0.0004$, $A(15,11) = 2.0004$, $A(15,15) = -2.0008 - C_{B4}$, $A(15,19) = 0.0004$, $A(16,12) = 2.0004$, $A(16,16) = -2.0008$, $A(16,20) = 0.0004$, $A(17,13) =$

2.0004, $A(17,17) = -2.0008-C_{B5}$, $A(17,21) = 0.0004$, $A(18,14) = 2.0004$, $A(18,18) = -2.0008-C_{A5}-C_{C5}$, $A(18,22) = 0.0004$, $A(19,15) = 2.0004$, $A(19,19) = -2.0008-C_{B5}$, $A(19,23) = 0.0004$, $A(20,16) = 2.0004$, $A(20,20) = -2.0008$, $A(20,24) = 0.0004$, $A(21,17) = 2.0004$, $A(21,21) = -2.0008-C_{B6}$, $A(21,25) = 0.0004$, $A(22,18) = 2.0004$, $A(22,22) = -2.0008-CA_6-C_{C6}$, $A(22,26) = 0.0004$, $A(23,19) = 2.0004$, $A(23,23) = -2.0008-C_{B6}$, $A(23,27) = 0.0004$, $A(24,20) = 2.0004$, $A(24,24) = -2.0008$, $A(24,28) = 0.0004$, $A(25,21) = 2.0004$, $A(25,25) = -2.0008-C_{B7}$, $A(25,29) = 0.0004$, $A(26,22) = 2.0004$, $A(26,26) = -2.0008-C_{A7}-C_{C7}$, $A(26,30) = 0.0004$, $A(27,23) = 2.0004$, $A(27,27) = -2.0008-C_{B7}$, $A(27,31) = 0.0004$, $A(28,24) = 2.0004$, $A(28,28) = -2.0008$, $A(28,32) = 0.0004$, $A(29,25) = 2.0004$, $A(29,29) = -2.0008-C_{B8}$, $A(29,33) = 0.0004$, $A(30,26) = 2.0004$, $A(30,30) = -2.0008-C_{A8}-C_{C8}$, $A(30,34) = 0.0004$, $A(31,27) = 2.0004$, $A(31,31) = -2.0008-C_{B8}$, $A(31,35) = 0.0004$, $A(32,28) = 2.0004$, $A(32,32) = -2.0008$, $A(32,36) = 0.0004$, $A(33,29) = 2.0004$, $A(33,33) = -2.0008-C_{B9}$, $A(33,37) = 0.0004$, $A(34,30) = 2.0004$, $A(34,34) = -2.0008-C_{A9}-C_{C9}$, $A(34,38) = 0.0004$, $A(35,31) = 2.0004$, $A(35,35) = -2.0008-C_{B9}$, $A(35,39) = 0.0004$, $A(36,32) = 2.0004$, $A(36,36) = -2.0008$, $A(36,40) = 0.0004$, $A(37,33) = 2.0004$, $A(37,37) = -2.0008-C_{B10}$, $A(37,41) = 0.0004$, $A(38,34) = 2.0004$, $A(38,38) = -2.0008-C_{A10}-C_{C10}$, $A(38,42) = 0.0004$, $A(39,35) = 2.0004$, $A(39,39) = -2.0008-C_{B10}$, $A(39,43) = 0.0004$, $A(40,36) = 2.0004$, $A(40,40) = -2.0008$, $A(40,44) = 0.0004$, $A(41,37) = 2.0004$, $A(41,41) = -2.0008-C_{B11}$, $A(41,45) = 0.0004$, $A(42,38) = 2.0004$, $A(42,42) = -2.0008-C_{A11}-C_{C11}$, $A(42,46) = 0.0004$, $A(43,39) = 2.0004$, $A(43,43) = -2.0008-C_{B11}$, $A(43,47) = 0.0004$, $A(44,40) = 2.0004$, $A(44,44) = -2.0008$, $A(44,48) = 0.0004$, $A(45,41) = 2.0004$, $A(45,45) = -2.0008-C_{B12}$, $A(45,49) = 0.0004$, $A(46,42) = 2.0004$, $A(46,46) = -2.0008-C_{A12}-C_{C12}$, $A(46,50) = 0.0004$, $A(47,43) = 2.0004$, $A(47,47) = -2.0008-C_{B12}$, $A(47,51) = 0.0004$, $A(48,44) = 2.0004$, $A(48,48) = -2.0008$, $A(48,52) = 0.0004$, $A(49,45) = 2.0004$, $A(49,49) = -2.0008-C_{B13}$, $A(49,53) = 0.0004$, $A(50,46) = 2.0004$, $A(50,50) = -2.0008-C_{A13}-C_{C13}$, $A(50,54) = 0.0004$, $A(51,47) = 2.0004$, $A(51,51) = -2.0008-C_{B13}$, $A(51,55) = 0.0004$, $A(52,48) = 2.0004$, $A(52,52) = -2.0008$, $A(52,56) = 0.0004$, $A(53,49) = 2.0004$, $A(53,53) = -2.0008-C_{B14}$, $A(53,57) = 0.0004$, $A(54,50) = 2.0004$, $A(54,54) = -2.0008-C_{A14}-C_{C14}$, $A(54,58) = 0.0004$, $A(55,51) = 2.0004$, $A(55,55) = -2.0008-C_{B14}$, $A(55,59) = 0.0004$, $A(56,52) = 2.0004$, $A(56,56) = -2.0008$, $A(56,60) = 0.0004$, $A(57,53) = 2.0004$, $A(57,57) = -2.0008-C_{B15}$, $A(57,61) = 0.0004$, $A(58,54) = 2.0004$, $A(58,58) = -2.0008-C_{A15}-C_{C15}$, $A(58,62) = 0.0004$, $A(59,55) = 2.0004$, $A(59,59) = -2.0008-C_{B15}$, $A(59,63) = 0.0004$, $A(60,56) = 2.0004$, $A(60,60) = -2.0008$, $A(60,64) = 0.0004$, $A(61,57) = 2.0004$, $A(61,61) = -2.0008-C_{B16}$, $A(61,65) = 0.0004$, $A(62,58) = 2.0004$, $A(62,62) = -2.0008-C_{A16}-C_{C16}$, $A(62,66) = 0.0004$, $A(63,59) = 2.0004$, $A(63,63) = -2.0008-C_{B16}$, $A(63,67) = 0.0004$, $A(64,60) = 2.0004$, $A(64,64) = -2.0008$, $A(64,68) = 0.0004$, $A(65,61) = 2.0004$, $A(65,65) = -2.0008-C_{B17}$, $A(65,69) = 0.0004$, $A(66,62) = 2.0004$, $A(66,66) = -2.0008-C_{A17}-C_{C17}$, $A(66,70) = 0.0004$, $A(67,63) = 2.0004$, $A(67,67) = -2.0008-C_{B17}$, $A(67,71) = 0.0004$, $A(68,64) = 2.0004$, $A(68,68) = -2.0008$, $A(68,72) = 0.0004$, $A(69,65) = 2.0004$, $A(69,69) = -2.0008-C_{B18}$, $A(69,73) = 0.0004$, $A(70,66) = 2.0004$, $A(70,70) = -2.0008-C_{A18}-C_{C18}$, $A(70,74) = 0.0004$, $A(71,67) = 2.0004$, $A(71,71) = -2.0008-C_{B18}$, $A(71,75) = 0.0004$, $A(72,68) = 2.0004$, $A(72,72) = -2.0008$, $A(72,76) = 0.0004$, $A(73,69) = 2.0004$, $A(73,73) = -2.0008-C_{B19}$, $A(73,77) = 0.0004$, $A(74,70) = 2.0004$, $A(74,74) = -2.0008-C_{A19}-C_{C19}$, $A(74,78) = 0.0004$, $A(75,71) = 2.0004$, $A(75,75) = -2.0008-C_{B19}$, $A(75,79) = 0.0004$, $A(76,72) = 2.0004$, $A(76,76) = -2.0008$, $A(76,80) = 0.0004$, $A(77,73) = 2.0004$, $A(77,77) = -2.0008-C_{B20}$, $A(77,81) = 0.0004$, $A(78,74) = 2.0004$, $A(78,78) = -2.0008-C_{A20}-C_{C20}$, $A(78,82) = 0.0004$, $A(79,75) = 2.0004$, $A(79,79) = -2.0008-C_{B20}$, $A(79,83) = 0.0004$, $A(80,76) = 2.0004$, $A(80,80) = -2.0008$, $A(80,84) = 0.0004$, $A(81,77) =$

2.0008, $A(81,81) = -2.0008 - C_{B21}$, $A(82,78) = 2.0008$, $A(82,82) = -2.0008 - C_{A21} - C_{C21}$, $A(83,79) = 2.0008$, $A(83,83) = -2.0008 - C_{B21}$, $A(84,80) = 2.0008$, $A(84,84) = -2.0008$

The nonzero right hand side terms are given in augmented matrix A form as

$A(1,85) = -20004$, $A(2,85) = -20004$, $A(3,85) = -C_{A1}C_{B1}$, $A(4,85) = -C_{B1}C_{C1}$, $A(7,85) = -C_{A2}C_{B2}$, $A(8,85) = -C_{B2}C_{C2}$, $A(11,85) = -C_{A3}C_{B3}$, $A(12,85) = -C_{B3}C_{C3}$, $A(15,85) = -C_{A4}C_{B4}$, $A(16,85) = -C_{B4}C_{C4}$, $A(19,85) = -C_{A5}C_{B5}$, $A(20,85) = -C_{B5}C_{C5}$, $A(23,85) = -C_{A6}C_{B6}$, $A(24,85) = -C_{B6}C_{C6}$, $A(27,85) = -C_{A7}C_{B7}$, $A(28,85) = -C_{B7}C_{C7}$, $A(31,85) = -C_{A8}C_{B8}$, $A(32,85) = -C_{B8}C_{C8}$, $A(35,85) = -C_{A9}C_{B9}$, $A(36,85) = -C_{B9}C_{C9}$, $A(39,85) = -C_{A10}C_{B10}$, $A(40,85) = -C_{B10}C_{C10}$, $A(43,85) = -C_{A11}C_{B11}$, $A(44,85) = -C_{B11}C_{C11}$, $A(47,85) = -C_{A12}C_{B12}$, $A(48,85) = -C_{B12}C_{C12}$, $A(51,85) = -C_{A13}C_{B13}$, $A(52,85) = -C_{B13}C_{C13}$, $A(55,85) = -C_{A14}C_{B14}$, $A(56,85) = -C_{B14}C_{C14}$, $A(59,85) = -C_{A15}C_{B15}$, $A(60,85) = -C_{B15}C_{C15}$, $A(63,85) = -C_{A16}C_{B16}$, $A(64,85) = -C_{B16}C_{C16}$, $A(67,85) = -C_{A17}C_{B17}$, $A(68,85) = -C_{B17}C_{C17}$, $A(71,85) = -C_{A18}C_{B18}$, $A(72,85) = -C_{B18}C_{C18}$, $A(75,85) = -C_{A19}C_{B19}$, $A(76,85) = -C_{B19}C_{C19}$, $A(79,85) = -C_{A20}C_{B20}$, $A(80,85) = -C_{B20}C_{C20}$, $A(83,85) = -C_{A21}C_{B21}$, $A(84,85) = -C_{B21}C_{C21}$

Program 7.2 for the solution of the above problem is given in the Appendix. The concentration of various species along the length of the reactor is obtained using the Gauss elimination method. The results are shown in Table 7.6.

Table 7.6 Results in Example 7.3

Node number	x (m)	C_A	C_B	C_C	C_D
1	0.0	0.999925	0.999918	0.000060	0.000006
2	0.5	0.745869	0.681292	0.189554	0.064577
3	1.0	0.602852	0.474505	0.268800	0.129276
4	1.5	0.516040	0.336482	0.304402	0.181438
5	2.0	0.460355	0.241939	0.321230	0.221265
6	2.5	0.423163	0.175791	0.329465	0.251137
7	3.0	0.397574	0.128732	0.333583	0.273464
8	3.5	0.379579	0.094823	0.335665	0.290175
9	4.0	0.366717	0.070151	0.336717	0.302718
10	4.5	0.357413	0.052067	0.337242	0.312168
11	5.0	0.350622	0.038739	0.337497	0.319310
12	5.5	0.345632	0.028875	0.337612	0.324724
13	6.0	0.341947	0.021552	0.337659	0.328835
14	6.5	0.339216	0.016103	0.337671	0.331960
15	7.0	0.337186	0.012040	0.337668	0.334332
16	7.5	0.335674	0.009008	0.337659	0.336124
17	8.0	0.334547	0.006742	0.337649	0.337466
18	8.5	0.333705	0.005048	0.337639	0.338454
19	9.0	0.333075	0.003780	0.337630	0.339160
20	9.5	0.332604	0.002831	0.337623	0.339638
21	10.0	0.332252	0.002121	0.337617	0.339996

EXAMPLE 7.4 Solve Example 7.3 by making 3 parts of the reactor of length 3 m.

Solution Since three parts are made, therefore the total number of nodes is 4.
The coefficients of equation 1 (node 1, species A) are:

Coefficient of $C_{A1} = -\dfrac{2\times 10^{-4}}{1^2} - \dfrac{3}{1} - C_{B1} - \dfrac{2}{10^{-4}} = -20003.0002 - C_{B1}$

Coefficient of C_{B1} = 0
Coefficient of C_{C1} = 0
Coefficient of C_{D1} = 0

Coefficient of $C_{A2} = \dfrac{2\times 10^{-4}}{1^2} + \dfrac{1}{1} = 1.0002$

Coefficient of C_{B2} = 0
Coefficient of C_{C2} = 0
Coefficient of C_{D2} = 0

Right hand side of equation 1 = $-\left(\dfrac{2u^2}{D} + \dfrac{2u}{\Delta x}\right)C_{A,\text{in}} = -\dfrac{2}{1} - \dfrac{2}{10^{-4}} = -20002$

The coefficients of equation 2 (node 1, species *B*) are:
Coefficient of C_{A1} = 0

Coefficient of $C_{B1} = -\dfrac{2\times 10^{-4}}{1^2} - \dfrac{3}{1} - C_{A1} - C_{C1} - \dfrac{2}{10^{-4}} = -20003.0002 - C_{A1} - C_{C1}$

Coefficient of C_{C1} = 0
Coefficient of C_{D1} = 0
Coefficient of C_{A2} = 0

Coefficient of $C_{B2} = \dfrac{2\times 10^{-4}}{1^2} + \dfrac{1}{1} = 1.0002$

Coefficient of C_{C2} = 0
Coefficient of C_{D2} = 0

Right hand side of equation 2 = $-\left(\dfrac{2u^2}{D} + \dfrac{2u}{\Delta x}\right)C_{B,\text{in}} = -\dfrac{2}{1} - \dfrac{2}{10^{-4}} = -20002$

The coefficients of equation 3 (node 1, species *C*) are:
Coefficient of C_{A1} = 0
Coefficient of C_{B1} = 0

Coefficient of $C_{C1} = -\dfrac{2\times 10^{-4}}{1^2} - \dfrac{3}{1} - C_{B1} - \dfrac{2}{10^{-4}} = -20003.0002 - C_{B1}$

Coefficient of C_{D1} = 0
Coefficient of C_{A2} = 0
Coefficient of C_{B2} = 0

Coefficient of $C_{C2} = \dfrac{2\times 10^{-4}}{1^2} + \dfrac{1}{1} = 1.0002$

Coefficient of C_{D2} = 0
Right hand side of equation 3 = $-C_{A1}C_{B1}$

The coefficients of equation 4 (node 1, species *D*) are:
Coefficient of C_{A1} = 0
Coefficient of C_{B1} = 0
Coefficient of C_{C1} = 0

Coefficient of $C_{D1} = -\dfrac{2\times 10^{-4}}{1^2} - \dfrac{3}{1} - \dfrac{2}{10^{-4}} = -20003.0002$

Coefficient of C_{A2} = 0
Coefficient of C_{B2} = 0
Coefficient of C_{C2} = 0

Coefficient of $C_{D2} = \dfrac{2\times 10^{-4}}{1^2} + \dfrac{1}{1} = 1.0002$

Right hand side of equation 4 = $-C_{B1}C_{C1}$

The coefficients of equation 5 (node 2, species *A*) are:

Coefficient of $C_{A1} = \dfrac{10^{-4}}{1^2} + \dfrac{1}{1} = 1.0001$

Coefficient of C_{B1} = 0
Coefficient of C_{C1} = 0
Coefficient of C_{D1} = 0

Coefficient of $C_{A2} = -\dfrac{2\times 10^{-4}}{1^2} - \dfrac{1}{1} - C_{B2} = -1.0002 - C_{B2}$

Coefficient of C_{B2} = 0
Coefficient of C_{C2} = 0
Coefficient of C_{D2} = 0

Coefficient of $C_{A3} = \dfrac{10^{-4}}{1^2} = 0.0001$

Coefficient of C_{B3} = 0
Coefficient of C_{C3} = 0
Coefficient of C_{D3} = 0
Right hand side of equation 5 = 0.
The coefficients of equation 6 (node 2, species *B*) are:
Coefficient of C_{A1} = 0

Coefficient of $C_{B1} = \dfrac{10^{-4}}{1^2} + \dfrac{1}{1} = 1.0001$

Coefficient of $C_{C1} = 0$
Coefficient of $C_{D1} = 0$
Coefficient of $C_{A2} = 0$

Coefficient of $C_{B2} = -\dfrac{2 \times 10^{-4}}{1^2} - \dfrac{1}{1} - C_{A2} - C_{C2} = -1.0002 - C_{A2} - C_{C2}$

Coefficient of $C_{C2} = 0$
Coefficient of $C_{D2} = 0$
Coefficient of $C_{A3} = 0$

Coefficient of $C_{B3} = \dfrac{10^{-4}}{1^2} = 0.0001$

Coefficient of $C_{C3} = 0$
Coefficient of $C_{D3} = 0$
Right hand side of equation 6 = 0.

The coefficients of equation 7 (node 2, species *C*) are:
Coefficient of $C_{A1} = 0$
Coefficient of $C_{B1} = 0$

Coefficient of $C_{C1} = \dfrac{10^{-4}}{1^2} + \dfrac{1}{1} = 1.0001$

Coefficient of $C_{D1} = 0$
Coefficient of $C_{A2} = 0$
Coefficient of $C_{B2} = 0$

Coefficient of $C_{C2} = -\dfrac{2 \times 10^{-4}}{1^2} - \dfrac{1}{1} - C_{B2} = -1.0002 - C_{B2}$

Coefficient of $C_{D2} = 0$
Coefficient of $C_{A3} = 0$
Coefficient of $C_{B3} = 0$

Coefficient of $C_{C3} = \dfrac{10^{-4}}{1^2} = 0.0001$

Coefficient of $C_{D3} = 0$
Right hand side of equation 7 = $-C_{A2}C_{B2}$.

The coefficients of equation 8 (node 2, species *D*) are:
Coefficient of $C_{A1} = 0$

Coefficient of C_{B1} = 0
Coefficient of C_{C1} = 0

$$\text{Coefficient of } C_{D1} = \frac{10^{-4}}{1^2} + \frac{1}{1} = 1.0001$$

Coefficient of C_{A2} = 0
Coefficient of C_{B2} = 0
Coefficient of C_{C2} = 0

$$\text{Coefficient of } C_{D2} = -\frac{2\times 10^{-4}}{1^2} - \frac{1}{1} = -1.0002$$

Coefficient of C_{A3} = 0
Coefficient of C_{B3} = 0
Coefficient of C_{C3} = 0

$$\text{Coefficient of } C_{D3} = \frac{10^{-4}}{1^2} = 0.0001$$

Right hand side of equation 8 = $-C_{B2}C_{C2}$

The coefficients of equation 13 (node 4, species *A*) are:

$$\text{Coefficient of } C_{A3} = \frac{2\times 10^{-4}}{1^2} + \frac{1}{1} = 1.0002$$

Coefficient of C_{B3} = 0
Coefficient of C_{C3} = 0
Coefficient of C_{D3} = 0

$$\text{Coefficient of } C_{A4} = -\frac{2\times 10^{-4}}{1^2} - \frac{1}{1} - C_{B4} = -1.0002 - C_{B4}$$

Coefficient of C_{B4} = 0
Coefficient of C_{C4} = 0
Coefficient of C_{D4} = 0
Right hand side of equation 13 = 0.

The coefficients of equation 14 (node 4, species *B*) are:
Coefficient of C_{A3} = 0

$$\text{Coefficient of } C_{B3} = \frac{2\times 10^{-4}}{1^2} + \frac{1}{1} = 1.0002$$

Coefficient of C_{C3} = 0
Coefficient of C_{D3} = 0
Coefficient of C_{A4} = 0

$$\text{Coefficient of } C_{B4} = -\frac{2\times 10^{-4}}{1^2} - \frac{1}{1} - C_{A4} - C_{C4} = -2.0008 - C_{A4} - C_{C4}$$

Coefficient of C_{C4} = 0
Coefficient of C_{D4} = 0
Right hand side of equation 14 = 0

The coefficients of equation 15 (node 4, species *C*) are:
Coefficient of C_{A3} = 0
Coefficient of C_{B3} = 0

Coefficient of $C_{C3} = \dfrac{2\times 10^{-4}}{1^2} + \dfrac{1}{1} = 1.0002$

Coefficient of C_{D3} = 0
Coefficient of C_{A4} = 0
Coefficient of C_{B4} = 0

Coefficient of $C_{C4} = -\dfrac{2\times 10^{-4}}{1^2} - \dfrac{1}{1} - C_{B4} = -1.0002 - C_{B4}$

Coefficient of C_{D4} = 0
Right hand side of equation 15 = $-C_{A4}C_{B4}$.
The coefficients of equation 16 (node 4, species *D*) are:
Coefficient of C_{A3} = 0
Coefficient of C_{B3} = 0
Coefficient of C_{C3} = 0

Coefficient of $C_{D3} = \dfrac{2\times 10^{-4}}{1^2} + \dfrac{1}{1} = 1.0002$

Coefficient of C_{A4} = 0
Coefficient of C_{B4} = 0
Coefficient of C_{C4} = 0

Coefficient of $C_{D4} = -\dfrac{2\times 10^{-4}}{1^2} - \dfrac{1}{1} = -1.0002$

Right hand side of equation 16 = $-C_{B4}C_{C4}$.

Thus the set of equations for concentration of species *A*, *B*, *C*, and *D* at nodes 1 to 4 can be written in the block tridiagonal form as

$$\begin{bmatrix} B_1 & C_1 & 0 & 0 \\ A_2 & B_2 & C_2 & 0 \\ 0 & A_3 & B_3 & C_3 \\ 0 & 0 & A_4 & B_4 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \end{bmatrix}$$

where

$$X_1 = \begin{bmatrix} C_{A1} \\ C_{B1} \\ C_{C1} \\ C_{D1} \end{bmatrix} \qquad X_2 = \begin{bmatrix} C_{A2} \\ C_{B2} \\ C_{C2} \\ C_{D2} \end{bmatrix} \qquad X_4 = \begin{bmatrix} C_{A4} \\ C_{B4} \\ C_{C4} \\ C_{D4} \end{bmatrix}$$

For node 1

$$B_1 = \begin{bmatrix} -20003.0002 - C_{B1} & 0 & 0 & 0 \\ 0 & -20003.0002 - C_{A1} - C_{C1} & 0 & 0 \\ 0 & 0 & -20003.0002 - C_{B1} & 0 \\ 0 & 0 & 0 & -20003.0002 \end{bmatrix}$$

$$C_1 = \begin{bmatrix} 1.0002 & 0 & 0 & 0 \\ 0 & 1.0002 & 0 & 0 \\ 0 & 0 & 1.0002 & 0 \\ 0 & 0 & 0 & 1.0002 \end{bmatrix}$$

$$D_1 = \begin{bmatrix} -20002 \\ -20002 \\ -C_{A1}C_{B1} \\ -C_{B1}C_{C1} \end{bmatrix}$$

For node 2

$$A_2 = \begin{bmatrix} 1.0001 & 0 & 0 & 0 \\ 0 & 1.0001 & 0 & 0 \\ 0 & 0 & 1.0001 & 0 \\ 0 & 0 & 0 & 1.0001 \end{bmatrix}$$

$$B_2 = \begin{bmatrix} -1.0002 - C_{B2} & 0 & 0 & 0 \\ 0 & -1.0002 - C_{A2} - C_{C2} & 0 & 0 \\ 0 & 0 & -1.0002 - C_{B2} & 0 \\ 0 & 0 & 0 & -1.0002 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} 0.0001 & 0 & 0 & 0 \\ 0 & 0.0001 & 0 & 0 \\ 0 & 0 & 0.0001 & 0 \\ 0 & 0 & 0 & 0.0001 \end{bmatrix}$$

$$D_2 = \begin{bmatrix} 0 \\ 0 \\ -C_{A2}C_{B2} \\ -C_{B2}C_{C2} \end{bmatrix}$$

For node 3

$$A_3 = \begin{bmatrix} 1.0001 & 0 & 0 & 0 \\ 0 & 1.0001 & 0 & 0 \\ 0 & 0 & 1.0001 & 0 \\ 0 & 0 & 0 & 1.0001 \end{bmatrix}$$

$$B_3 = \begin{bmatrix} -1.0002 - C_{B3} & 0 & 0 & 0 \\ 0 & -1.0002 - C_{A3} - C_{C3} & 0 & 0 \\ 0 & 0 & -1.0002 - C_{B3} & 0 \\ 0 & 0 & 0 & -1.0002 \end{bmatrix}$$

$$C_3 = \begin{bmatrix} 0.0001 & 0 & 0 & 0 \\ 0 & 0.0001 & 0 & 0 \\ 0 & 0 & 0.0001 & 0 \\ 0 & 0 & 0 & 0.0001 \end{bmatrix}$$

$$D_3 = \begin{bmatrix} 0 \\ 0 \\ -C_{A3}C_{B3} \\ -C_{B3}C_{C3} \end{bmatrix}$$

For node 4

$$A_4 = \begin{bmatrix} 1.0002 & 0 & 0 & 0 \\ 0 & 1.0002 & 0 & 0 \\ 0 & 0 & 1.0002 & 0 \\ 0 & 0 & 0 & 1.0002 \end{bmatrix}$$

$$B_4 = \begin{bmatrix} -1.0002 - C_{B4} & 0 & 0 & 0 \\ 0 & -1.0002 - C_{A4} - C_{C4} & 0 & 0 \\ 0 & 0 & -1.0002 - C_{B4} & 0 \\ 0 & 0 & 0 & -1.0002 \end{bmatrix}$$

$$D_4 = \begin{bmatrix} 0 \\ 0 \\ -C_{A4}C_{B4} \\ -C_{B4}C_{C4} \end{bmatrix}$$

The 16 linear algebraic equations can be written in the form $Ax = d$, where A is a 16×16 matrix, x is the vector of size 16×1 containing the variables to be determined, and d is also a vector of size 16×1. The variables can be written as

$$x = \begin{bmatrix} C_{A1} & C_{B1} & C_{C1} & C_{D1} & \cdots & \cdots & \cdots & \cdots & C_{A4} & C_{B4} & C_{C4} & C_{D4} \end{bmatrix}^T$$

The Gauss elimination method can be used to solve these 16 linear algebraic equations (see Program 1.2 given in the Appendix). The results are given in Table 7.7.

Table 7.7 Results in Example 7.4

Node number	x (m)	C_A	C_B	C_C	C_D
1	0	0.999933	0.999927	0.000060	0.000006
2	1	0.652683	0.532064	0.226697	0.120620
3	2	0.503350	0.296694	0.289994	0.206656
4	3	0.430048	0.170485	0.310390	0.259562

Exercises

7.1 Consider a reaction $A \rightarrow B$ carried out in a tubular reactor. The differential equation for species A along the length of the tubular reactor of length 10 m is

$$D\frac{d^2C_A}{dx^2} - u\frac{dC_A}{dx} - kC_A = 0$$

The boundary conditions are
At $x = 0$ (inlet)

$$uC_{A,\text{in}} = uC_A - D\frac{dC_A}{dx}$$

At $x = 10$ m (exit)

$$\frac{dC_A}{dx} = 0$$

A fluid medium comprising initially only A flows through the reactor with a mean axial velocity $u = 1$ m/s. The axial dispersion coefficient, $D = 10^{-4}$ m^2/s and the rate constant of the reaction is 0.1 s^{-1}. The inlet concentration $C_{A,\text{in}} = 1$ mol/m^3. Make 10 parts of the reactor. List the tridiagonal set of equations and determine the concentration of A at various positions along the length of the tubular reactor.
(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -20003.1002 & 1.0002 & & & \\ 1.0001 & -1.1002 & 0.0001 & & \\ & \cdots & \cdots & \cdots & \\ & & 1.0001 & -1.1002 & 0.0001 \\ & & & 1.0002 & -1.1002 \end{bmatrix} \begin{bmatrix} C_{A1} \\ C_{A2} \\ \cdots \\ C_{A10} \\ C_{A11} \end{bmatrix} = \begin{bmatrix} -20002 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

$C_{A1} = C_A(0.0) = 0.999991$ $\quad C_{A2} = C_A(1.0) = 0.909083$
$C_{A3} = C_A(2.0) = 0.826440$ $\quad C_{A4} = C_A(3.0) = 0.751310$
$C_{A5} = C_A(4.0) = 0.683009$ $\quad C_{A6} = C_A(5.0) = 0.620918$
$C_{A7} = C_A(6.0) = 0.564471$ $\quad C_{A8} = C_A(7.0) = 0.513156$
$C_{A9} = C_A(8.0) = 0.466506$ $\quad C_{A10} = C_A(9.0) = 0.424097$
$C_{A11} = C_A(10.0) = 0.385549$

7.2 Consider a reaction $A \rightarrow B$ carried out in a tubular reactor. The differential equation for species A along the length of the tubular reactor of length 10 m is

$$D\frac{d^2C_A}{dx^2} - u\frac{dC_A}{dx} - kC_A^2 = 0$$

The boundary conditions are

$$\text{At } x = 0 \text{ (inlet): } uC_{A,in} = uC_A - D\frac{dC_A}{dx}$$

$$\text{At } x = 10 \text{ m (exit): } \frac{dC_A}{dx} = 0$$

A fluid medium comprising initially only A flows through the reactor with a mean axial velocity u = 1 m/s. The axial dispersion coefficient, $D = 10^{-4}$ m^2/s and rate constant of the reaction is 0.1 m^3/mol-s. The inlet concentration $C_{A,\text{in}}$ = 1 mol/m^3. Make 10 parts of the reactor. List the tridiagonal set of equations and determine the concentration of A at various positions along the length of the tubular reactor.
(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -20003.0002 - 0.1C_{A1} & 1.0002 & & & \\ 1.0001 & -1.0002 - 0.1C_{A2} & 0.0001 & & \\ & \cdots & \cdots & \cdots & \\ & & 1.0001 & -1.0002 - 0.1C_{A10} & 0.0001 \\ & & & 1.0002 & -1.0002 - 0.1C_{A11} \end{bmatrix} \begin{bmatrix} C_{A1} \\ C_{A2} \\ \cdots \\ C_{A10} \\ C_{A11} \end{bmatrix} = \begin{bmatrix} -20002 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}$$

$C_{A1} = C_A(0.0) = 0.999991$ $\quad C_{A2} = C_A(1.0) = 0.916073$
$C_{A3} = C_A(2.0) = 0.844719$ $\quad C_{A4} = C_A(3.0) = 0.783356$
$C_{A5} = C_A(4.0) = 0.730059$ $\quad C_{A6} = C_A(5.0) = 0.683363$
$C_{A7} = C_A(6.0) = 0.642133$ $\quad C_{A8} = C_A(7.0) = 0.605478$
$C_{A9} = C_A(8.0) = 0.572688$ $\quad C_{A10} = C_A(9.0) = 0.543192$
$C_{A11} = C_A(10.0) = 0.516529$

Chapter 8

Chemical Reaction and Diffusion in Spherical Catalyst Pellet

Chemical reaction and diffusion in a spherical catalyst pellet is a boundary value problem, because at the surface of the pellet the concentration of the species is known and at the centre of the pellet the gradient of concentration is zero. The finite difference method is used for the numerical solution of the first and second order reactions along with the diffusion term in a spherical catalyst pellet. The numerical solution under nonisothermal conditions is also discussed in this chapter.

8.1 First Order Reaction

The differential equation for diffusion and reaction in a spherical catalyst pellet is given by

$$D\left(\frac{d^2C}{dr^2}+\frac{2}{r}\frac{dC}{dr}\right)-kC=0 \tag{8.1}$$

It is assumed that the pellet is isothermal and therefore the rate constant is also fixed. D is the effective binary diffusivity of A within the catalyst pellet. The boundary conditions are
at $r = R$

$$C = C_S \tag{8.1b}$$

and at $r = 0$

$$\frac{dC}{dr}=0 \tag{8.1b}$$

where C_S is the concentration at the surface of the spherical catalyst pellet.

EXAMPLE 8.1 The chemical reaction and diffusion in a spherical catalyst pellet is given by

$$D\frac{d^2C_A}{dr^2}+\frac{2}{r}D\frac{dC_A}{dr}-kC_A=0$$

where D is the effective binary diffusivity of A within the catalyst pellet. The pellet is isothermal. The concentration at the surface of the spherical catalyst pellet is 1 mol/m^3, thus the boundary conditions are at $r = R$

$$C_A = 1$$

at $r = 0$

$$\frac{dC_A}{dr} = 0$$

The radius of the catalyst pellet is 1.0 cm. Make 100 parts of the radius. Take the rate constant, $k = 10^{-3}$ s^{-1} and $D = 10^{-9}$ m^2/s. Determine the concentration of species A at various nodes along the radius of the catalyst pellet.

Solution The differential equation for diffusion and reaction in a spherical catalyst pellet is

$$\frac{d^2C}{dr^2} + \frac{2}{r}\frac{dC}{dr} - \frac{k}{D}C = 0$$

It is given that $\frac{k}{D} = \frac{10^{-3}}{10^{-9}} = 10^6 \text{ m}^{-2}$.

The radius is 1 cm = 10^{-2} m and 100 parts are made, thus $\Delta r = \frac{10^{-2}}{100} = 10^{-4}$ m. The schematic diagram of the spherical catalyst pellet is shown in Fig. 8.1. The first node is labelled 0 and therefore the last node is the 100th node as 100 parts are made.

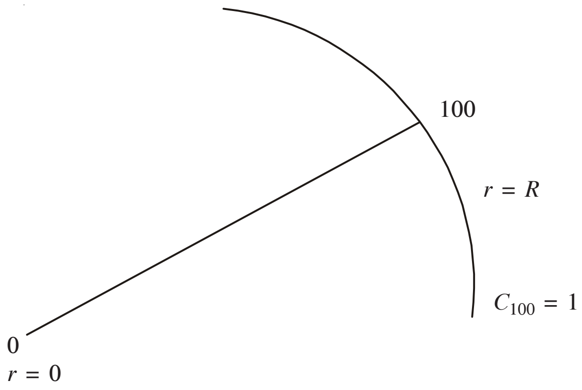


Fig. 8.1 Diffusion and reaction in spherical catalyst pellet.

The boundary conditions are:

at $r = 1$ cm

$$C = 1$$

$r = 0$

$$\frac{dC}{dr} = 0$$

Discretizing the differential equation at node *i*, we get

$$\frac{C_{i+1}+C_{i-1}-2C_i}{\Delta r^2}+\frac{2}{m\Delta r}\left(\frac{C_{i+1}-C_{i-1}}{2\Delta r}\right)-10^6 C_i=0$$

$$C_{i+1}+C_{i-1}-2C_i+\frac{1}{m}\left(C_{i+1}-C_{i-1}\right)-10^6\,\Delta r^2 C_i=0$$

$$C_{i+1}+C_{i-1}-2C_i+\frac{1}{m}\left(C_{i+1}-C_{i-1}\right)-0.01C_i=0$$

$$C_{i-1}\left(1-\frac{1}{m}\right)-2.01C_i+C_{i+1}\left(1+\frac{1}{m}\right)=0$$

At node 0 (centre of spherical catalyst pellet) the differential equation becomes

$$3\frac{d^2C}{dr^2}-10^6 C=0$$

Discretizing, we get

$$3\left(\frac{C_1+C_{-1}-2C_0}{\Delta r^2}\right)-10^6 C_0=0$$

$$3\left(C_1+C_{-1}-2C_0\right)-10^6\,\Delta r^2 C_0=0$$

$$3\left(C_1+C_{-1}-2C_0\right)-0.01C_0=0$$

At node 0, $\frac{dC}{dr}=0$; thus $\frac{C_1-C_{-1}}{2\Delta r}=0$, and therefore $C_{-1}=C_1$. Therefore the above equation becomes

$$3\left(2C_1-2C_0\right)-0.01C_0=0$$

$$-6.01C_0+6C_1=0$$

At node 1 (m = 1)

$$C_{i-1}\left(1-\frac{1}{m}\right)-2.01C_i+C_{i+1}\left(1+\frac{1}{m}\right)=0$$

$$-2.01C_1+C_2\left(1+\frac{1}{1}\right)=0$$

At node 2 (m = 2)

$$C_1\left(1-\frac{1}{2}\right)-2.01C_2+C_3\left(1+\frac{1}{2}\right)=0$$

At node 3 (m = 3)

$$C_2\left(1-\frac{1}{3}\right)-2.01C_3+C_4\left(1+\frac{1}{3}\right)=0$$

At node 99 (m = 99)

$$C_{98}\left(1-\frac{1}{99}\right)-2.01C_{99}+C_{100}\left(1+\frac{1}{99}\right)=0$$

Since C_{100} = 1, we get

$$C_{98}\left(1-\frac{1}{99}\right)-2.01C_{99}=-\left(1+\frac{1}{99}\right)$$

$$C_{98}\left(1-\frac{1}{99}\right)-2.01C_{99}=-\frac{100}{99}$$

The 100 equations can be written in tridiagonal form as

$$\begin{bmatrix} -6.01 & 6 & & & & & & & & \\ 1-\frac{1}{1} & -2.01 & 1+\frac{1}{1} & & & & & & & \\ & 1-\frac{1}{2} & -2.01 & 1+\frac{1}{2} & & & & & & \\ & & 1-\frac{1}{3} & -2.01 & 1+\frac{1}{3} & & & & & \\ & & & \cdots & \cdots & \cdots & & & & \\ & & & & \cdots & \cdots & \cdots & & & \\ & & & & & 1-\frac{1}{97} & -2.01 & 1+\frac{1}{97} & & \\ & & & & & & 1-\frac{1}{98} & -2.01 & 1+\frac{1}{98} & \\ & & & & & & & 1-\frac{1}{99} & -2.01 & \end{bmatrix}\begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ \cdots \\ \cdots \\ C_{97} \\ C_{98} \\ C_{99} \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \\ 0 \\ \cdots \\ \cdots \\ \cdots \\ 0 \\ 0 \\ -\frac{100}{99} \end{bmatrix}$$

The solution can be obtained by modifying the parameters a_i (i = 2 to N), b_i (i = 1 to N) and c_i (i = 1 to N – 1) in Program 1.1 given in the Appendix. The results for nodes 77 to 99 are presented in Table 8.1 given in the next section.

8.2 Second Order Reaction

The differential equation for diffusion and second order reaction in a spherical catalyst pellet is given by

$$D\left(\frac{d^2C}{dr^2}+\frac{2}{r}\frac{dC}{dr}\right)-kC^2=0 \tag{8.2}$$

It is assumed that the pellet is isothermal and therefore the rate constant is also fixed. D is the effective binary diffusivity of A within the catalyst pellet. The boundary conditions are

At $r = R$: $C = C_S$

At $r = 0$: $\frac{dC}{dr}=0$

where C_S is the concentration at the surface of the spherical catalyst pellet.

EXAMPLE 8.2 The chemical reaction and diffusion in a spherical catalyst pellet is given by

$$D\frac{d^2C_A}{dr^2}+\frac{2}{r}D\frac{dC_A}{dr}-kC_A^2=0$$

where D is the effective binary diffusivity of A within the catalyst pellet. The pellet is isothermal. The concentration at the surface of the spherical catalyst pellet is 1 mol/m^3; thus the boundary conditions are

$$\text{At } r = R: \qquad C_A = 1$$

$$\text{At } r = 0: \qquad \frac{dC_A}{dr}=0$$

The radius of the catalyst pellet is 1.0 cm. Make 100 parts of the radius. Take the rate constant, $k = 10^{-3}$ m^3/mol-s and $D = 10^{-9}$ m^2/s. Determine the concentration of species A at various nodes along the radius of the catalyst pellet.

Solution The differential equation for diffusion and reaction in a spherical catalyst pellet is

$$\frac{d^2C}{dr^2}+\frac{2}{r}\frac{dC}{dr}-\frac{k}{D}C^2=0$$

It is given that $\frac{k}{D}=\frac{10^{-3}}{10^{-9}}=10^6$.

The radius is 1 cm = 10^{-2} m and 100 parts are made, thus $\Delta r=\frac{10^{-2}}{100}=10^{-4}$ m. The schematic diagram of the spherical catalyst pellet is given in Fig. 8.1. The first node is labelled 0 and therefore the last node is the 100th node as 100 parts are made. Discretizing the differential equation at node *i,* we get

$$\frac{C_{i+1}+C_{i-1}-2C_i}{\Delta r^2}+\frac{2}{m\Delta r}\left(\frac{C_{i+1}-C_{i-1}}{2\Delta r}\right)-10^6C_i^2=0$$

$$C_{i+1}+C_{i-1}-2C_i+\frac{1}{m}\left(C_{i+1}-C_{i-1}\right)-10^6\Delta r^2C_i^2=0$$

$$C_{i+1}+C_{i-1}-2C_i+\frac{1}{m}\left(C_{i+1}-C_{i-1}\right)-0.01C_i^2=0$$

$$C_{i-1}\left(1-\frac{1}{m}\right)+C_i\left(-2-0.01C_i\right)+C_{i+1}\left(1+\frac{1}{m}\right)=0$$

At node 0 (centre of spherical catalyst pellet) the differential equation becomes

$$3\frac{d^2C}{dr^2}-10^6C^2=0$$

Discretizing, we get

$$3\left(\frac{C_1 + C_{-1} - 2C_0}{\Delta r^2}\right) - 10^6 C_0^2 = 0$$

$$3\left(C_1 + C_{-1} - 2C_0\right) - 10^6 \Delta r^2 C_0^2 = 0$$

$$3\left(C_1 + C_{-1} - 2C_0\right) - 0.01C_0^2 = 0$$

At node 0, $\frac{dC}{dr} = 0$; thus $\frac{C_1 - C_{-1}}{2\Delta r} = 0$, and therefore $C_{-1} = C_1$. Therefore the above equation becomes

$$3\left(2C_1 - 2C_0\right) - 0.01C_0^2 = 0$$

$$C_0\left(-6 - 0.01C_0\right) + 6C_1 = 0$$

At node 1 ($m = 1$)

$$C_{i-1}\left(1 - \frac{1}{m}\right) + \left(-2 - 0.01C_i\right)C_i + C_{i+1}\left(1 + \frac{1}{m}\right) = 0$$

$$\left(-2 - 0.01C_1\right)C_1 + C_2\left(1 + \frac{1}{1}\right) = 0$$

At node 2 ($m = 2$)

$$C_1\left(1 - \frac{1}{2}\right) + \left(-2 - 0.01C_2\right)C_2 + C_3\left(1 + \frac{1}{2}\right) = 0$$

At node 3 ($m = 3$)

$$C_2\left(1 - \frac{1}{3}\right) + \left(-2 - 0.01C_3\right)C_3 + C_4\left(1 + \frac{1}{3}\right) = 0$$

At node 99 ($m = 99$)

$$C_{98}\left(1 - \frac{1}{99}\right) + \left(-2 - 0.01C_{99}\right)C_{99} + C_{100}\left(1 + \frac{1}{99}\right) = 0$$

Since $C_{100} = 1$, we get

$$C_{98}\left(1 - \frac{1}{99}\right) + \left(-2 - 0.01C_{99}\right)C_{99} = -\left(1 + \frac{1}{99}\right)$$

$$C_{98}\left(1 - \frac{1}{99}\right) + \left(-2 - 0.01C_{99}\right)C_{99} = -\frac{100}{99}$$

The 100 equations can be written in tridiagonal form as

$$\begin{bmatrix} -6-0.01C_0 & 6 & & & \\ 1-\frac{1}{1} & -2-0.01C_1 & 1+\frac{1}{1} & & \\ & & \cdots & & \\ & & 1-\frac{1}{98} & -2-0.01C_{98} & 1+\frac{1}{98} \\ & & & 1-\frac{1}{99} & -2-0.01C_{99} \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ \cdots \\ C_{98} \\ C_{99} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -\frac{100}{99} \end{bmatrix}$$

It is seen that the coefficient matrix also depends on the concentrations. Therefore, to start the program the concentrations are assumed, the coefficients are calculated and TDMA is used to determine the new concentrations. At these concentrations the coefficients are re-calculated and TDMA is used to determine the new concentrations. The procedure is repeated till there is no change in the concentration profile. Program 8.1 for the solution of the above problem is given in the Appendix. The results for nodes 77 to 99 are presented in Table 8.1.

Table 8.1 Concentration of reactants in spherical catalyst pellet for first and second order reactions under isothermal condition

Node number	r (cm)	C (first order reaction)	C (second order reaction)
99	0.99	0.914015	0.930360
98	0.98	0.835509	0.868043
97	0.97	0.763826	0.812053
96	0.96	0.698366	0.761560
95	0.95	0.638586	0.715865
94	0.94	0.583988	0.674377
93	0.93	0.534119	0.636593
92	0.92	0.488564	0.602084
91	0.91	0.446948	0.570482
90	0.90	0.408925	0.541468
89	0.89	0.374184	0.514766
88	0.88	0.342438	0.490138
87	0.87	0.313425	0.467374
86	0.86	0.286908	0.446290
85	0.85	0.262670	0.426724
84	0.84	0.240513	0.408536
83	0.83	0.220257	0.391599
82	0.82	0.201735	0.375800
81	0.81	0.184799	0.361041
80	0.80	0.169310	0.347233
79	0.79	0.155144	0.334296
78	0.78	0.142186	0.322160
77	0.77	0.130331	0.310759

8.3 Nonisothermal Conditions

The differential equation for diffusion and reaction in a spherical catalyst pellet is given by

$$D\left(\frac{d^2C}{dr^2}+\frac{2}{r}\frac{dC}{dr}\right)-k(T)C=0 \tag{8.3}$$

where the rate constant is a function of the temperature, or

$$k(T)=k(T_S)\exp\left[-\frac{E}{RT_S}\left(\frac{T_S}{T}-1\right)\right] \tag{8.4}$$

Consider the case of a non-isothermal first order reaction $A \rightarrow B$ occurring in the interior of a spherical catalyst pellet. We wish to compute the effect of internal heat and mass transfer resistance upon the reaction rate and the concentration and temperature profiles within the pellet. The concentration profile $C_A(r)$ is governed by the mole balance

$$\frac{d}{dr}\left(r^2 D_A \frac{dC_A}{dr}\right) - r^2 k(T) C_A = 0 \tag{8.5}$$

where D_A is the effective binary diffusivity of A within the pellet. If k is the effective thermal conductivity of the pellet, the temperature profile $T(r)$ is governed by the energy balance

$$\frac{d}{dr}\left(r^2 k \frac{dT}{dr}\right) + r^2\left(-\Delta H^0_{\text{rxn}}\right)\left[k(T) C_A\right] = 0 \tag{8.6}$$

Neglecting external heat and mass transfer resistance, we have known values of the concentration and temperature at the surface, $r = R$: $C_A(R) = C_{AS}$ and $T(R) = T_S$. Also, at the centre of the pellet, $r = 0$: $\left.\frac{dC_A}{dr}\right|_{r=0} = 0$ and $\left.\frac{dT}{dr}\right|_{r=0} = 0$. The temperature dependence of the rate constant is

$$k(T) = k(T_S)\exp\left[-\frac{E}{RT_S}\left(\frac{T_S}{T} - 1\right)\right] \tag{8.7}$$

If we assume constant D_A, k and ΔH^0_{rxn} the problem reduces to a single ordinary differential equation. Dividing the energy balance equation by $-\Delta H^0_{\text{rxn}}$ and adding to the mole balance equation, we get

$$\frac{d}{dr}\left(r^2 D_A \frac{dC_A}{dr}\right) + \frac{d}{dr}\left(r^2 \frac{k}{\left(-\Delta H^0_{\text{rxn}}\right)} \frac{dT}{dr}\right) = 0 \tag{8.8}$$

Integrating, we get

$$r^2\left[D_A \frac{dC_A}{dr} + \frac{k}{\left(-\Delta H^0_{\text{rxn}}\right)} \frac{dT}{dr}\right] = C_1 \tag{8.9}$$

where C_1 is the constant of integration. Dividing by r^2 gives

$$\frac{d}{dr}\left[D_A C_A + \frac{k}{\left(-\Delta H^0_{\text{rxn}}\right)} T\right] = \frac{C_1}{r^2} \tag{8.10}$$

From the symmetry boundary condition $C_1 = 0$ and a second integration

$$D_A C_A + \frac{k}{\left(-\Delta H^0_{\text{rxn}}\right)} T = C_2 \tag{8.11}$$

where C_2 is the constant of integration. At the surface, we get the value of constant C_2 as

$$C_2 = D_A C_{AS} + \frac{k}{\left(-\Delta H^0_{\text{rxn}}\right)} T_S \tag{8.12}$$

Comparing Eqs. (8.11) and (8.12), we get

$$D_A C_A + \frac{k}{\left(-\Delta H_{\text{rxn}}^0\right)} T = D_A C_{AS} + \frac{k}{\left(-\Delta H_{\text{rxn}}^0\right)} T_S \tag{8.13}$$

Thus there exists the following linear relation between $C_A(r)$ and $T(r)$:

$$T(r) - T_S = \frac{D_A \Delta H_{\text{rxn}}^0}{k}\left[C_A(r) - C_{AS}\right] \tag{8.14}$$

Thus only the mole balance equation has to be solved. Thus, if we assume constant D_A, k and ΔH_{rxn}^0, we can show that at any point along the radius the temperature and concentration of the reactant are related by Eq. (8.14). A parameter is defined as

$$\beta = \frac{D\left(-\Delta H_{\text{rxn}}^0\right) C_S}{k T_S} \tag{8.15}$$

From Eq. (8.14), we get

$$\frac{T}{T_S} = 1 + \frac{D \Delta H_{\text{rxn}}^0}{k T_S}(C - C_S)$$

Therefore

$$\frac{T_S}{T} = \frac{1}{1 + \frac{D \Delta H_{\text{rxn}}^0}{k T_S}(C - C_S)}$$

Subtracting one from both the sides, we get

$$\frac{T_S}{T} - 1 = \frac{-\frac{D \Delta H_{\text{rxn}}^0}{k T_S}(C - C_S)}{1 + \frac{D \Delta H_{\text{rxn}}^0}{k T_S}(C - C_S)} \tag{8.16}$$

Let us define a parameter as

$$\gamma = \frac{E}{R T_S} \tag{8.17}$$

If C_S = 1, then $\beta = \frac{D\left(-\Delta H_{\text{rxn}}^0\right)}{k T_S}$ and the expression for rate constant given in Eq. (8.7) becomes

$$k(T) = k(T_S)\exp\left[-\frac{\gamma\beta(C - C_S)}{1 - \beta(C - C_S)}\right] \tag{8.18}$$

EXAMPLE 8.3 Diffusion and reaction take place in a non-isothermal spherical catalyst pellet of radius 1 cm. The rate constant of the reaction $k(T_S) = 10^{-3}\ \text{s}^{-1}$ and effective diffusivity of species, $D = 10^{-9}\ \text{m}^2/\text{s}$. Make 100 parts of the radius and determine the concentration within the catalyst pellet. The concentration at the surface of the spherical catalyst pellet $C_S = 1$ mol/m^3. Take $\beta = 1$ and $\gamma = 1$.

Solution The differential equation for diffusion and reaction in a non-isothermal spherical catalyst pellet is

$$\frac{d^2C}{dr^2} + \frac{2}{r}\frac{dC}{dr} - \frac{k}{D}C = 0$$

where

$$k(T) = k(T_S)\exp\left[-\frac{\gamma\beta(C - C_S)}{1 - \beta(C - C_S)}\right]$$

Thus the differential equation becomes

$$\frac{d^2C}{dr^2} + \frac{2}{r}\frac{dC}{dr} - \frac{k(T_S)}{D}\left[\exp\left(-\frac{\gamma\beta(C - C_S)}{1 - \beta(C - C_S)}\right)\right]C = 0$$

It is given that $\dfrac{k(T_S)}{D} = \dfrac{10^{-3}}{10^{-9}} = 10^6\ \text{m}^{-2}$.

The radius is 1 cm = 10^{-2} m and 100 parts are made; thus $\Delta r = \dfrac{10^{-2}}{100} = 10^{-4}$ m. The schematic diagram of the spherical catalyst pellet is given in Fig. 8.1. The boundary conditions are

$$\text{At } r = 1 \text{ cm:} \qquad C = 1$$

$$\text{At } r = 0: \qquad \frac{dC}{dr} = 0$$

Since $\beta = 1$, $\gamma = 1$, and $C_S = 1$ mol/m^3, the differential equation becomes

$$\frac{d^2C}{dr^2} + \frac{2}{r}\frac{dC}{dr} - 10^6\left[\exp\left(\frac{1 - C}{2 - C}\right)\right]C = 0$$

Discretizing the differential equation at node i, we get

$$\frac{C_{i+1} + C_{i-1} - 2C_i}{\Delta r^2} + \frac{2}{m\Delta r}\left(\frac{C_{i+1} - C_{i-1}}{2\Delta r}\right) - 10^6\left[\exp\left(\frac{1 - C_i}{2 - C_i}\right)\right]C_i = 0$$

$$C_{i+1} + C_{i-1} - 2C_i + \frac{1}{m}(C_{i+1} - C_{i-1}) - 0.01\left[\exp\left(\frac{1 - C_i}{2 - C_i}\right)\right]C_i = 0$$

$$C_{i-1}\left(1-\frac{1}{m}\right)+C_i\left[-2-0.01\exp\left(\frac{1-C_i}{2-C_i}\right)\right]+C_{i+1}\left(1+\frac{1}{m}\right)=0$$

At node 0 (centre of spherical catalyst pellet), the differential equation becomes

$$3\frac{d^2C}{dr^2}-10^6\left[\exp\left(\frac{1-C}{2-C}\right)\right]C=0$$

Discretizing, we get

$$3\left(\frac{C_1+C_{-1}-2C_0}{\Delta r^2}\right)-10^6\left[\exp\left(\frac{1-C_0}{2-C_0}\right)\right]C_0=0$$

$$3\left(C_1+C_{-1}-2C_0\right)-0.01\left[\exp\left(\frac{1-C_0}{2-C_0}\right)\right]C_0=0$$

At node 0, $\frac{dC}{dr}=0$; thus $\frac{C_1-C_{-1}}{2\Delta r}=0$, and therefore $C_{-1} = C_1$. Therefore the above equation becomes

$$3\left(2C_1-2C_0\right)-0.01\left[\exp\left(\frac{1-C_0}{2-C_0}\right)\right]C_0=0$$

$$\left[-6-0.01\exp\left(\frac{1-C_0}{2-C_0}\right)\right]C_0+6C_1=0$$

At node 1 ($m = 1$)

$$C_{i-1}\left(1-\frac{1}{m}\right)+\left[-2-0.01\exp\left(\frac{1-C_i}{2-C_i}\right)\right]C_i+C_{i+1}\left(1+\frac{1}{m}\right)=0$$

$$\left[-2-0.01\exp\left(\frac{1-C_1}{2-C_1}\right)\right]C_1+C_2\left(1+\frac{1}{1}\right)=0$$

At node 2 ($m = 2$)

$$C_1\left(1-\frac{1}{2}\right)+\left[-2-0.01\exp\left(\frac{1-C_2}{2-C_2}\right)\right]C_2+C_3\left(1+\frac{1}{2}\right)=0$$

At node 3 ($m = 3$)

$$C_2\left(1-\frac{1}{3}\right)+\left[-2-0.01\exp\left(\frac{1-C_3}{2-C_3}\right)\right]C_3+C_4\left(1+\frac{1}{3}\right)=0$$

At node 99 ($m = 99$)

$$C_{98}\left(1-\frac{1}{99}\right)+\left[-2-0.01\exp\left(\frac{1-C_{99}}{2-C_{99}}\right)\right]C_{99}+C_{100}\left(1+\frac{1}{99}\right)=0$$

Since $C_{100} = 1$, we get

$$C_{98}\left(1-\frac{1}{99}\right)+\left[-2-0.01\exp\left(\frac{1-C_{99}}{2-C_{99}}\right)\right]C_{99}=-\frac{100}{99}$$

The 100 equations can be written in tridiagonal form as

$$\begin{bmatrix} -6-0.01\exp\left(\frac{1-C_0}{2-C_0}\right) & 6 & & & & \\ 1-\frac{1}{1} & -2-0.01\exp\left(\frac{1-C_1}{2-C_1}\right) & 1+\frac{1}{1} & & & \\ & & \cdots & & & \\ & & & 1-\frac{1}{98} & -2-0.01\exp\left(\frac{1-C_{98}}{2-C_{98}}\right) & 1+\frac{1}{98} \\ & & & & 1-\frac{1}{99} & -2-0.01\exp\left(\frac{1-C_{99}}{2-C_{99}}\right) \end{bmatrix}\begin{bmatrix} C_0 \\ C_1 \\ \cdots \\ C_{98} \\ C_{99} \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -\frac{100}{99} \end{bmatrix}$$

It is seen that the coefficient matrix also depends on the concentrations. Therefore, to start the program the concentrations are assumed, the coefficients are calculated and TDMA is used to determine the new concentrations. At these concentrations the coefficients are re-calculated and TDMA is used to determine the new concentrations. The procedure is repeated till there is no change in the concentration profile. Program 8.2 for the solution of the above problem is given in the Appendix. The results for nodes 77 to 100 are presented in Table 8.2.

EXAMPLE 8.4 Solve Example 8.3 for $\beta = 10$ and $\gamma = 1$.

Solution Since $\beta = 10$, $\gamma = 1$, and $C_S = 1$ mol/m^3, the differential equation becomes

$$\frac{d^2C}{dr^2}+\frac{2}{r}\frac{dC}{dr}-10^6\left[\exp\left(\frac{10-10C}{11-10C}\right)\right]C=0$$

Discretizing the differential equation at node *i,* we get

$$\frac{C_{i+1}+C_{i-1}-2C_i}{\Delta r^2}+\frac{2}{m\Delta r}\left(\frac{C_{i+1}-C_{i-1}}{2\Delta r}\right)-10^6\left[\exp\left(\frac{10-10C_i}{11-10C_i}\right)\right]C_i=0$$

$$C_{i+1}+C_{i-1}-2C_i+\frac{1}{m}(C_{i+1}-C_{i-1})-0.01\left[\exp\left(\frac{10-10C_i}{11-10C_i}\right)\right]C_i=0$$

$$C_{i-1}\left(1-\frac{1}{m}\right)+C_i\left[-2-0.01\exp\left(\frac{10-10C_i}{11-10C_i}\right)\right]+C_{i+1}\left(1+\frac{1}{m}\right)=0$$

At node 0 (centre of spherical catalyst pellet), the differential equation becomes

$$3\frac{d^2C}{dr^2}-10^6\left[\exp\left(\frac{10-10C}{11-10C}\right)\right]C=0$$

Discretizing, we get

$$3\left(\frac{C_1 + C_{-1} - 2C_0}{\Delta r^2}\right) - 10^6\left[\exp\left(\frac{10 - 10C_0}{11 - 10C_0}\right)\right]C_0 = 0$$

$$3\left(C_1 + C_{-1} - 2C_0\right) - 0.01\left[\exp\left(\frac{10 - 10C_0}{11 - 10C_0}\right)\right]C_0 = 0$$

At node 0, $\frac{dC}{dr} = 0$; thus $\frac{C_1 - C_{-1}}{2\Delta r} = 0$, and therefore $C_{-1} = C_1$. Therefore the above equation becomes

$$3\left(2C_1 - 2C_0\right) - 0.01\left[\exp\left(\frac{10 - 10C_0}{11 - 10C_0}\right)\right]C_0 = 0$$

$$\left[-6 - 0.01\exp\left(\frac{10 - 10C_0}{11 - 10C_0}\right)\right]C_0 + 6C_1 = 0$$

At node 1 ($m = 1$)

$$C_{i-1}\left(1 - \frac{1}{m}\right) + \left[-2 - 0.01\exp\left(\frac{10 - 10C_i}{11 - 10C_i}\right)\right]C_i + C_{i+1}\left(1 + \frac{1}{m}\right) = 0$$

$$\left[-2 - 0.01\exp\left(\frac{10 - 10C_1}{11 - 10C_1}\right)\right]C_1 + C_2\left(1 + \frac{1}{1}\right) = 0$$

At node 2 ($m = 2$)

$$C_1\left(1 - \frac{1}{2}\right) + \left[-2 - 0.01\exp\left(\frac{10 - 10C_2}{11 - 10C_2}\right)\right]C_2 + C_3\left(1 + \frac{1}{2}\right) = 0$$

At node 3 ($m = 3$)

$$C_2\left(1 - \frac{1}{3}\right) + \left[-2 - 0.01\exp\left(\frac{10 - 10C_3}{11 - 10C_3}\right)\right]C_3 + C_4\left(1 + \frac{1}{3}\right) = 0$$

At node 99 ($m = 99$)

$$C_{98}\left(1 - \frac{1}{99}\right) + \left[-2 - 0.01\exp\left(\frac{10 - 10C_{99}}{11 - 10C_{99}}\right)\right]C_{99} + C_{100}\left(1 + \frac{1}{99}\right) = 0$$

Since $C_{100} = 1$, we get

$$C_{98}\left(1 - \frac{1}{99}\right) + \left[-2 - 0.01\exp\left(\frac{10 - 10C_{99}}{11 - 10C_{99}}\right)\right]C_{99} = -\frac{100}{99}$$

The 100 equations can be written in tridiagonal form as

$$\begin{bmatrix} -6-0.01\exp\left(\dfrac{10-10C_0}{11-10C_0}\right) & 6 & & & \\ 1-\dfrac{1}{1} & -2-0.01\exp\left(\dfrac{10-10C_1}{11-10C_1}\right) & 1+\dfrac{1}{1} & & \\ & & \cdots & & \\ & & 1-\dfrac{1}{98} & -2-0.01\exp\left(\dfrac{10-10C_{98}}{11-10C_{98}}\right) & 1+\dfrac{1}{98} \\ & & & 1-\dfrac{1}{99} & -2-0.01\exp\left(\dfrac{10-10C_{99}}{11-10C_{99}}\right) \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ \cdots \\ C_{98} \\ C_{99} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -\dfrac{100}{99} \end{bmatrix}$$

It is seen that the coefficient matrix also depends on the concentrations. Therefore, to start the program the concentrations are assumed, the coefficients are calculated and TDMA is used to determine the new concentrations. At these concentrations the coefficients are re-calculated and TDMA is used to determine the new concentrations. The procedure is repeated till there is no change in the concentration profile. Program 8.2 can be modified to solve this problem. The results for nodes 77 to 100 are presented in Table 8.2.

Table 8.2 Concentration of reactant in spherical catalyst pellet under non-isothermal conditions for first order reaction for $\beta = 1$ and $\beta = 10$

Node number	r (cm)	C ($\beta = 1$)	C ($\beta = 10$)
100	1.00	1.000000	1.000000
99	0.99	0.901657	0.873620
98	0.98	0.803074	0.752422
97	0.97	0.713959	0.646573
96	0.96	0.633761	0.554827
95	0.95	0.561849	0.475639
94	0.94	0.497557	0.407470
93	0.93	0.440217	0.348888
92	0.92	0.389179	0.298610
91	0.91	0.343828	0.255496
90	0.90	0.303586	0.218553
89	0.89	0.267922	0.186914
88	0.88	0.236345	0.159829
87	0.87	0.208414	0.136650
86	0.86	0.183724	0.116820
85	0.85	0.161913	0.099585
84	0.84	0.142658	0.085352
83	0.83	0.125665	0.072949
82	0.82	0.110677	0.062345
81	0.81	0.097460	0.053280
80	0.80	0.085810	0.045531
79	0.79	0.075543	0.038908
78	0.78	0.066497	0.033247
77	0.77	0.058529	0.028409

Exercises

8.1 The chemical reaction and diffusion in a spherical catalyst pellet is given by

$$D\frac{d^2C_A}{dr^2}+\frac{2}{r}D\frac{dC_A}{dr}-kC_A=0$$

where D is the effective binary diffusivity of A within the catalyst pellet. The pellet is isothermal. The concentration at the surface of the spherical catalyst pellet is 1 mol/m^3 thus the boundary conditions are:

$$\text{At } r = R: \qquad C_A = 1$$

$$\text{At } r = 0: \qquad \frac{dC_A}{dr}=0$$

The radius of the catalyst pellet is 1.0 cm. Make 10 parts of the radius. Take the rate constant, $k = 0.1$ s^{-1} and $D = 10^{-9}$ m^2/s. Determine the concentration of species A at various positions along the radius of the catalyst pellet.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -106 & 6 & & & \\ 1-\frac{1}{1} & -102 & 1+\frac{1}{1} & & \\ & \cdots & \cdots & \cdots & \\ & & 1-\frac{1}{8} & -102 & 1+\frac{1}{8} \\ & & & 1-\frac{1}{9} & -102 \end{bmatrix}\begin{bmatrix} C_{A0} \\ C_{A1} \\ \cdots \\ C_{A8} \\ C_{A9} \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -\frac{10}{9} \end{bmatrix}$$

$C_{A0} = C_A(0.0) = 0.000000$ $\quad$ $C_{A1} = C_A(0.1) = 0.000000$

$C_{A2} = C_A(0.2) = 0.000000$ $\quad$ $C_{A3} = C_A(0.3) = 0.000000$

$C_{A4} = C_A(0.4) = 0.000000$ $\quad$ $C_{A5} = C_A(0.5) = 0.000000$

$C_{A6} = C_A(0.6) = 0.000000$ $\quad$ $C_{A7} = C_A(0.7) = 0.000001$

$C_{A8} = C_A(0.8) = 0.000120$ $\quad$ $C_{A9} = C_A(0.9) = 0.010894$

Distance (in cm) is measured from the centre of the spherical pellet.

8.2 The chemical reaction and diffusion in a spherical catalyst pellet is given by

$$D\frac{d^2C_A}{dr^2}+\frac{2}{r}D\frac{dC_A}{dr}-kC_A^2=0$$

where D is the effective binary diffusivity of A within the catalyst pellet. The pellet is isothermal. The concentration at the surface of the spherical catalyst pellet is 1 mol/m^3, thus the boundary conditions are

$$\text{At } r = R: \qquad C_A = 1$$

$$\text{At } r = 0: \qquad \frac{dC_A}{dr}=0$$

The radius of the catalyst pellet is 1.0 cm. Make 10 parts of the radius. Take the rate constant, $k = 0.1$ m^3/mol-s and $D = 10^{-9}$ m^2/s. Determine the concentration of species A at various positions along the radius of the catalyst pellet.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -6-100C_{A0} & 6 & & & \\ 1-\frac{1}{1} & -2-100C_{A1} & 1+\frac{1}{1} & & \\ & \cdots & \cdots & \cdots & \\ & & 1-\frac{1}{8} & -2-100C_{A8} & 1+\frac{1}{8} \\ & & & 1-\frac{1}{9} & -2-100C_{A9} \end{bmatrix} \begin{bmatrix} C_{A0} \\ C_{A1} \\ \cdots \\ C_{A8} \\ C_{A9} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -\frac{10}{9} \end{bmatrix}$$

$C_{A0} = C_A(0.0) = 0.001837$ $\qquad C_{A1} = C_A(0.1) = 0.001894$

$C_{A2} = C_A(0.2) = 0.002073$ $\qquad C_{A3} = C_A(0.3) = 0.002419$

$C_{A4} = C_A(0.4) = 0.003030$ $\qquad C_{A5} = C_A(0.5) = 0.004131$

$C_{A6} = C_A(0.6) = 0.006286$ $\qquad C_{A7} = C_A(0.7) = 0.011211$

$C_{A8} = C_A(0.8) = 0.025902$ $\qquad C_{A9} = C_A(0.9) = 0.096965$

Distance (in cm) is measured from the centre of the spherical pellet.

8.3 Diffusion and reaction take place in a non-isothermal spherical catalyst pellet of radius 1 cm. The rate constant of the reaction $k(T_S) = 0.1$ s^{-1} and effective diffusivity of species, $D = 10^{-9}$ m^2/s. Make 10 parts of the radius and determine the concentration within the catalyst pellet. The concentration at the surface of the spherical catalyst pellet, $C_S = 1$ mol/m^3. Take $\beta = 1$ and $\gamma = 1$.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -6-100\exp\left(\frac{1-C_0}{2-C_0}\right) & 6 & & & \\ 1-\frac{1}{1} & -2-100\exp\left(\frac{1-C_1}{2-C_1}\right) & 1+\frac{1}{1} & & \\ & & \cdots & & \\ & & 1-\frac{1}{8} & -2-100\exp\left(\frac{1-C_8}{2-C_8}\right) & 1+\frac{1}{8} \\ & & & 1-\frac{1}{9} & -2-100\exp\left(\frac{1-C_9}{2-C_9}\right) \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ \cdots \\ C_8 \\ C_9 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ -\frac{10}{9} \end{bmatrix}$$

$C_{A0} = C_A(0.0) = 0.000000$ $\qquad C_{A1} = C_A(0.1) = 0.000000$

$C_{A2} = C_A(0.2) = 0.000000$ $\qquad C_{A3} = C_A(0.3) = 0.000000$

$C_{A4} = C_A(0.4) = 0.000000$ $\qquad C_{A5} = C_A(0.5) = 0.000000$

$C_{A6} = C_A(0.6) = 0.000000$ $\qquad C_{A7} = C_A(0.7) = 0.000000$

$C_{A8} = C_A(0.8) = 0.000045$ $\qquad C_{A9} = C_A(0.9) = 0.006659$

Distance (in cm) is measured from the centre of the spherical pellet.

Chapter 9

One-Dimensional Transient Heat Conduction

The numerical solution of one-dimensional transient heat conduction in a rectangular slab, cylinder, and sphere is discussed in this chapter using the finite difference method. The one-dimensional transient heat conduction in a rectangular slab is given by

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{9.1}$$

In a cylinder it is given by

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) \tag{9.2}$$

and in a sphere it is given by

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) \tag{9.3}$$

where $\alpha = \dfrac{k}{\rho C_P}$. Discretization is carried out using the forward in time and central in space (FTCS) difference scheme. The explicit, implicit and Crank–Nicolson discretizations are discussed. An example of one-dimensional transient diffusion is also discussed. Von Neumann stability analysis, which is used to determine the criteria under which the explicit scheme is stable, is also discussed.

9.1 Classification of Partial Differential Equations

Consider the two-dimensional partial differential equation (PDE)

$$A \frac{\partial^2 f}{\partial x^2} + B \frac{\partial^2 f}{\partial x \partial y} + C \frac{\partial^2 f}{\partial y^2} + D \frac{\partial f}{\partial x} + E \frac{\partial f}{\partial y} + Ff + G = 0 \tag{9.4}$$

When $B^2 - 4AC < 0$, characteristics do not exist and it is elliptic PDE.
When $B^2 - 4AC = 0$, one set of characteristics exists and it is parabolic PDE.
When $B^2 - 4AC > 0$, two sets of characteristics exist and it is hyperbolic PDE.
A summary of the above result with examples is presented in Table 9.1.

Table 9.1 Classification of partial differential equations

PDE	*Parameters*	*Classification of PDE*
$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=0$	$A = 1$ $B = 0$ $C = 1$	$B^2 - 4AC = -4 < 0$ Elliptic
$\frac{\partial T}{\partial t}-\alpha\frac{\partial^2 T}{\partial x^2}=0 \quad (\alpha > 0)$	$A = -\alpha$ $B = 0$ $C = 0$	$B^2 - 4AC = 0$ Parabolic
1-D wave equation $\frac{\partial u}{\partial t}+a\frac{\partial u}{\partial x}=0 \quad (a > 0) \qquad (9.5)$	$A = 1$ $B = 0$ $C = -a^2$	$B^2 - 4AC = 4a^2 > 0$ Hyperbolic

The coefficients in the 1D wave equation are determined using the following. Differentiating Eq. (9.5) with respect to x, we get

$$\frac{\partial^2 u}{\partial t\partial x}+a\frac{\partial^2 u}{\partial x^2}=0$$

Differentiating Eq. (9.5) with respect to t, we get

$$\frac{\partial^2 u}{\partial t^2}+a\frac{\partial^2 u}{\partial t\partial x}=0$$

Combining the above two equations, we get

$$\frac{\partial^2 u}{\partial t^2}-a^2\frac{\partial^2 u}{\partial x^2}=0$$

A linear PDE is one in which A, B, C, D, E, F, and G are functions of x and y only.

9.2 Explicit and Implicit Discretization

Consider conduction in a one-dimensional rectangular slab. The partial differential equation is [see Eq. (9.1)]

$$\frac{\partial T}{\partial t}=\alpha\frac{\partial^2 T}{\partial x^2}$$

Using the forward in time and central in space explicit difference scheme, we get

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}=\alpha\frac{T_{i+1}^n+T_{i-1}^n-2T_i^n}{(\Delta x)^2} \tag{9.6}$$

If the solution is known at time n, then it is very easy to determine the solution at time $n + 1$ using the explicit method.

$$T_i^{n+1} = M\left(T_{i+1}^n + T_{i-1}^n - 2T_i^n\right) + T_i^n \tag{9.7}$$

where $M = \dfrac{\alpha \Delta t}{(\Delta x)^2}$.

Thus if the temperature at all the nodes is known at time t, the temperature at time $t + \Delta t$ can be computed and from this temperature at time $t + \Delta t$, the temperature at time $t + 2\Delta t$ can be computed. Thus the temperature at any required time can be computed. Thus the values of all the nodes can be updated to compute the temperature profile at the required time. But there is a disadvantage, which is that explicit discretization is not stable for all values of Δt and Δx. It is stable only when

$$\alpha \frac{\Delta t}{(\Delta x)^2} \le \frac{1}{2} \tag{9.8}$$

Thus the choice of Δt and Δx is not independent. If the condition $\alpha \dfrac{\Delta t}{(\Delta x)^2} \le \dfrac{1}{2}$ is not satisfied, then convergence shall not be obtained and the solution shall start diverging. The implicit method is an unconditionally stable method and the implicit discretization of Eq. (9.1) is given by

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1}}{(\Delta x)^2} \tag{9.9}$$

When the temperature at time t is known, then to calculate the temperature at time $t + \Delta t$ the tridiagonal set of linear algebraic equations is solved. Thus T_i^n are known and T_i^{n+1} are calculated. Thus marching in time can be carried out to obtain the temperature at various nodes at the next time step for the parabolic PDE.

9.3 Crank-Nicolson Discretization

Consider conduction in a rectangular slab. The partial differential equation is [see Eq. (9.1)]

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Crank–Nicolson discretization is given by

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{\alpha}{2}\left[\frac{T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1}}{(\Delta x)^2} + \frac{T_{i+1}^n + T_{i-1}^n - 2T_i^n}{(\Delta x)^2}\right] \tag{9.10}$$

In the Crank–Nicolson method the discretization of space term is carried out using the central difference scheme at time n and at time $n + 1$ and taking the mean of the two. It is an unconditionally stable method. It is an more accurate than the implicit method. The accuracy of the implicit method is O(Δt,Δx^2), whereas that of Crank–Nicolson is O(Δt^2,Δx^2). The central difference scheme is not used in time because it would require high storage, as there would be terms of three types—T^{n+1}, T^n, T^{n-1}.

9.4 Von Neumann Stability Analysis

Von Neumann stability analysis is also called the *Fourier method*. The method shall be described for the one-dimensional transient heat conduction [see Eq. (9.1)]

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Discretizing using the FTCS explicit scheme, we get at node i [see Eq. (9.6)]

$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{\Delta x^2}\left(T_{i+1}^n + T_{i-1}^n - 2T_i^n\right)$$

Let the exact solution of this equation be D. This is the solution that would be obtained using a computer with infinite accuracy (infinite storage of each variable). Let the numerical solution on a real machine with finite accuracy be N. Then, round-off error = $N - D = \varepsilon$. Thus, $N = D + \varepsilon$ and the above equation becomes

$$\frac{D_i^{n+1} + \varepsilon_i^{n+1} - D_i^n - \varepsilon_i^n}{\Delta t} = \alpha\left(\frac{D_{i+1}^n + \varepsilon_{i+1}^n + D_{i-1}^n + \varepsilon_{i-1}^n - 2D_i^n - 2\varepsilon_i^n}{\Delta x^2}\right) \tag{9.11}$$

Since the exact solution D must satisfy the difference equation, the same is true of the error, that is

$$\frac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = \alpha\left(\frac{\varepsilon_{i+1}^n + \varepsilon_{i-1}^n - 2\varepsilon_i^n}{\Delta x^2}\right) \tag{9.12}$$

Thus the exact solution D and the error ε must both satisfy the same difference equation. Consider a distribution of errors at any time. The error $\varepsilon(x, t)$ can be written as a series of the form

$$\varepsilon(x,t) = \sum_m e^{at} e^{ik_m x} \tag{9.13}$$

where

$$k_m = \frac{m\pi}{L} \qquad m = 0, 1, 2, \ldots, M' \tag{9.14}$$

M' is the number of intervals (Δx units long) contained in length L. Since the difference equation is linear, superposition may be used and we may examine the behaviour of a single term of the series. Thus, when the finite difference equation (FDE) is linear, it is sufficient to investigate only one component of the Fourier series. The error is in the form of Fourier series. Consider the term

$$\varepsilon_m(x,t) = e^{at} e^{ik_m x} \tag{9.15}$$

where k_m is real but a may be complex. Substituting $\varepsilon_m(x,t) = e^{at} e^{ik_m x}$ into Eq. (9.12), we get

$$e^{a(t+\Delta t)} e^{ik_m x} - e^{at} e^{ik_m x} = M\left(e^{at} e^{ik_m(x+\Delta x)} - 2e^{at} e^{ik_m x} + e^{at} e^{ik_m(x-\Delta x)}\right) \tag{9.16}$$

where $M = \dfrac{\alpha \Delta t}{\Delta x^2}$. If we divide by $e^{at} e^{ik_m x}$, we get

$$e^{a\Delta t} - 1 = M\left(e^{ik_m \Delta x} + e^{-ik_m \Delta x} - 2\right)$$

and if we utilize the relation

$$\cos\beta = \frac{e^{i\beta} + e^{-i\beta}}{2} \tag{9.17}$$

we get

$$e^{a\Delta t} = 1 + 2M(\cos\beta - 1) \tag{9.18}$$

where

$$\beta = k_m \Delta x \tag{9.19}$$

We know

$$\sin^2\frac{\beta}{2} = \frac{1 - \cos\beta}{2} \tag{9.20}$$

Thus

$$e^{a\Delta t} = 1 - 4M\sin^2\frac{\beta}{2} \tag{9.21}$$

Since $\varepsilon_i^{n+1} = e^{a\Delta t}\varepsilon_i^n$ for each frequency present in the solution for the error, it is clear that if $\left|e^{a\Delta t}\right|$ is less than or equal to one, a general component of the error will not grow from one time step to the next. Stability means that error should not grow. This requires that

$$\left|1 - 4M\sin^2\frac{\beta}{2}\right| \le 1 \tag{9.22}$$

The factor $1 - 4M\sin^2\dfrac{\beta}{2}$ (representing $\dfrac{\varepsilon_i^{n+1}}{\varepsilon_i^n}$) is called the *amplification factor*. If the sign on the left hand side of Eq. (9.22) is either positive or negative, two conditions result.

For positive sign

$$4M\sin^2\frac{\beta}{2} > 0 \tag{9.23}$$

For negative sign

$$4M\sin^2\frac{\beta}{2} - 1 \le 1 \tag{9.24}$$

Since M is positive, the first condition is always satisfied. The second inequality is satisfied only if $M \le \frac{1}{2}$, which is the stability requirement. Thus for the explicit finite difference equation $T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{\Delta x^2}\left(T_{i+1}^n + T_{i-1}^n - 2T_i^n\right)$ to be stable

$$\frac{\alpha \Delta t}{\Delta x^2} \le \frac{1}{2} \tag{9.25}$$

The two-dimensional transient heat conduction equation is

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \tag{9.26}$$

Discretizing at node (*i*, *j*) using the FTCS explicit scheme, we get

$$T_{i,j}^{n+1} = T_{i,j}^n + \frac{\alpha \Delta t}{\Delta x^2}\left(T_{i+1,j}^n + T_{i-1,j}^n - 2T_{i,j}^n\right) + \frac{\alpha \Delta t}{\Delta y^2}\left(T_{i,j+1}^n + T_{i,j-1}^n - 2T_{i,j}^n\right) \tag{9.27}$$

From the von Neumann stability analysis, we get the explicit FTCS discretization to be stable when

$$\frac{\alpha \Delta t}{\Delta x^2} + \frac{\alpha \Delta t}{\Delta y^2} \le \frac{1}{2} \tag{9.28}$$

When $\Delta x = \Delta y = \Delta$, the discretized form of Eq. (9.26) becomes

$$T_{i,j}^{n+1} = T_{i,j}^n + \frac{\alpha \Delta t}{\Delta^2}\left(T_{i+1,j}^n + T_{i-1,j}^n + T_{i,j+1}^n + T_{i,j-1}^n - 4T_{i,j}^n\right) \tag{9.29}$$

and the stability criterion for explicit discretization becomes

$$\frac{\alpha \Delta t}{\Delta^2} \le \frac{1}{4} \tag{9.30}$$

9.5 Transient Conduction in Rectangular Slab

One-dimensional transient heat conduction in a rectangular slab using the implicit method is described in the example below.

EXAMPLE 9.1 Consider transient heat conduction in a rectangular slab. The partial differential equation is

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

The total width of the rectangular slab is 0.8 cm. Initially the temperature is uniform at 20°C. The temperature of the end faces of the rectangular slab is made 300°C at $t = 0$ s. Use implicit discretization and take $\Delta x = 0.1$ cm, $\Delta t = 0.1$ s, and $\alpha = 10^{-5}$ m^2/s. List the tridiagonal system of equations and determine the temperature at the centre and the intermediate points of the slab up to 3.1 s.

Solution The schematic diagram of the rectangular slab is shown in Fig. 9.1.

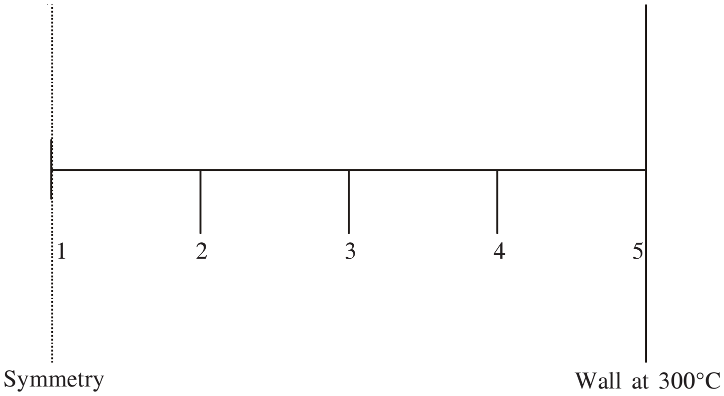


Fig. 9.1 Transient heat conduction in rectangular slab.

Using forward in time and central in space implicit difference scheme, we get

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1}}{(\Delta x)^2}$$

$$T_i^{n+1} - T_i^n = M\left(T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1}\right)$$

where $M = \dfrac{\alpha \Delta t}{(\Delta x)^2}$.

$$(M)T_{i-1}^{n+1} - (2M+1)T_i^{n+1} + (M)T_{i+1}^{n+1} = -T_i^n$$

At node 2

$$(M)T_1^{n+1} - (2M+1)T_2^{n+1} + (M)T_3^{n+1} = -T_2^n$$

At node 3

$$(M)T_2^{n+1} - (2M+1)T_3^{n+1} + (M)T_4^{n+1} = -T_3^n$$

At node 4

$$(M)T_3^{n+1} - (2M+1)T_4^{n+1} + (M)T_5^{n+1} = -T_4^n$$

where T_5 = 300°C. At node 1 the finite difference equation is

$$(M)T_0^{n+1} - (2M+1)T_1^{n+1} + (M)T_2^{n+1} = -T_1^n$$

where 0 is a hypothetical node to the left of node 1. Since at $x = 0$ (node 1) the symmetry condition is satisfied, we get $\frac{\partial T}{\partial x} = 0$; thus $\frac{T_2^{n+1} - T_0^{n+1}}{2\Delta x} = 0$ and so $T_0^{n+1} = T_2^{n+1}$.

Thus at $i = 1$, we get

$$(-2M - 1)T_1^{n+1} + (2M)T_2^{n+1} = -T_1^n$$

The following tridiagonal set of linear algebraic equations is obtained:

$$\begin{bmatrix} \frac{-2M-1}{2} & M & 0 & 0 \\ M & -2M-1 & M & 0 \\ 0 & M & -2M-1 & M \\ 0 & 0 & M & -2M-1 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \end{bmatrix} = \begin{bmatrix} -\frac{T_1^n}{2} \\ -T_2^n \\ -T_3^n \\ -T_4^n - 300M \end{bmatrix}$$

where the old values are at time n and the computed values are at time $n + 1$. Here $\alpha = 10^{-5}$ m²/s, $\Delta t = 0.1$ s, $\Delta x = 0.1$ cm, $T_1^n = T_2^n = T_3^n = T_4^n = 20$ °C, $T_5 = 300$°C. Thus

$$M = \frac{\alpha \Delta t}{(\Delta x)^2} = \frac{10^{-5} \times 0.1}{(0.1 \times 10^{-2})^2} = 1$$

$$\begin{bmatrix} -1.5 & 1 & 0 & 0 \\ 1 & -3 & 1 & 0 \\ 0 & 1 & -3 & 1 \\ 0 & 0 & 1 & -3 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \end{bmatrix} = \begin{bmatrix} -0.5T_1^n \\ -T_2^n \\ -T_3^n \\ -T_4^n - 300 \end{bmatrix}$$

At time $t = 0$, $T_1^n = T_2^n = T_3^n = T_4^n = 20$°C and the solution by TDMA is obtained at time $t = 0.1$s. These become the old values for solution by TDMA at $t = 0.2$ s and so on. Note that in this sort of discretization a tridiagonal matrix is bound to get formed because, for discretization at node *i,* use is made of the values at nodes $i - 1$, $i + 1$, and *i*. Program 9.1 for the solution of the above problem is given in the Appendix. The coefficient matrix parameters are constant, but the right hand side of the linear algebraic equations each time is updated. The results of Program 9.1 are presented in Table 9.2.

Table 9.2 Results of Program 9.1

Time (s)	T_1	T_2	T_3	T_4
0.1	31.91	37.87	61.70	127.23
0.2	53.21	63.86	100.49	175.91
0.3	78.59	91.28	131.40	202.44
0.4	104.35	117.22	156.04	219.49
0.5	128.55	140.66	176.20	231.90
0.6	150.45	161.40	193.09	241.66
0.7	169.87	179.57	207.45	249.71
0.8	186.90	195.42	219.79	256.50
0.9	201.78	209.21	230.44	262.31
1.0	214.72	221.20	239.65	267.32
1.1	225.98	231.60	247.64	271.65
1.2	235.75	240.64	254.56	275.40
1.3	244.24	248.48	260.57	278.66
1.4	251.60	255.29	265.78	281.48
1.5	258.00	261.19	270.30	283.93
1.6	263.55	266.32	274.22	286.05
1.7	268.36	270.77	277.63	287.89
1.8	272.54	274.63	280.58	289.49
1.9	276.17	277.98	283.15	290.88
2.0	279.32	280.89	285.38	292.09
2.1	282.05	283.42	287.31	293.13
2.2	284.42	285.61	288.99	294.04
2.3	286.48	287.51	290.44	294.83
2.4	288.27	289.16	291.70	295.51
2.5	289.82	290.59	292.80	296.10
2.6	291.16	291.84	293.75	296.62
2.7	292.33	292.91	294.58	297.07
2.8	293.34	293.85	295.29	297.45
2.9	294.22	294.66	295.92	297.79
3.0	294.99	295.37	296.46	298.08
3.1	295.65	295.98	296.92	298.33

EXAMPLE 9.2 A brick wall with a thickness of 0.5 m is initially at a uniform temperature of 300 K. At time $t = 0$ the left surface is maintained at 425 K and right at 600 K. Determine the time required for its centre temperature to reach 425 K. Use implicit discretization and take $\Delta x = 0.05$ m, $\alpha = 10^{-5}\text{m}^2/\text{s}$, and $\Delta t = 1.0$ s.

Solution The schematic diagram is shown in Fig. 9.2.

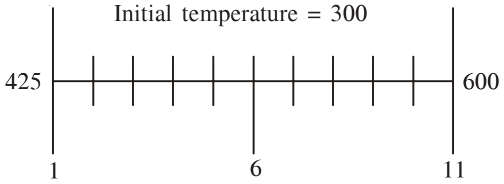


Fig. 9.2 Example 9.2.

In a rectangular slab

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Discretizing using implicit FTCS at node *i*, we get

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \left(\frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta x^2} \right)$$

Δx = 0.05 m and Δt = 1.0 s; thus $\alpha \frac{\Delta t}{\Delta x^2} = \frac{10^{-5}}{0.05 \times 0.05} = 0.004$. Therefore

$$T_i^{n+1} - T_i^n = 0.004\left(T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}\right)$$

$$-0.004T_{i-1}^{n+1} + 1.008T_i^{n+1} - 0.004T_{i+1}^{n+1} = T_i^n$$

At node 2

$$-0.004T_1^{n+1} + 1.008T_2^{n+1} - 0.004T_3^{n+1} = T_2^n$$

Since T_1 = 425, we get

$$1.008T_2^{n+1} - 0.004T_3^{n+1} = T_2^n + 0.004 \times 425$$

At node 3

$$-0.004T_2^{n+1} + 1.008T_3^{n+1} - 0.004T_4^{n+1} = T_3^n$$

At node 9

$$-0.004T_8^{n+1} + 1.008T_9^{n+1} - 0.004T_{10}^{n+1} = T_9^n$$

At node 10

$$-0.004T_9^{n+1} + 1.008T_{10}^{n+1} - 0.004T_{11}^{n+1} = T_{10}^n$$

Since T_{11} = 600, we get

$$-0.004T_9^{n+1} + 1.008T_{10}^{n+1} = T_{10}^n + 0.004 \times 600$$

Thus the unknowns are T_2 to T_{10}. The tridiagonal set of 9 linear algebraic equations is

$$\begin{bmatrix} 1.008 & -0.004 & & & \\ -0.004 & 1.008 & -0.004 & & \\ & \cdots & \cdots & \cdots & \\ & & -0.004 & 1.008 & -0.004 \\ & & & -0.004 & 1.008 \end{bmatrix} \begin{bmatrix} T_2^{n+1} \\ T_3^{n+1} \\ \cdots \\ T_9^{n+1} \\ T_{10}^{n+1} \end{bmatrix} = \begin{bmatrix} T_2^n + 1.7 \\ T_3^n \\ \cdots \\ T_9^n \\ T_{10}^n + 2.4 \end{bmatrix}$$

Initially $T_2^n = T_3^n = T_4^n = T_5^n = T_6^n = T_7^n = T_8^n = T_9^n = T_{10}^n = 300$. After every iteration the time is incremented by 1 s. We have to determine the time when T_6 = 425. Program 9.1 can be modified by changing the coefficients and the following solution is obtained at 2865 s: $T_2 = 415.87$, $T_3 = 409.24$, $T_4 = 407.40$, $T_5 = 412.24$, $T_6 = 425.06$, $T_7 = 446.44$, $T_8 = 476.11$, $T_9 = 512.95$, and $T_{10} = 555.07$.

9.6 Transient Conduction in Cylinder

One-dimensional transient heat conduction in a cylinder using the implicit method is described in the example below.

EXAMPLE 9.3 Consider a cylinder of radius 0.4 cm. Initially the temperature is uniform at 20°C. The temperature of the cylinder surface is made 300°C at $t = 0$ s. Use implicit discretization and take $\Delta r = 0.1$ cm, $\Delta t = 0.1$ s, and $\alpha = 10^{-5}\text{m}^2/\text{s}$. List the tridiagonal system of equations and determine the temperature at the centre and the intermediate points of the cylinder up to 2.1 s.

Solution The partial differential equation is

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right)$$

Using the forward in time and central in space implicit difference scheme, we get

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha\left[\frac{T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1}}{(\Delta r)^2} + \frac{1}{m\Delta r}\left(\frac{T_{i+1}^{n+1} - T_{i-1}^{n+1}}{2\Delta r}\right)\right]$$

$$T_i^{n+1} - T_i^n = M\left[T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1} + \frac{1}{2m}\left(T_{i+1}^{n+1} - T_{i-1}^{n+1}\right)\right]$$

where $M = \dfrac{\alpha\Delta t}{(\Delta r)^2}$.

$$T_i^{n+1} - T_i^n = T_{i+1}^{n+1}\left(M + \frac{M}{2m}\right) + T_{i-1}^{n+1}\left(M - \frac{M}{2m}\right) - 2MT_i^{n+1}$$

$$\left(M - \frac{M}{2m}\right)T_{i-1}^{n+1} - (2M+1)T_i^{n+1} + \left(M + \frac{M}{2m}\right)T_{i+1}^{n+1} = -T_i^n$$

At node 2 ($m = 1$)

$$\left(M - \frac{M}{2}\right)T_1^{n+1} - (2M+1)T_2^{n+1} + \left(M + \frac{M}{2}\right)T_3^{n+1} = -T_2^n$$

At node 3 ($m = 2$)

$$\left(M - \frac{M}{4}\right)T_2^{n+1} - (2M+1)T_3^{n+1} + \left(M + \frac{M}{4}\right)T_4^{n+1} = -T_3^n$$

At node 4 (m = 3)

$$\left(M-\frac{M}{6}\right)T_3^{n+1}-(2M+1)T_4^{n+1}+\left(M+\frac{M}{6}\right)T_5^{n+1}=-T_4^n$$

where T_5 = 300°C. On using L'Hospital's rule at node 1, the PDE becomes $\frac{\partial T}{\partial t}=2\frac{\partial^2 T}{\partial r^2}$. Using implicit FTCS to discretize, we get

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}=\frac{2\left(T_{i+1}^{n+1}+T_{i-1}^{n+1}-2T_i^{n+1}\right)}{(\Delta r)^2}$$

$$T_i^{n+1}-T_i^n=2M\left(T_{i+1}^{n+1}+T_{i-1}^{n+1}-2T_i^{n+1}\right)$$

$$(2M)T_{i-1}^{n+1}-(4M+1)T_i^{n+1}+(2M)T_{i+1}^{n+1}=-T_i^n$$

At i = 1, we get

$$(2M)T_0^{n+1}-(4M+1)T_1^{n+1}+(2M)T_2^{n+1}=-T_1^n$$

where 0 is a hypothetical node to the left of node 1.

Since at r = 0, $\frac{\partial T}{\partial r}=0$, $\frac{T_2^{n+1}-T_0^{n+1}}{2\Delta r}=0$; thus $T_0^{n+1}=T_2^{n+1}$.

Thus at i = 1, we get

$$(-4M-1)T_1^{n+1}+(4M)T_2^{n+1}=-T_1^n$$

The following tridiagonal set of linear algebraic equations is obtained.

$$\begin{bmatrix}-4M-1 & 4M & 0 & 0\\ \frac{M}{2} & -2M-1 & \frac{3M}{2} & 0\\ 0 & \frac{3M}{4} & -2M-1 & \frac{5M}{4}\\ 0 & 0 & \frac{5M}{6} & -2M-1\end{bmatrix}\begin{bmatrix}T_1^{n+1}\\ T_2^{n+1}\\ T_3^{n+1}\\ T_4^{n+1}\end{bmatrix}=\begin{bmatrix}-T_1^n\\ -T_2^n\\ -T_3^n\\ -T_4^n-\frac{7M}{6}\times 300\end{bmatrix}$$

where the old values are at time n and the computed values are at time n + 1. Here $\alpha = 10^{-5}$ m^2/s, Δt = 0.1 s, Δr = 0.1 cm, $T_1^n=T_2^n=T_3^n=T_4^n=20\,^\circ\text{C}$, T_5 = 300°C. Thus

$$M=\frac{\alpha\Delta t}{(\Delta r)^2}=\frac{10^{-5}\times 0.1}{\left(0.1\times 10^{-2}\right)^2}=1$$

$$\begin{bmatrix}-5 & 4 & 0 & 0\\ 0.5 & -3 & 1.5 & 0\\ 0 & 0.75 & -3 & 1.25\\ 0 & 0 & 0.833 & -3\end{bmatrix}\begin{bmatrix}T_1^{n+1}\\ T_2^{n+1}\\ T_3^{n+1}\\ T_4^{n+1}\end{bmatrix}=\begin{bmatrix}-T_1^n\\ -T_2^n\\ -T_3^n\\ -T_4^n-350\end{bmatrix}$$

At time $t = 0$, $T_1^n = T_2^n = T_3^n = T_4^n = 20\,^\circ\text{C}$, and the solution by TDMA is obtained at time $t = 0.1$ s. These become the old values for solution by TDMA at $t = 0.2$ s and so on. Program 9.1 can be modified to solve this problem and the results are given in Table 9.3.

Table 9.3 Results in Example 9.3

Time (s)	T_1	T_2	T_3	T_4
0.1	48.29	55.37	81.30	145.91
0.2	91.65	102.48	137.51	203.48
0.3	135.90	146.97	180.31	234.56
0.4	174.33	183.93	211.78	253.66
0.5	205.21	212.93	234.84	266.43
0.6	229.08	235.05	251.79	275.39
0.7	247.17	251.69	264.29	281.85
0.8	260.72	264.11	273.53	286.56
0.9	270.83	273.36	280.36	290.04
1.0	278.34	280.22	285.43	292.60
1.1	283.92	285.32	289.18	294.49
1.2	288.06	289.09	291.96	295.90
1.3	291.13	291.89	294.02	296.94
1.4	293.40	293.97	295.54	297.71
1.5	295.09	295.51	296.67	298.28
1.6	296.34	296.65	297.51	298.70
1.7	297.26	297.49	298.13	299.02
1.8	297.95	298.12	298.60	299.25
1.9	298.46	298.58	298.94	299.42
2.0	298.83	298.93	299.19	299.55
2.1	299.11	299.18	299.38	299.64

The number of parts can be increased to obtain a better solution.

9.7 Transient Conduction in Sphere

One-dimensional transient heat conduction in a sphere using the implicit method is described in the example below.

EXAMPLE 9.4 Consider a sphere of radius 0.4 cm. Initially the temperature is uniform at 20°C. The temperature of the sphere surface is made 300°C at $t = 0$ s. Use implicit discretization and take $\Delta r = 0.1$ cm, $\Delta t = 0.1$ s, and $\alpha = 10^{-5}$ m^2/s. List the tridiagonal system of equations and determine the temperature at the centre and the intermediate points of the sphere up to 1.4 s.

Solution The partial differential equation is

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r}\right)$$

Using the forward in time and central in space implicit difference scheme, we get

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}=\alpha\left[\frac{T_{i+1}^{n+1}+T_{i-1}^{n+1}-2T_i^{n+1}}{(\Delta r)^2}+\frac{2}{m\Delta r}\left(\frac{T_{i+1}^{n+1}-T_{i-1}^{n+1}}{2\Delta r}\right)\right]$$

$$T_i^{n+1}-T_i^n=M\left[T_{i+1}^{n+1}+T_{i-1}^{n+1}-2T_i^{n+1}+\frac{1}{m}\left(T_{i+1}^{n+1}-T_{i-1}^{n+1}\right)\right]$$

where $M=\frac{\alpha\Delta t}{(\Delta r)^2}$.

$$T_i^{n+1}-T_i^n=T_{i+1}^{n+1}\left(M+\frac{M}{m}\right)+T_{i-1}^{n+1}\left(M-\frac{M}{m}\right)-2MT_i^{n+1}$$

$$T_{i+1}^{n+1}\left(M+\frac{M}{m}\right)+T_{i-1}^{n+1}\left(M-\frac{M}{m}\right)+T_i^{n+1}(-2M-1)=-T_i^n$$

At node 2 (m = 1)

$$T_3^{n+1}(M+M)+T_1^{n+1}(0)+T_2^{n+1}(-2M-1)=-T_2^n$$

At node 3 (m = 2)

$$T_4^{n+1}\left(M+\frac{M}{2}\right)+T_2^{n+1}\left(M-\frac{M}{2}\right)+T_3^{n+1}(-2M-1)=-T_3^n$$

At node 4 (m = 3)

$$T_5^{n+1}\left(M+\frac{M}{3}\right)+T_3^{n+1}\left(M-\frac{M}{3}\right)+T_4^{n+1}(-2M-1)=-T_4^n$$

where T_5 = 300°C

At node 1 the PDE becomes $\frac{\partial T}{\partial t}=3\frac{\partial^2 T}{\partial r^2}$.

Again, using the implicit FTCS, we get

$$\frac{T_i^{n+1}-T_i^n}{\Delta t}=\frac{3\left(T_{i+1}^{n+1}+T_{i-1}^{n+1}-2T_i^{n+1}\right)}{(\Delta r)^2}$$

$$T_i^{n+1}-T_i^n=3M\left(T_{i+1}^{n+1}+T_{i-1}^{n+1}-2T_i^{n+1}\right)$$

$$T_{i+1}^{n+1}(3M)+T_{i-1}^{n+1}(3M)+T_i^{n+1}(-6M-1)=-T_i^n$$

At i =1, we get

$$T_2^{n+1}(3M)+T_0^{n+1}(3M)+T_1^{n+1}(-6M-1)=-T_1^n$$

where 0 is a hypothetical node to the left of node 1.

At r = 0, $\frac{\partial T}{\partial r}=0$; thus $\frac{T_2^{n+1}-T_0^{n+1}}{2\Delta r}=0$ and so $T_0^{n+1}=T_2^{n+1}$.

Thus at $i = 1$, we get

$$T_2^{n+1}(6M) + T_1^{n+1}(-6M - 1) = -T_1^n$$

The following tridiagonal set of linear algebraic equations is obtained:

$$\begin{bmatrix} -6M-1 & 6M & 0 & 0 \\ 0 & -2M-1 & 2M & 0 \\ 0 & \dfrac{M}{2} & -2M-1 & \dfrac{3M}{2} \\ 0 & 0 & \dfrac{2M}{3} & -2M-1 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \end{bmatrix} = \begin{bmatrix} -T_1^n \\ -T_2^n \\ -T_3^n \\ -T_4^n - \dfrac{4M}{3} \times 300 \end{bmatrix}$$

where the old values are at time n and the computed values are at time $n + 1$. Here $\alpha = 10^{-5}$ m^2/s, $\Delta t = 0.1$ s, $\Delta r = 0.1$ cm, $T_1^n = T_2^n = T_3^n = T_4^n = 20\,°\text{C}$, $T_5 = 300°\text{C}$. Thus

$$M = \frac{\alpha \Delta t}{(\Delta r)^2} = \frac{10^{-5} \times 0.1}{(0.1 \times 10^{-2})^2} = 1$$

$$\begin{bmatrix} -7 & 6 & 0 & 0 \\ 0 & -3 & 2 & 0 \\ 0 & 0.5 & -3 & 1.5 \\ 0 & 0 & 0.667 & -3 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \end{bmatrix} = \begin{bmatrix} -T_1^n \\ -T_2^n \\ -T_3^n \\ -T_4^n - 400 \end{bmatrix}$$

At time $t = 0$, $T_1^n = T_2^n = T_3^n = T_4^n = 20°\text{C}$ and the solution by TDMA is obtained at time $t = 0.1$ s. These become the old values for solution by TDMA at $t = 0.2$ s and so on. Program 9.1 can be modified to solve this problem and the results are given in Table 9.4.

Table 9.4 Results in Example 9.4

Time (s)	T_1	T_2	T_3	T_4
0.1	65.71	73.33	100.00	162.22
0.2	126.67	136.83	168.57	224.87
0.3	180.57	189.55	215.92	256.27
0.4	220.93	227.66	246.71	273.58
0.5	248.79	253.44	266.33	283.71
0.6	267.24	270.32	278.75	289.85
0.7	279.18	281.17	286.60	293.64
0.8	286.82	288.09	291.55	296.00
0.9	291.67	292.48	294.67	297.48
1.0	294.74	295.25	296.64	298.41
1.1	296.68	297.00	297.88	299.00
1.2	297.91	298.11	298.66	299.37
1.3	298.68	298.81	299.16	299.60
1.4	299.17	299.25	299.47	299.75

9.8 Transient Diffusion in Sphere

One-dimensional transient diffusion in a sphere using the implicit method is described in the example below.

EXAMPLE 9.5 Consider a 6.52 mm diameter bead which contains 10 mg of a certain drug in gel matrix. The diffusion coefficient of drug in gel matrix is 3.0×10^{-7} cm^2/s. The drug is immediately swept away once it reaches the bulk solution, that is, $C_S = 0$. The transient diffusion of the drug is given by

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right)$$

The boundary conditions are

$$\text{At } r = 0: \quad \frac{\partial C}{\partial r} = 0 \qquad t \ge 0$$

$$\text{At } r = R: \quad C = C_S = 0 \qquad t > 0$$

The initial condition is

$$\text{At } t = 0: \quad C = C_0 \qquad 0 \le r \le R$$

Determine the concentration of the drug in the centre of the bead after 3, 12, 24, and 48 h. Make 10 parts of the radius from $r = 0$ to $r = R$. Take $\Delta t = 1.0$ s.

Solution The radius of the bead is 0.326 cm and the initial concentration of the drug in the bead is = $\dfrac{10\,\text{mg}}{\frac{4}{3}\pi R^3} = 68.9\,\text{mg/cm}^3$. The schematic diagram of the bead from $r = 0$ to $r = R$ with 10 parts is shown in Fig. 9.3.

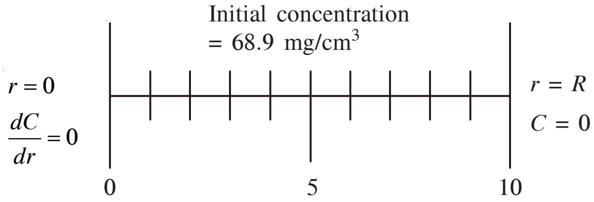


Fig. 9.3 Example 9.5.

In a sphere

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right)$$

Discretizing using FTCS at node *i*, we get

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}=D\left(\frac{C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}}{\Delta r^2}+\frac{2}{m\Delta r}\frac{C_{i+1}^{n+1}-C_{i-1}^{n+1}}{2\Delta r}\right)$$

$$C_i^{n+1}-C_i^n=\frac{D\Delta t}{\Delta r^2}\left[C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}+\frac{1}{m}\left(C_{i+1}^{n+1}-C_{i-1}^{n+1}\right)\right]$$

Δr = 0.0326 cm and Δt = 1.0 s. Thus

$$D\frac{\Delta t}{\Delta r^2}=\frac{3\times10^{-7}}{0.0326\times0.0326}=2.82\times10^{-4}$$

Thus at node i

$$C_i^{n+1}-C_i^n=2.82\times10^{-4}\left[C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}+\frac{1}{m}\left(C_{i+1}^{n+1}-C_{i-1}^{n+1}\right)\right]$$

$$-C_{i-1}^{n+1}\left(1-\frac{1}{m}\right)+3544.5C_i^{n+1}-C_{i+1}^{n+1}\left(1+\frac{1}{m}\right)=3542.5C_i^n$$

Using L'Hospital's rule, the PDE at node 0 becomes

$$\frac{\partial C}{\partial t}=3D\frac{\partial^2 C}{\partial r^2}$$

Discretizing the above equation at node 0, we get

$$\frac{C_0^{n+1}-C_0^n}{\Delta t}=\frac{3D}{\Delta r^2}\left(C_1^{n+1}-2C_0^{n+1}+C_{-1}^{n+1}\right)$$

$$3542.5\left(C_0^{n+1}-C_0^n\right)=3\left(C_1^{n+1}-2C_0^{n+1}+C_{-1}^{n+1}\right)$$

At node 0, $\frac{\partial C}{\partial r}=0$; thus $\frac{C_1-C_{-1}}{2\Delta r}=0$, and therefore C_1 = C_{-1}. Thus the above equation becomes

$$3542.5\left(C_0^{n+1}-C_0^n\right)=3\left(2C_1^{n+1}-2C_0^{n+1}\right)$$

$$590.4\left(C_0^{n+1}-C_0^n\right)=C_1^{n+1}-C_0^{n+1}$$

Thus the equation at node 0 is

$$591.4C_0^{n+1}-C_1^{n+1}=590.4C_0^n$$

At node 1

$$-C_0^{n+1}\left(1-\frac{1}{1}\right)+3544.5C_1^{n+1}-C_2^{n+1}\left(1+\frac{1}{1}\right)=3542.5C_1^n$$

At node 2

$$-C_1^{n+1}\left(1-\frac{1}{2}\right)+3544.5C_2^{n+1}-C_3^{n+1}\left(1+\frac{1}{2}\right)=3542.5C_2^n$$

At node 8

$$-C_7^{n+1}\left(1-\frac{1}{8}\right)+3544.5C_8^{n+1}-C_9^{n+1}\left(1+\frac{1}{8}\right)=3542.5C_8^n$$

At node 9

$$-C_8^{n+1}\left(1-\frac{1}{9}\right)+3544.5C_9^{n+1}-C_{10}^{n+1}\left(1+\frac{1}{9}\right)=3542.5C_9^n$$

Since C_{10} = 0, the equation for node 9 becomes

$$-C_8^{n+1}\left(1-\frac{1}{9}\right)+3544.5C_9^{n+1}=3542.5C_9^n$$

The above set of 10 equations (at nodes 0 to 9) can be written in tridiagonal form as

$$\begin{bmatrix} 591.4 & -1 & & & \\ -\left(1-\frac{1}{1}\right) & 3544.5 & -\left(1+\frac{1}{1}\right) & & \\ & \cdots & \cdots & \cdots & \\ & & -\left(1-\frac{1}{8}\right) & 3544.5 & -\left(1+\frac{1}{8}\right) \\ & & & -\left(1-\frac{1}{9}\right) & 3544.5 \end{bmatrix}\begin{bmatrix} C_0^{n+1} \\ C_1^{n+1} \\ \cdots \\ C_8^{n+1} \\ C_9^{n+1} \end{bmatrix}=\begin{bmatrix} 590.4C_0^n \\ 3542.5C_1^n \\ \cdots \\ 3542.5C_8^n \\ 3542.5C_9^n \end{bmatrix}$$

Initially $C_0^n = C_1^n = C_2^n = C_3^n = C_4^n = C_5^n = C_6^n = C_7^n = C_8^n = C_9^n = 68.9$ mg/cm^3. At the completion of an iteration, time is incremented by 1 s. Program 9.2 for the solution of the above problem is given in the Appendix. The following concentration of drug at the centre of the bead is obtained from Program 9.2: after 3 h the concentration is 62.39 mg/cm^3; after 12 h the concentration is 26.36 mg/cm^3, after 24 h the concentration is 7.99 mg/cm^3; and after 48 h the concentration is 0.73 mg/cm^3.

Exercises

9.1 Consider transient heat conduction in a rectangular slab. The total width of the rectangular slab is 1 cm. Initially the temperature is uniform at 25°C. The temperature of the end-faces of the rectangular slab is made 300°C at t = 0 s. Use implicit discretization and take Δx = 0.1 cm, Δt = 0.1 s, and $\alpha = 10^{-5}$ m^2/s. List the tridiagonal system of equations and determine the temperature at the centre and the intermediate points of the slab after 5 s.

(**Ans:** The tridiagonal set of equations is

$$\begin{bmatrix} -1.5 & 1 & & & \\ 1 & -3 & 1 & & \\ & 1 & -3 & 1 & \\ & & 1 & -3 & 1 \\ & & & 1 & -3 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \\ T_5^{n+1} \end{bmatrix} = \begin{bmatrix} -0.5T_1^n \\ -T_2^n \\ -T_3^n \\ -T_4^n \\ -T_5^n - 300.0 \end{bmatrix}$$

$T_1 = T(0.0) = 87.43$ $\qquad$ $T_2 = T(0.1) = 96.08$
$T_3 = T(0.2) = 122.44$ $\qquad$ $T_4 = T(0.3) = 166.98$
$T_5 = T(0.4) = 228.16$.
Distance (in cm) is measured from the centre.

9.2 Consider a cylinder of radius 0.5 cm. Initially the temperature is uniform at 25°C. The temperature of the cylinder surface is made 300°C at $t = 0$ s. Use implicit discretization and take $\Delta r = 0.1$ cm, $\Delta t = 0.1$ s, and $\alpha = 10^{-5}$ m^2/s. List the tridiagonal system of equations and determine the temperature at the centre and the intermediate points of the cylinder after 5 s.

(**Ans:** The tridiagonal set of equations is

$$\begin{bmatrix} -5 & 4 & & & \\ 0.5 & -3 & 1.5 & & \\ & 0.75 & -3 & 1.25 & \\ & & \frac{5}{6} & -3 & \frac{7}{6} \\ & & & \frac{7}{8} & -3 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \\ T_5^{n+1} \end{bmatrix} = \begin{bmatrix} -T_1^n \\ -T_2^n \\ -T_3^n \\ -T_4^n \\ -T_5^n - \frac{2700}{8} \end{bmatrix}$$

$T_1 = T(0.0) = 150.81$ $\qquad$ $T_2 = T(0.1) = 158.06$
$T_3 = T(0.2) = 179.46$ $\qquad$ $T_4 = T(0.3) = 213.45$
$T_5 = T(0.4) = 256.06$
Distance (in cm) is measured from the centre.

9.3 Consider a sphere of radius 0.5 cm. Initially the temperature is uniform at 25°C. The temperature of the sphere surface is made 300°C at $t = 0$ s. Use implicit discretization and take $\Delta r = 0.1$ cm, $\Delta t = 0.1$ s, and $\alpha = 10^{-5}$ m^2/s. List the tridiagonal system of equations and determine the temperature at the centre and the intermediate points of the sphere after 5 s.

(**Ans:** The tridiagonal set of equations is

$$\begin{bmatrix} -7 & 6 & & & \\ 0 & -3 & 2 & & \\ & 0.5 & -3 & 1.5 & \\ & & \frac{2}{3} & -3 & \frac{4}{3} \\ & & & 0.75 & -3 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \\ T_5^{n+1} \end{bmatrix} = \begin{bmatrix} -T_1^n \\ -T_2^n \\ -T_3^n \\ -T_4^n \\ -T_5^n - \frac{1500}{4} \end{bmatrix}$$

$T_1 = T(0.0) = 200.21$ $\quad$ $T_2 = T(0.1) = 205.72$
$T_3 = T(0.2) = 221.68$ $\quad$ $T_4 = T(0.3) = 245.88$
$T_5 = T(0.4) = 274.07$
Distance (in cm) is measured from the centre.

9.4 Consider a concrete wall 0.5 m thick. Initially the temperature is uniform at 20°C. The temperature of one surface of the wall $x = 0$ is suddenly raised to 80°C and the right surface at $x = 0.5$ m remains always at 20°C. Use implicit discretization and take $\Delta x = 0.1$ m, $\Delta t = 10$ s, and $\alpha = 1.25 \times 10^{-5}$ m^2/s. List the tridiagonal system of equations and determine the temperature distribution throughout the slab after 1 h.

(**Ans:** The tridiagonal set of equations are

$$\begin{bmatrix} -1.025 & 0.0125 & & \\ 0.0125 & -1.025 & 0.0125 & \\ & 0.0125 & -1.025 & 0.0125 \\ & & 0.0125 & -1.025 \end{bmatrix} \begin{bmatrix} T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \\ T_5^{n+1} \end{bmatrix} = \begin{bmatrix} -T_2^n - 1.0 \\ -T_3^n \\ -T_4^n \\ -T_5^n - 0.25 \end{bmatrix}$$

$T_2 = T(0.1) = 64.06$ $\quad$ $T_3 = T(0.2) = 49.66$
$T_4 = T(0.3) = 37.70$ $\quad$ $T_5 = T(0.4) = 28.13$
Distance (in m) is measured from surface at 80°C.

9.5 A large flat slab of clay is to be dried. The slab is dried from both sides, is 4 cm thick and has an initial uniform water concentration of 0.5 g of water per cm^3. The movement of water within the clay occurs by diffusion. It is known that, with the proposed drying conditions, the drying will occur in the constant rate period at a rate of 0.1 g/cm^2-h of water as long as the surface moisture concentration remains above 0.2257 g of water per cm^3. Use implicit discretization and take $\Delta x = 0.2$ cm, $\Delta t = 0.01$ h, and $D = 0.25$ cm^2/h. List the tridiagonal system of equations and determine the duration of the constant rate period and the distribution of water within the clay at the end of the constant rate period. The partial differential equation is

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

and the boundary conditions are: at $x = 0$ (centre), $\frac{\partial C}{\partial x} = 0$ and at $x = 2$ cm,

$$-D\frac{\partial C}{\partial x} = 0.1$$

(**Ans:** The solution of the problem is obtained by calculating the time required for the surface concentration to fall to 0.2257 g/cm^3. This concentration is obtained at 1.5 h. The tridiagonal set of equations is

$$\begin{bmatrix} -1.125 & 0.125 & & & \\ 0.0625 & -1.125 & 0.0625 & & \\ & \dots & \dots & \dots & \\ & & 0.0625 & -1.125 & 0.0625 \\ & & & 0.125 & -1.125 \end{bmatrix} \begin{bmatrix} C_1^{n+1} \\ C_2^{n+1} \\ \dots \\ C_{10}^{n+1} \\ C_{11}^{n+1} \end{bmatrix} = \begin{bmatrix} -C_1^n \\ -C_2^n \\ \dots \\ -C_{10}^n \\ -C_{11}^n + 0.01 \end{bmatrix}$$

At $t = 1.5$ h:

$C_1 = C(0.0) = 0.4947$ $C_2 = C(0.2) = 0.4937$ $C_3 = C(0.4) = 0.4904$

$C_4 = C(0.6) = 0.4841$ $C_5 = C(0.8) = 0.4738$ $C_6 = C(1.0) = 0.4578$

$C_7 = C(1.2) = 0.4342$ $C_8 = C(1.4) = 0.4011$ $C_9 = C(1.6) = 0.3563$

$C_{10} = C(1.8) = 0.2983$ $C_{11} = C(2.0) = 0.2257$

Distance (in cm) is measured from the centre.

Chapter 10

Two-Dimensional Steady and Transient Heat Conduction

Two-dimensional steady heat conduction is given by

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \tag{10.1}$$

This is an elliptic partial differential equation and the temperature $T(x, y)$ must satisfy this equation as well as the boundary conditions along the entire boundary of the plate. Two-dimensional transient heat conduction is given by [see Eq. (9.26)]

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$

This is a parabolic partial differential equation. Relaxation techniques are used for the numerical solution of elliptic equations, whereas marching in time is used for parabolic equations. The numerical solution of two-dimensional steady heat conduction is carried out by the Gauss–Seidel, Red–Black Gauss–Seidel, and Alternating Direction Implicit (ADI) methods. The boundary conditions like convection, exterior corner with convection, interior corner with convection and insulation are discussed in this chapter. The numerical solution of two-dimensional transient heat conduction is discussed using ADI method, which is an implicit method and is therefore unconditionally stable. It is also called *line-by-line TDMA*.

10.1 Discretization in Two-Dimensional Space

Consider a two-dimensional body as shown in Fig. 10.1. Around each node a control volume is made. If there is no net accumulation of mass in the body, then the mass balance equation at a node can be interpreted as indicating that the net mass entering through all the four sides of the control volume is zero. The depth of the body in the z-direction may be taken to be unity. The temperature in the control volume is uniform and under steady conditions the heat input through all the sides of the control volume is zero. The heat inputs are given by terms like $-kA\frac{\partial T}{\partial x}$ and $-kA\frac{\partial T}{\partial y}$. Therefore the derivatives $\frac{\partial T}{\partial x}$ and $\frac{\partial T}{\partial y}$ have to be evaluated at the control volume boundaries. The temperature gradients around the control volume (i, j) may be written as

$$\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2},j} \approx \frac{T_{i+1,j} - T_{i,j}}{\Delta x} \tag{10.2}$$

$$\left.\frac{\partial T}{\partial x}\right|_{i-\frac{1}{2},j} \approx \frac{T_{i,j} - T_{i-1,j}}{\Delta x} \tag{10.3}$$

$$\left.\frac{\partial T}{\partial y}\right|_{i,j+\frac{1}{2}} \approx \frac{T_{i,j+1} - T_{i,j}}{\Delta y} \tag{10.4}$$

$$\left.\frac{\partial T}{\partial y}\right|_{i,j-\frac{1}{2}} \approx \frac{T_{i,j} - T_{i,j-1}}{\Delta y} \tag{10.5}$$

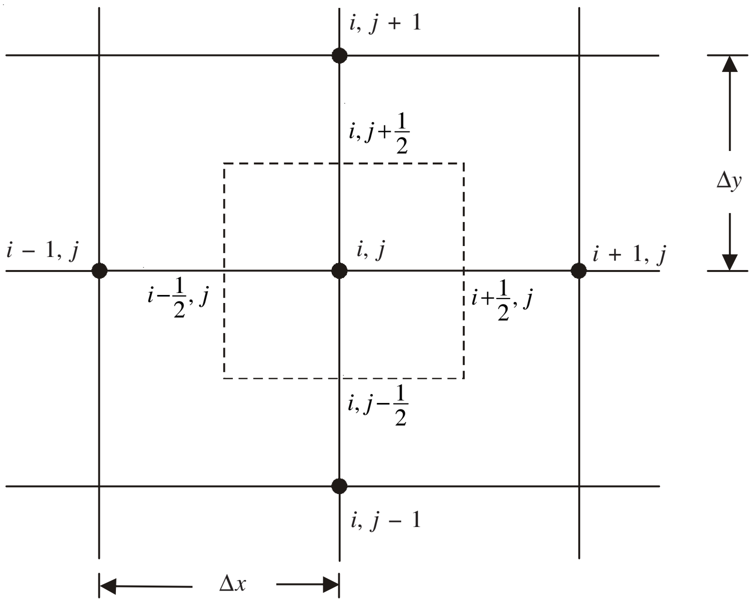


Fig. 10.1 Control volume around node.

The second derivatives may be written as

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_{i,j} \approx \frac{\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2},j} - \left.\frac{\partial T}{\partial x}\right|_{i-\frac{1}{2},j}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} = \frac{T_{i+1,j} - T_{i,j} - \left(T_{i,j} - T_{i-1,j}\right)}{\Delta x^2} = \frac{T_{i+1,j} + T_{i-1,j} - 2T_{i,j}}{\Delta x^2} \tag{10.6}$$

$$\left.\frac{\partial^2 T}{\partial y^2}\right|_{i,j} \approx \frac{\left.\frac{\partial T}{\partial y}\right|_{i,j+\frac{1}{2}} - \left.\frac{\partial T}{\partial y}\right|_{i,j-\frac{1}{2}}}{y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}} = \frac{T_{i,j+1} - T_{i,j} - \left(T_{i,j} - T_{i,j-1}\right)}{\Delta y^2} = \frac{T_{i,j+1} + T_{i,j-1} - 2T_{i,j}}{\Delta y^2} \tag{10.7}$$

Discretizing the equation $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$ for any interior node in which the source term is zero, we get

$$\frac{T_{i+1,j} + T_{i-1,j} - 2T_{i,j}}{\Delta x^2} + \frac{T_{i,j+1} + T_{i,j-1} - 2T_{i,j}}{\Delta y^2} = 0 \tag{10.8}$$

For $\Delta x = \Delta y$, we get

$$T_{i+1,j} + T_{i-1,j} - 2T_{i,j} + T_{i,j+1} + T_{i,j-1} - 2T_{i,j} = 0$$

or

$$T_{i,j} = \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}}{4} \tag{10.9}$$

10.2 Gauss-Seidel Method

In calculating $T_{i,j}$ the values of the temperatures on the right hand side of Eq. (10.9) consist initially of estimated values or known boundary values. However, as soon as an appropriate temperature at a node is calculated, this calculated value supersedes the estimated value and is used as the temperature at that point until it is, in turn, superseded by a new calculated value. Thus the latest calculated values of the temperatures are always used in calculating newer and better values.

Consider nodes in a two-dimensional space, with the bottom left node being (0,0) and the top right node being (10,10). Suppose that node (0,0) is updated first followed by node (1,0), (2,0),…, (10,0), (0,1), (1,1),…, (10,1), (0,2), (1,2),…, (10,2),…, (0,10), (1,10),…, (10,10). Then, by the time the value of $T_{i,j}$ is updated, the values $T_{i-1,j}$ and $T_{i,j-1}$ have already been updated. On using the Gauss–Seidel method, Eq. (10.9) becomes

$$T_{i,j}^{n+1} = \frac{T_{i+1,j}^{n} + T_{i-1,j}^{n+1} + T_{i,j+1}^{n} + T_{i,j-1}^{n+1}}{4} \tag{10.10}$$

10.3 Relaxation Parameter

The temperature taken at the beginning of an iteration is T^n and the new temperature computed during the iteration is T^{n+1}. Now, for the next iteration the temperature can be taken to be either T^{n+1}, between T^n and T^{n+1}, or more than T^{n+1}, and is given by

$$T^{n+1} = T^n + \omega \Delta T^{n+1} \tag{10.11}$$

The parameter ω is known as the *relaxation parameter*. The various cases are described in Table 10.1.

Table 10.1 Relaxation parameter values

Temperature taken at the beginning of iteration	New temperature computed during iteration	Temperature taken at the beginning of next iteration	Relaxation parameter	Type of Relaxation
100	110	110	1	Gauss–Seidel
100	110	105	0.5	Underrelaxation
100	110	115	1.5	Overrelaxation

The method is convergent only for $0 < \omega < 2$. For overrelaxation the relaxation parameter lies between 1 and 2 and for underrelaxation between 0 and 1. When $\omega = 1$, it becomes the Gauss–Seidel method. The optimum value of ω is different for each problem. It has to be determined by hit and trial.

10.4 Red–Black Gauss–Seidel Method

When the Gauss–Seidel method is used, the nodes are processed down the rows (or columns) or the mesh is divided into black and red nodes as shown in Fig. 10.2. This method for solution of elliptic PDE is Red–Black Gauss–Seidel. Both Gauss–Seidel and Red–Black Gauss–Seidel are pointwise methods. The Alternating Direction Implicit (ADI) method described in the next section is a line-by-line method.

R B R B R B R B R B R B R B R B
B R B R B R B R B R B R B R B R
R B R B R B R B **R** B R B R B R B
B R B R B R B **R B R** B R B R B R
R B R **B** R B R B **R** B R B R B R B
B R **B R B** R B R B R B R B R B R
R B R **B** R B R B R B R B R B R B
B R B R B R B R B R B R B R B R

Fig. 10.2 Red–black nodes in two-dimensional space.

The nodes surrounding the black node are all red and the nodes surrounding the red node are all black. The surrounding nodes are those nodes which are to the east, west, north and south of a node. The other four nodes are called the *corner nodes* of node (i, j). Consider again the finite difference equation (10.9):

$$T_{i,j} = \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}}{4}$$

Red points depend only on the black points and black points depend only on the red points. Thus we can carry out one half-sweep updating the red points and then another half-sweep updating the black points with the new red values. Thus, the Red–Black Gauss–Seidel method is the one in which the red nodes are updated using black nodes and then the black nodes are updated using the updated red nodes. This procedure is repeated till the following convergence criterion is satisfied: $\left|T_{i,j}^{n+1} - T_{i,j}^{n}\right| < \varepsilon$.

EXAMPLE 10.1 Determine the temperature at various nodes shown in Fig. 10.3. The two-dimensional heat transfer is given by the equation $\dfrac{\partial^2 T}{\partial x^2} + \dfrac{\partial^2 T}{\partial y^2} = 0$. The boundary conditions are shown in Fig. 10.3. The size of the slab is 2 m × 2 m and $\Delta x = \Delta y = 0.5$ m. Use the Gauss–Seidel method.

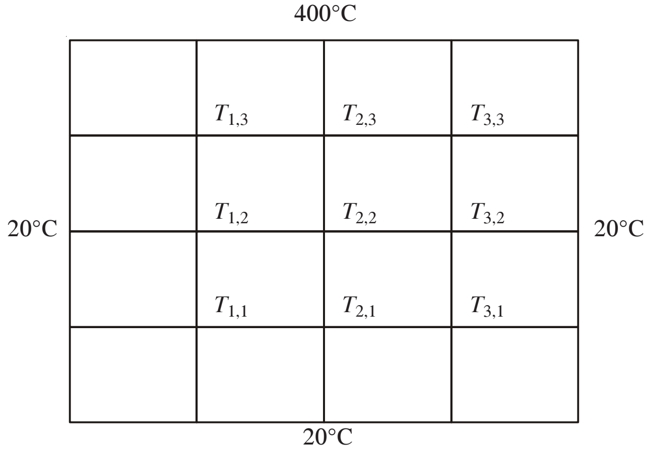


Fig. 10.3 Example 10.1

Solution Since all the nodes are interior nodes, therefore the discretized equation at node (*i*, *j*) is given by

$$T_{i,j} = \frac{T_{i-1,j} + T_{i+1,j} + T_{i,j+1} + T_{i,j-1}}{4}$$

Thus

$$T_{1,1}^{n+1} = \frac{20 + T_{1,2}^{n} + T_{2,1}^{n} + 20}{4}$$

$$T_{1,2}^{n+1} = \frac{T_{1,1}^{n+1} + T_{1,3}^{n} + T_{2,2}^{n} + 20}{4}$$

$$T_{1,3}^{n+1} = \frac{T_{1,2}^{n+1} + T_{2,3}^{n} + 400 + 20}{4}$$

$$T_{2,1}^{n+1} = \frac{T_{1,1}^{n+1} + T_{2,2}^{n} + T_{3,1}^{n} + 20}{4}$$

$$T_{2,2}^{n+1} = \frac{T_{1,2}^{n+1} + T_{2,1}^{n+1} + T_{2,3}^{n} + T_{3,2}^{n}}{4}$$

$$T_{2,3}^{n+1} = \frac{T_{1,3}^{n+1} + T_{2,2}^{n+1} + T_{3,3}^{n} + 400}{4}$$

$$T_{3,1}^{n+1} = \frac{20 + T_{2,1}^{n+1} + T_{3,2}^{n} + 20}{4}$$

$$T_{3,2}^{n+1} = \frac{T_{2,2}^{n+1} + T_{3,1}^{n+1} + T_{3,3}^{n} + 20}{4}$$

$$T_{3,3}^{n+1} = \frac{400 + T_{3,2}^{n+1} + T_{2,3}^{n+1} + 20}{4}$$

Note that the coefficient of the term on the left hand side is the highest among all the other coefficients in the linear algebraic equation. That is why convergence is obtained when the Gauss–Seidel method is used for solving the above set of linear algebraic equations. To start the iteration, some initial values of all the nine variables are assumed and thereafter their latest values are used to update the solution. The iterations are performed till there is no change in the value of temperature $\left|T_{i,j}^{n+1} - T_{i,j}^{n}\right| < \varepsilon$. Program 10.1 for the solution of the above problem is given in the Appendix. The converged solution is

$T_{1,1} = 47.14 \qquad T_{2,1} = 57.32 \qquad T_{3,1} = 47.14$

$T_{1,2} = 91.25 \qquad T_{2,2} = 115.00 \qquad T_{3,2} = 91.25$

$T_{1,3} = 182.86 \qquad T_{2,3} = 220.18 \qquad T_{3,3} = 182.86$

EXAMPLE 10.2 Consider the following body in which the inner face is at 200°C and the outer face is at 100°C. The body is very long so that heat transfer takes place in two dimensions only. The thermal conductivity of the body is 1.21 W/m-K. The dimensions of the body are shown in Fig. 10.4. Take $\Delta x = \Delta y = \frac{1}{2}$ m.

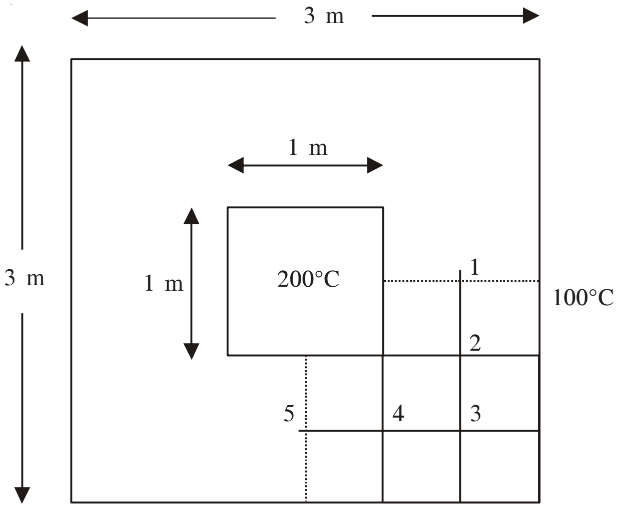


Fig. 10.4 Example 10.2.

Using the Gauss–Seidel method, solve for the temperatures at nodes 1 to 5.

Solution Since there is no source term, we get

$$T_1^{n+1} = \frac{2T_2^n + 300}{4}$$

$$T_2^{n+1} = \frac{T_1^{n+1} + T_3^n + 300}{4}$$

$$T_3^{n+1} = \frac{T_2^{n+1} + T_4^n + 200}{4}$$

$$T_4^{n+1} = \frac{T_3^{n+1} + T_5^n + 300}{4}$$

$$T_5^{n+1} = \frac{2T_4^{n+1} + 300}{4}$$

On modifying the Program 10.1, the following solution is obtained: T_1 = 145.83°C, T_2 = 141.67°C, T_3 = 120.83°C, T_4 = 141.67°C, T_5 = 145.83°C.

EXAMPLE 10.3 Determine the temperature at various nodes shown in Fig. 10.5. The heat transfer is given by the equation $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$. The boundary conditions are shown in the figure. The size of the slab is 2 m × 2 m and $\Delta x = \Delta y = 0.5$ m. Use the Red–Black Gauss–Seidel method.

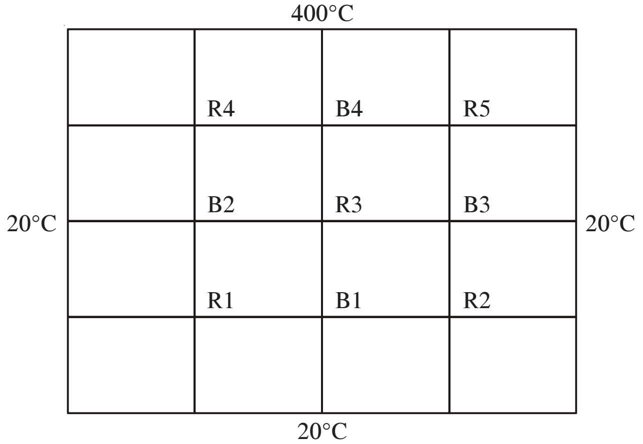


Fig. 10.5 Example 10.3.

Solution Before starting the iterations the following initial values of temperatures at the black nodes are assumed: $B1$ = 55, $B2$ = 90, $B3$ = 90, $B4$ = 220°C. Now we compute values at the red nodes using the assumed values at the black nodes.

$$R1 = \frac{90 + 20 + 20 + 55}{4} = \frac{185}{4} = 46.25°\text{C}$$

$$R2 = \frac{55 + 20 + 90 + 20}{4} = \frac{185}{4} = 46.25°\text{C}$$

$$R3 = \frac{90 + 90 + 220 + 55}{4} = \frac{455}{4} = 113.75°\text{C}$$

$$R4 = \frac{20 + 220 + 400 + 90}{4} = \frac{730}{4} = 182.5°\text{C}$$

$$R5 = \frac{400 + 90 + 220 + 20}{4} = \frac{730}{4} = 182.5°\text{C}$$

Now let us update the black node values using the updated values at the red nodes.

$$B1 = \frac{113.75 + 20 + 46.25 + 46.25}{4} = 56.5625°\text{C}$$

$$B2 = \frac{113.75 + 20 + 182.5 + 46.25}{4} = 90.625°\text{C}$$

$$B3 = \frac{113.75 + 20 + 46.25 + 182.5}{4} = 90.625°\text{C}$$

$$B4 = \frac{113.75 + 400 + 182.5 + 182.5}{4} = 219.6875°\text{C}$$

Updating the red nodes using the updated black node values, we get: $R1$ = 46.80, $R2$ = 46.80, $R3$ = 114.375, $R4$ = 182.578, $R5$ = 182.578°C. Updating the black nodes using updated red node values, we get: $B1$ = 56.994, $B2$ = 90.938, $B3$ = 90.938, $B4$ = 219.88°C. Note that even after two iterations the temperatures are close to the converged values obtained using the Gauss–Seidel method in Example 10.1. The iterations are performed till there is no change in the value of temperature, $\left|T_{i,j}^{n+1} - T_{i,j}^{n}\right| < \varepsilon$.

EXAMPLE 10.4 Discretize the equation $\dfrac{\partial^2 T}{\partial x^2} + \dfrac{\partial^2 T}{\partial y^2} = 0$ at node (i, j) of a convection boundary as shown in Fig. 10.6.

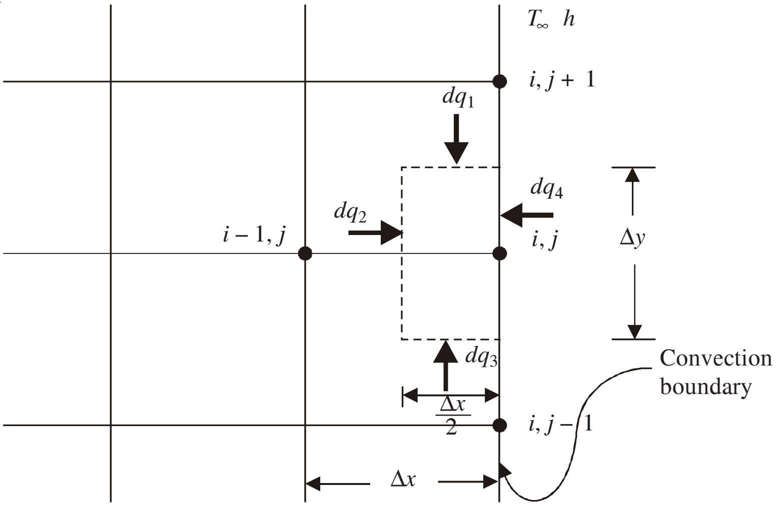


Fig. 10.6 Convection boundary condition.

Solution The given differential equation is at steady state and therefore in the control volume around node (i, j), the summation of $\dot{q}$ entering the control volume from all the four sides is zero. From the left and right sides, $\frac{dq}{dt} = -kA\frac{\partial T}{\partial x}$, and from top and bottom, $\frac{dq}{dt} = -kA\frac{\partial T}{\partial y}$. To determine the area for heat transfer into the control volume, the depth is taken to be unity. The various energy inputs into the control volume around node (i, j) are

$$\frac{dq_1}{dt} = -k\frac{\Delta x}{2}\left(\frac{T_{i,j} - T_{i,j+1}}{\Delta y}\right)$$

$$\frac{dq_2}{dt} = -k\Delta y\left(\frac{T_{i,j} - T_{i-1,j}}{\Delta x}\right)$$

$$\frac{dq_3}{dt} = -k\frac{\Delta x}{2}\left(\frac{T_{i,j} - T_{i,j-1}}{\Delta y}\right)$$

$$\frac{dq_4}{dt} = h\Delta y\left(T_\infty - T_{i,j}\right)$$

Thus, from the energy balance at node (i, j), we get

$$\frac{dq_1}{dt} + \frac{dq_2}{dt} + \frac{dq_3}{dt} + \frac{dq_4}{dt} = 0$$

Thus

$$-k\frac{\Delta x}{2}\left(\frac{T_{i,j} - T_{i,j+1}}{\Delta y}\right) - k\Delta y\left(\frac{T_{i,j} - T_{i-1,j}}{\Delta x}\right) - k\frac{\Delta x}{2}\left(\frac{T_{i,j} - T_{i,j-1}}{\Delta y}\right) = h\Delta y\left(T_{i,j} - T_\infty\right)$$

where T_∞ is the free stream temperature of the surrounding fluid and h is the convective heat transfer coefficient between the convection boundary surface and fluid.

If $\Delta x = \Delta y$, the equation becomes

$$\frac{k}{2}\left(T_{i,j} - T_{i,j+1}\right) + k\left(T_{i,j} - T_{i-1,j}\right) + \frac{k}{2}\left(T_{i,j} - T_{i,j-1}\right) = -h\Delta x\left(T_{i,j} - T_\infty\right)$$

Collecting the terms of $T_{i,j}$ on one side and the rest of the terms on the other side, we get

$$T_{i,j} = \frac{T_{i-1,j} + 0.5\left(T_{i,j+1} + T_{i,j-1}\right) + BiT_\infty}{Bi + 2}$$

where the Biot number is given by

$$Bi = \frac{h\Delta x}{k}$$

An equation of this type is applicable for each node along the convection boundary surface.

EXAMPLE 10.5 Discretize the equation $\dfrac{\partial^2 T}{\partial x^2}+\dfrac{\partial^2 T}{\partial y^2}=0$ at node (*i*, *j*) of an exterior corner with convection boundary condition as shown in Fig. 10.7.

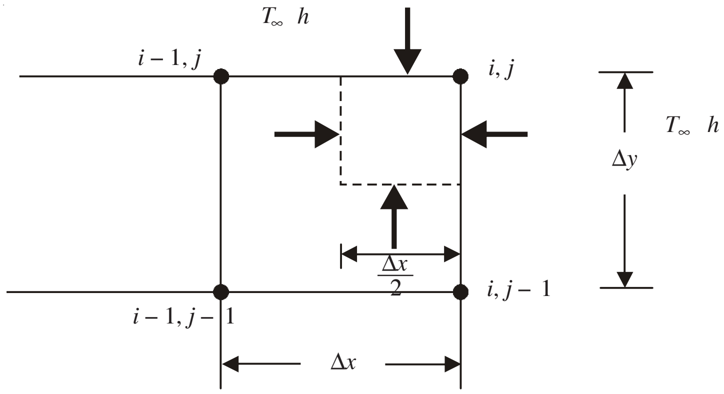


Fig. 10.7 Exterior corner with convection boundary condition.

Solution From the energy balance at node (*i*, *j*), we get

$$-k\frac{\Delta y}{2}\left(\frac{T_{i,j}-T_{i-1,j}}{\Delta x}\right)-k\frac{\Delta x}{2}\left(\frac{T_{i,j}-T_{i,j-1}}{\Delta y}\right)=h\frac{\Delta x}{2}\left(T_{i,j}-T_\infty\right)+h\frac{\Delta y}{2}\left(T_{i,j}-T_\infty\right)$$

where T_∞ is the free stream temperature of the surrounding fluid and h is the convective heat transfer coefficient between the convection boundary surface and the fluid. If $\Delta x = \Delta y$, the equation becomes

$$-\frac{k}{2}\left(T_{i,j}-T_{i-1,j}\right)-\frac{k}{2}\left(T_{i,j}-T_{i,j-1}\right)=h\Delta x\left(T_{i,j}-T_\infty\right)$$

Collecting the terms of $T_{i,j}$ on one side and the rest of the terms on the other side, we get

$$T_{i,j}=\frac{0.5\left(T_{i-1,j}+T_{i,j-1}\right)+BiT_\infty}{Bi+1}$$

EXAMPLE 10.6 Discretize the equation $\dfrac{\partial^2 T}{\partial x^2}+\dfrac{\partial^2 T}{\partial y^2}=0$ at node (*i*, *j*) of an interior corner with the convection boundary condition as shown in Fig. 10.8.

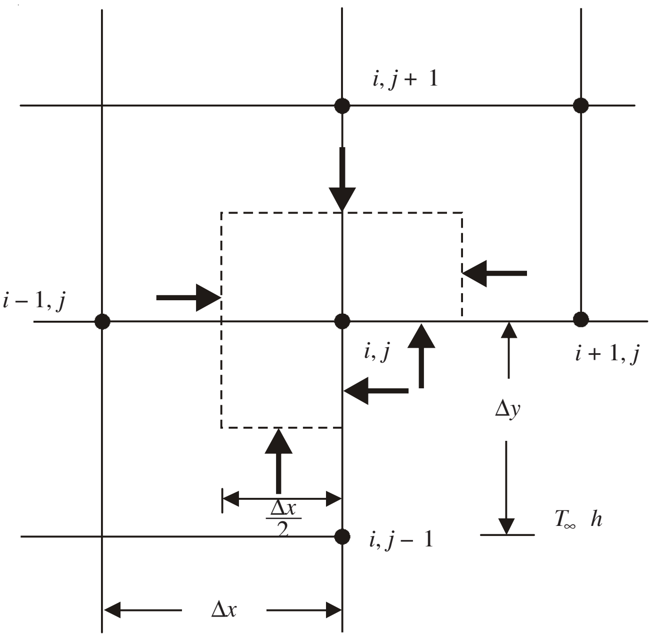


Fig. 10.8 Interior corner with convection boundary condition.

Solution From the energy balance at node (*i*, *j*), we get

$$-k\frac{\Delta y}{2}\left(\frac{T_{i,j}-T_{i+1,j}}{\Delta x}\right)-k\Delta x\left(\frac{T_{i,j}-T_{i,j+1}}{\Delta y}\right)-k\Delta y\left(\frac{T_{i,j}-T_{i-1,j}}{\Delta x}\right)-k\frac{\Delta x}{2}\left(\frac{T_{i,j}-T_{i,j-1}}{\Delta y}\right)$$

$$=h\frac{\Delta x}{2}\left(T_{i,j}-T_\infty\right)+h\frac{\Delta y}{2}\left(T_{i,j}-T_\infty\right)$$

where T_∞ is the free stream temperature of the surrounding fluid and h is the convective heat transfer coefficient between the convection boundary surface and the fluid. Taking $\Delta x = \Delta y$ and dividing by k, we get

$$\frac{1}{2}\left(T_{i,j}-T_{i+1,j}\right)+\frac{1}{2}\left(T_{i,j}-T_{i,j-1}\right)+T_{i,j}-T_{i,j+1}+T_{i,j}-T_{i-1,j}=-Bi\left(T_{i,j}-T_\infty\right)$$

Collecting the terms of $T_{i,j}$ on one side and the rest of the terms on the other side, we get

$$T_{i,j}=\frac{T_{i,j+1}+T_{i-1,j}+0.5\left(T_{i+1,j}+T_{i,j-1}\right)+BiT_\infty}{Bi+3}$$

EXAMPLE 10.7 Discretize the equation $\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=0$ at node (*i*, *j*) of an insulation boundary as shown in Fig. 10.9.

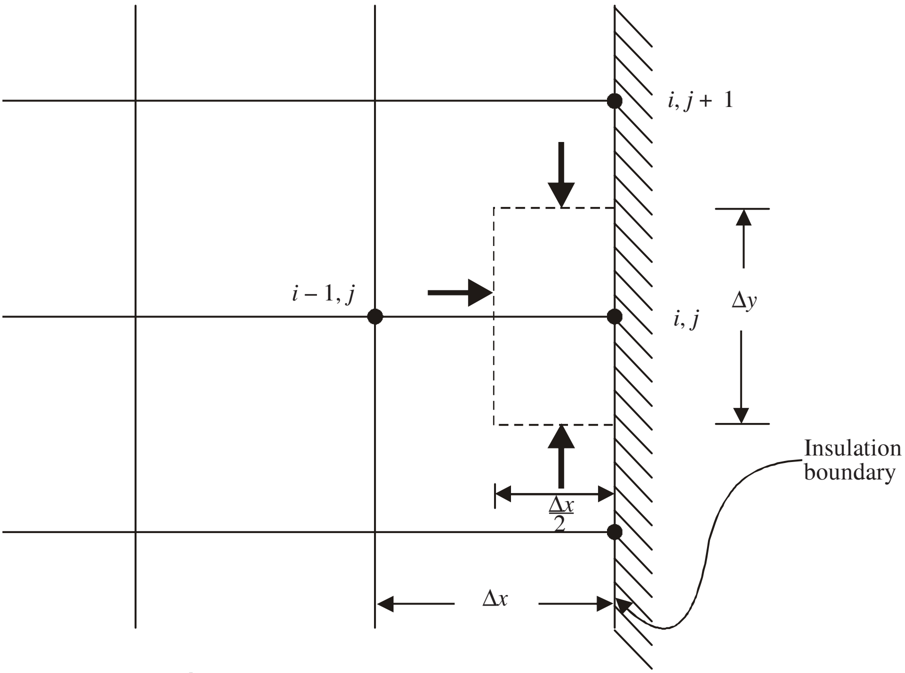


Fig. 10.9 Insulation boundary condition.

Solution The given differential equation is at steady state and therefore in the control volume around node (i, j) the summation of $\dot{q}$ entering the control volume from all the three sides is zero. There is no heat flux across the insulation boundary. From the energy balance at node (i, j), we get

$$-k\frac{\Delta x}{2}\left(\frac{T_{i,j}-T_{i,j+1}}{\Delta y}\right)-k\Delta y\left(\frac{T_{i,j}-T_{i-1,j}}{\Delta x}\right)-k\frac{\Delta x}{2}\left(\frac{T_{i,j}-T_{i,j-1}}{\Delta y}\right)=0$$

If $\Delta x = \Delta y$, the equation becomes

$$\frac{1}{2}\left(T_{i,j}-T_{i,j+1}\right)+T_{i,j}-T_{i-1,j}+\frac{1}{2}\left(T_{i,j}-T_{i,j-1}\right)=0$$

Collecting the terms of $T_{i,j}$ on one side and the rest of the terms on the other side, we get

$$T_{i,j}=\frac{2T_{i-1,j}+T_{i,j+1}+T_{i,j-1}}{4}$$

Note that the insulation boundary equation is obtained by setting $h = 0$ in the equation for convection boundary.

EXAMPLE 10.8 Determine the temperature at various nodes shown in Fig. 10.10. The steady heat transfer is given by the equation $\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=0$. The left face is maintained at

100°C and the top face at 500°C, while the other two faces are exposed to an environment at 100°C. The convective heat transfer coefficient between the right and bottom walls to the surrounding fluid is 10 W/m^2-K. The block is 1 m × 1 m. Use the Gauss–Seidel method.

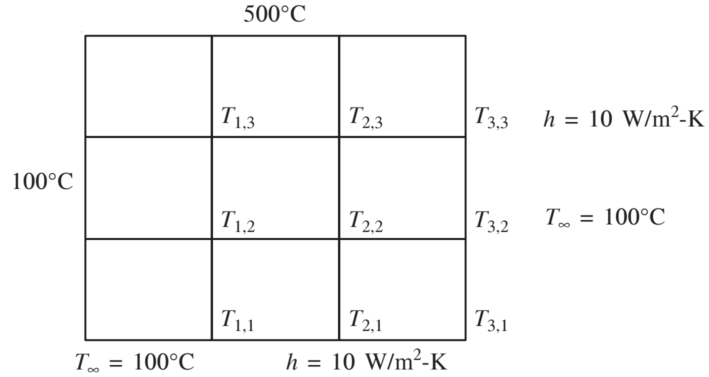


Fig. 10.10 Example 10.8.

Solution $\Delta x = \Delta y = \frac{1}{3}$ m.

At the interior nodes the discretized equation is

$$T_{i,j} = \frac{T_{i-1,j} + T_{i+1,j} + T_{i,j+1} + T_{i,j-1}}{4}$$

At nodes $T_{1,1}$, $T_{2,1}$, $T_{3,2}$, and $T_{3,3}$ the convection boundary condition exists, and at node $T_{3,1}$ the exterior corner convection boundary condition exists. These convection boundary conditions have been described in previous examples. Thus the following nodal equations are obtained:

$$T_{1,1}^{n+1} = \frac{T_{1,2}^{n} + 0.5\left(100 + T_{2,1}^{n}\right) + \frac{100}{3}}{2 + \frac{1}{3}}$$

$$T_{1,2}^{n+1} = \frac{T_{1,1}^{n+1} + T_{1,3}^{n} + 100 + T_{2,2}^{n}}{4}$$

$$T_{1,3}^{n+1} = \frac{500 + T_{1,2}^{n+1} + 100 + T_{2,3}^{n}}{4}$$

$$T_{2,1}^{n+1} = \frac{T_{2,2}^{n} + 0.5\left(T_{3,1}^{n} + T_{1,1}^{n+1}\right) + \frac{100}{3}}{2 + \frac{1}{3}}$$

$$T_{2,2}^{n+1} = \frac{T_{2,1}^{n+1} + T_{2,3}^{n} + T_{1,2}^{n+1} + T_{3,2}^{n}}{4}$$

$$T_{2,3}^{n+1} = \frac{500 + T_{2,2}^{n+1} + T_{1,3}^{n+1} + T_{3,3}^{n}}{4}$$

$$T_{3,1}^{n+1} = \frac{0.5\left(T_{3,2}^{n} + T_{2,1}^{n+1}\right) + \frac{100}{3}}{1 + \frac{1}{3}}$$

$$T_{3,2}^{n+1} = \frac{T_{2,2}^{n+1} + 0.5\left(T_{3,1}^{n+1} + T_{3,3}^{n}\right) + \frac{100}{3}}{2 + \frac{1}{3}}$$

$$T_{3,3}^{n+1} = \frac{T_{2,3}^{n+1} + 0.5\left(T_{3,2}^{n+1} + 500\right) + \frac{100}{3}}{2 + \frac{1}{3}}$$

Note that the coefficient of the term on the left hand side is the highest among all the other coefficients in the linear algebraic equation and that is why convergence is obtained when the Gauss–Seidel method is used. To start the iteration, some initial values of all the nine variables are assumed and thereafter their latest values are used to update the solution. The iterations are performed till there is no change in the value of the temperature at the given node, that is, $\left|T_{i,j}^{n+1} - T_{i,j}^{n}\right| < \varepsilon$. Program 10.1 can be modified for the solution of this problem. The converged solution is (all T in °C)

$T_{1,1} = 157.68$ $\quad T_{2,1} = 184.51$ $\quad T_{3,1} = 175.32$
$T_{1,2} = 192.34$ $\quad T_{2,2} = 231.03$ $\quad T_{3,2} = 217.01$
$T_{1,3} = 280.65$ $\quad T_{2,3} = 330.25$ $\quad T_{3,3} = 309.32$

EXAMPLE 10.9 For the *L*-shaped body shown in Fig. 10.11, determine the temperatures at nodes 1 to 9. Steady heat conduction takes place in the body, $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$. The left surface is insulated and the bottom surface is at a uniform temperature of 90°C. The entire top surface is subjected to convection to ambient air at 25°C. The heat transfer coefficient between the top surface and the ambient air is 75 W/m^2-K. The right surface is subjected to uniform heat flux of 4500 W/m^2. $\Delta x = \Delta y = 1$ cm. The thermal conductivity of the body, $k = 15$ W/m-K.

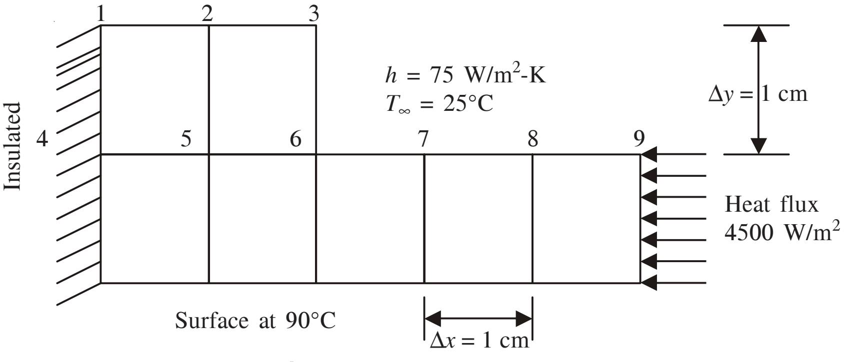


Fig. 10.11 Example 10.9.

Solution Equation for node 1:

$$-k\frac{\Delta x}{2}\left(\frac{T_1 - T_4}{\Delta y}\right) - k\frac{\Delta y}{2}\left(\frac{T_1 - T_2}{\Delta x}\right) = h\frac{\Delta x}{2}\left(T_1 - T_\infty\right)$$

$$-k\left(T_1 - T_4\right) - k\left(T_1 - T_2\right) = h\Delta x\left(T_1 - T_\infty\right)$$

$$T_1 - T_4 + T_1 - T_2 + \frac{h\Delta x}{k}\left(T_1 - T_\infty\right) = 0$$

where $\frac{h\Delta x}{k} = \frac{75 \times 0.01}{15} = 0.05$.
Thus the equation for node 1 becomes

$$2.05T_1 - T_2 - T_4 + 0.05\left(-T_\infty\right) = 0$$

The coefficient of T_1 is the highest; therefore

$$T_1 = \frac{T_2 + T_4 + 1.25}{2.05}$$

Equation for node 2:

$$-k\frac{\Delta y}{2}\left(\frac{T_2 - T_1}{\Delta x}\right) - k\frac{\Delta y}{2}\left(\frac{T_2 - T_3}{\Delta x}\right) - k\Delta x\left(\frac{T_2 - T_5}{\Delta y}\right) = h\Delta x\left(T_2 - T_\infty\right)$$

$$\frac{1}{2}\left(T_2 - T_1\right) + \frac{1}{2}\left(T_2 - T_3\right) + \left(T_2 - T_5\right) = \frac{h\Delta x}{k}\left(T_\infty - T_2\right)$$

$$T_2 = \frac{0.5\left(T_1 + T_3\right) + T_5 + 1.25}{2.05}$$

Equation for node 3:

$$-k\frac{\Delta y}{2}\left(\frac{T_3 - T_2}{\Delta x}\right) - k\frac{\Delta x}{2}\left(\frac{T_3 - T_6}{\Delta y}\right) = h\frac{\Delta x}{2}\left(T_3 - T_\infty\right) + h\frac{\Delta y}{2}\left(T_3 - T_\infty\right)$$

$$\frac{T_3 - T_2}{2} + \frac{T_3 - T_6}{2} = \frac{h\Delta x}{k}\left(T_\infty - T_3\right)$$

$$T_3 = \frac{0.5\left(T_2 + T_6\right) + 1.25}{1.05}$$

Equation for node 4:

$$-k\frac{\Delta x}{2}\left(\frac{T_4 - T_1}{\Delta y}\right) - k\frac{\Delta x}{2}\left(\frac{T_4 - 90}{\Delta y}\right) - k\Delta y\left(\frac{T_4 - T_5}{\Delta x}\right) = 0$$

$$\frac{T_4 - T_1}{2} + \frac{T_4 - 90}{2} + T_4 - T_5 = 0$$

$$T_4 = \frac{T_5 + 0.5T_1 + 45}{2}$$

Equation for node 5:

$$-k\Delta y\left(\frac{T_5 - T_4}{\Delta x}\right) - k\Delta y\left(\frac{T_5 - T_6}{\Delta x}\right) - k\Delta x\left(\frac{T_5 - T_2}{\Delta y}\right) - k\Delta x\left(\frac{T_5 - T_{11}}{\Delta y}\right) = 0$$

$$T_5 = \frac{T_4 + T_6 + T_2 + 90}{4}$$

Equation for node 6:

$$-k\frac{\Delta x}{2}\left(\frac{T_6 - T_3}{\Delta y}\right) - k\Delta y\left(\frac{T_6 - T_5}{\Delta x}\right) - k\Delta x\left(\frac{T_6 - T_{12}}{\Delta y}\right) - k\frac{\Delta y}{2}\left(\frac{T_6 - T_7}{\Delta x}\right)$$

$$= h\frac{\Delta x}{2}\left(T_6 - T_\infty\right) + h\frac{\Delta y}{2}\left(T_6 - T_\infty\right)$$

$$\frac{T_6 - T_3}{2} + T_6 - T_5 + T_6 - T_{12} + \frac{T_6 - T_7}{2} = \frac{h\Delta x}{k}\left(T_\infty - T_6\right)$$

$$T_6 = \frac{T_5 + 90 + 0.5\left(T_3 + T_7\right) + 1.25}{3.05}$$

Equation for node 7:

$$-k\frac{\Delta y}{2}\left(\frac{T_7 - T_6}{\Delta x}\right) - k\frac{\Delta y}{2}\left(\frac{T_7 - T_8}{\Delta x}\right) - k\Delta x\left(\frac{T_7 - 90}{\Delta y}\right) = h\Delta x\left(T_7 - T_\infty\right)$$

$$\frac{1}{2}\left(T_7 - T_6\right) + \frac{1}{2}\left(T_7 - T_8\right) + \left(T_7 - 90\right) = \frac{h\Delta x}{k}\left(T_\infty - T_7\right)$$

$$T_7 = \frac{0.5\left(T_6 + T_8\right) + 90 + 1.25}{2.05}$$

Equation for node 8:

$$-k\frac{\Delta y}{2}\left(\frac{T_8 - T_7}{\Delta x}\right) - k\frac{\Delta y}{2}\left(\frac{T_8 - T_9}{\Delta x}\right) - k\Delta x\left(\frac{T_8 - 90}{\Delta y}\right) = h\Delta x\left(T_8 - T_\infty\right)$$

$$\frac{1}{2}\left(T_8 - T_7\right) + \frac{1}{2}\left(T_8 - T_9\right) + \left(T_8 - 90\right) = \frac{h\Delta x}{k}\left(T_\infty - T_8\right)$$

$$T_8 = \frac{0.5\left(T_7 + T_9\right) + 90 + 1.25}{2.05}$$

Equation for node 9:

$$-k\frac{\Delta y}{2}\left(\frac{T_9 - T_8}{\Delta x}\right) - k\frac{\Delta x}{2}\left(\frac{T_9 - 90}{\Delta y}\right) + 4500\frac{\Delta y}{2} = h\frac{\Delta x}{2}\left(T_9 - T_\infty\right)$$

$$\frac{1}{2}\left(T_9 - T_8\right) + \frac{1}{2}\left(T_9 - 90\right) - \frac{4500}{15}\frac{\Delta y}{2} = \frac{h\Delta x}{2k}\left(T_\infty - T_9\right)$$

$$T_9 = \frac{0.5T_8 + 47.125}{1.025}$$

Program 10.1 can be modified for the solution of this problem. The converged solution is: $T_1 = 83.19$, $T_2 = 82.86$, $T_3 = 81.49$, $T_4 = 86.43$, $T_5 = 86.27$, $T_6 = 85.78$, $T_7 = 86.72$, $T_8 = 87.26$, and $T_9 = 88.54$°C.

10.5 ADI Method for Steady Heat Conduction

The Alternating Direction Implicit (ADI) method can also be applied for the solution of the two-dimensional steady heat conduction equation (10.1)

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Using the central difference scheme, we get

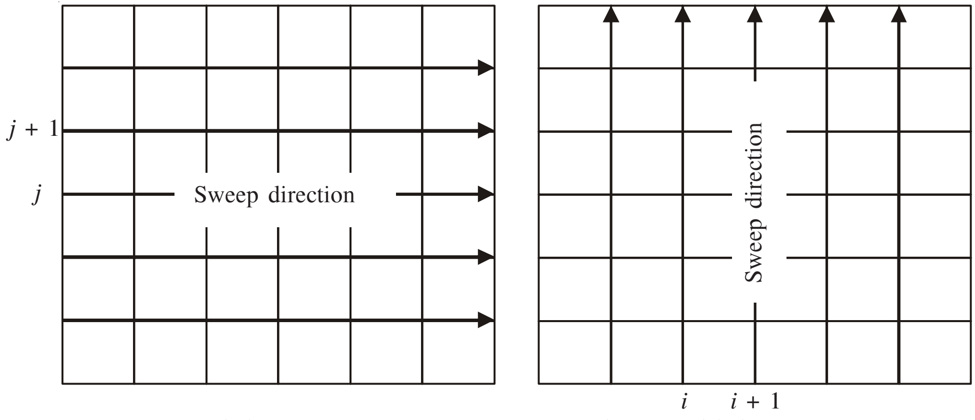
$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} = 0 \qquad \text{[see Eq. (10.8)]}$$

This equation can be split into the following two half-steps:

$$\frac{T_{i+1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} = -\left(\frac{T_{i,j+1}^{n} - 2T_{i,j}^{n} + T_{i,j-1}^{n}}{\Delta y^2}\right) \tag{10.12}$$

$$\frac{T_{i,j+1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j-1}^{n+1}}{\Delta y^2} = -\left(\frac{T_{i+1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right) \tag{10.13}$$

The first half-step is executed on all the nodes. This is followed by computation of the second half- step on all the nodes (see Fig. 10.12). The ADI method is also called the *line-by-line*



(a) First half-step of iteration (b) Second half-step of iteration

Fig. 10.12 First half-step and second half-step in ADI iteration.

TDMA, as in each line of nodes taken a tridiagonal set of linear algebraic equations is formed. TDMA can be used to solve them, and thus the values of nodes along a line are updated. Initially, Eq. (10.12) is considered for the first half of iteration, in which the sweep direction is along the x-axis and each line of nodes along the x-axis is updated. Then Eq. (10.13) is considered for the second half of iteration, in which the sweep direction is along the y-axis and each line of nodes along the y-axis is updated. The iterations are performed till convergence in temperature is achieved, $\left|T_{i,j}^{n+1} - T_{i,j}^{n}\right| < \varepsilon$. ADI is a *line-by-line* method, whereas Gauss–Seidel is a pointwise method.

EXAMPLE 10.10 Determine the temperature at various nodes shown in Fig. 10.13. The heat transfer is given by the equation $\dfrac{\partial^2 T}{\partial x^2} + \dfrac{\partial^2 T}{\partial y^2} = 0$. The boundary conditions are shown in Fig. 10.13. The size of the slab is 2 m × 2 m and $\Delta x = \Delta y = 0.5$ m. Use the ADI method.

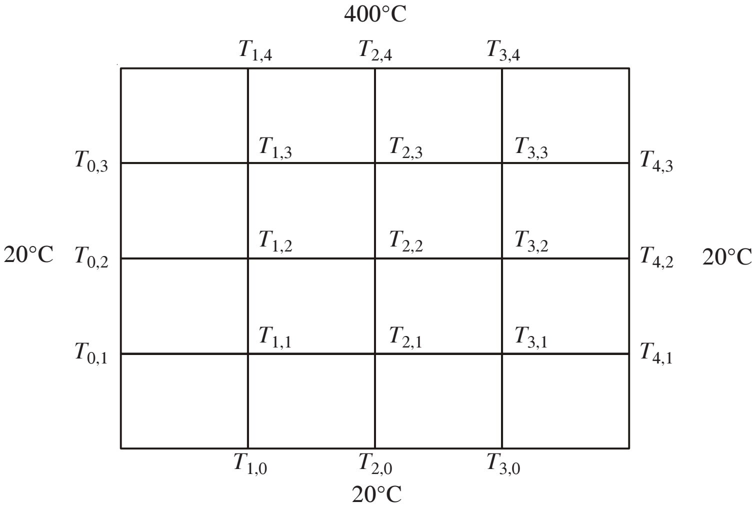


Fig. 10.13 Example 10.10.

Solution The first half iteration is performed (scanning various i nodes for given j) using the discretized equation

$$\frac{T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j+1}^{n} + T_{i,j-1}^{n} - 2T_{i,j}^{n}}{\Delta y^2} = 0$$

Since $\Delta x = \Delta y$, the discretized equation becomes

$$T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 4T_{i,j}^{n+\frac{1}{2}} = -T_{i,j+1}^{n} - T_{i,j-1}^{n}$$

At node 1,1

$$T_{2,1}^{n+\frac{1}{2}} + T_{0,1}^{n+\frac{1}{2}} - 4T_{1,1}^{n+\frac{1}{2}} = -T_{1,2}^{n} - T_{1,0}^{n}$$

Let us assume the following initial temperatures: $T_{1,2}$ = 90, $T_{2,2}$ = 110, $T_{3,2}$ = 90. Since $T_{0,1}$ is always at 20°C, the above equation becomes

$$-4T_{1,1}^{n+\frac{1}{2}} + T_{2,1}^{n+\frac{1}{2}} = -T_{0,1}^{n+\frac{1}{2}} - T_{1,2}^{n} - T_{1,0}^{n} = -20 - 90 - 20 = -130$$

At node 2,1

$$T_{3,1}^{n+\frac{1}{2}} + T_{1,1}^{n+\frac{1}{2}} - 4T_{2,1}^{n+\frac{1}{2}} = -T_{2,2}^{n} - T_{2,0}^{n}$$

$$T_{1,1}^{n+\frac{1}{2}} - 4T_{2,1}^{n+\frac{1}{2}} + T_{3,1}^{n+\frac{1}{2}} = -T_{2,2}^{n} - T_{2,0}^{n} = -110 - 20 = -130$$

At node 3,1

$$T_{4,1}^{n+\frac{1}{2}} + T_{2,1}^{n+\frac{1}{2}} - 4T_{3,1}^{n+\frac{1}{2}} = -T_{3,2}^{n} - T_{3,0}^{n}$$

$$T_{2,1}^{n+\frac{1}{2}} - 4T_{3,1}^{n+\frac{1}{2}} = -T_{4,1}^{n+\frac{1}{2}} - T_{3,2}^{n} - T_{3,0}^{n}$$

Since $T_{4,1}$ is always at 20°C, the above equation becomes

$$T_{2,1}^{n+\frac{1}{2}} - 4T_{3,1}^{n+\frac{1}{2}} = -T_{4,1}^{n+\frac{1}{2}} - T_{3,2}^{n} - T_{3,0}^{n} = -20 - 90 - 20 = -130$$

The following tridiagonal set of linear algebraic equations is obtained for various i nodes at j = 1

$$\begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_{1,1}^{n+\frac{1}{2}} \\ T_{2,1}^{n+\frac{1}{2}} \\ T_{3,1}^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} -130 \\ -130 \\ -130 \end{bmatrix}$$

The solution by TDMA is $T_{1,1}^{n+\frac{1}{2}}$ = 46.43, $T_{2,1}^{n+\frac{1}{2}}$ = 55.71, $T_{3,1}^{n+\frac{1}{2}}$ = 46.43°C.

Now let us write the equations for various i nodes at j = 2.

At node 1,2

$$T_{2,2}^{n+\frac{1}{2}} + T_{0,2}^{n+\frac{1}{2}} - 4T_{1,2}^{n+\frac{1}{2}} = -T_{1,3}^{n} - T_{1,1}^{n}$$

Let us assume the following initial temperatures: $T_{1,3}$ = 180, $T_{2,3}$ = 220, $T_{3,3}$ = 180. Since $T_{0,2}$ is always at 20°C, the above equation becomes

$$-4T_{1,2}^{n+\frac{1}{2}} + T_{2,2}^{n+\frac{1}{2}} = -T_{0,2}^{n+\frac{1}{2}} - T_{1,3}^{n} - T_{1,1}^{n} = -20 - 180 - 46.43 = -246.43$$

At node 2,2

$$T_{3,2}^{n+\frac{1}{2}} + T_{1,2}^{n+\frac{1}{2}} - 4T_{2,2}^{n+\frac{1}{2}} = -T_{2,3}^{n} - T_{2,1}^{n}$$

$$T_{1,2}^{n+\frac{1}{2}} - 4T_{2,2}^{n+\frac{1}{2}} + T_{3,2}^{n+\frac{1}{2}} = -T_{2,3}^{n} - T_{2,1}^{n} = -220 - 55.71 = -275.71$$

At node 3,2

$$T_{4,2}^{n+\frac{1}{2}} + T_{2,2}^{n+\frac{1}{2}} - 4T_{3,2}^{n+\frac{1}{2}} = -T_{3,3}^{n} - T_{3,1}^{n}$$

$$T_{2,2}^{n+\frac{1}{2}} - 4T_{3,2}^{n+\frac{1}{2}} = -T_{4,2}^{n+\frac{1}{2}} - T_{3,3}^{n} - T_{3,1}^{n}$$

Since $T_{4,2}$ is always at 20°C, the above equation becomes

$$T_{2,2}^{n+\frac{1}{2}} - 4T_{3,2}^{n+\frac{1}{2}} = -T_{4,2}^{n+\frac{1}{2}} - T_{3,3}^{n} - T_{3,1}^{n} = -20 - 180 - 46.43 = -246.43$$

The following tridiagonal set of linear algebraic equations is obtained for various i nodes at j = 2:

$$\begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_{1,2}^{n+\frac{1}{2}} \\ T_{2,2}^{n+\frac{1}{2}} \\ T_{3,2}^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} -246.43 \\ -275.71 \\ -246.43 \end{bmatrix}$$

The solution by TDMA is: $T_{1,2}^{n+\frac{1}{2}} = 90.10$, $T_{2,2}^{n+\frac{1}{2}} = 113.98$, $T_{3,2}^{n+\frac{1}{2}} = 90.10$°C.

Now let us write the equations for various i nodes at j = 3.

At node 1,3

$$T_{2,3}^{n+\frac{1}{2}} + T_{0,3}^{n+\frac{1}{2}} - 4T_{1,3}^{n+\frac{1}{2}} = -T_{1,4}^{n} - T_{1,2}^{n}$$

Since $T_{0,3}$ is always at 20°C, the above equation becomes

$$-4T_{1,3}^{n+\frac{1}{2}} + T_{2,3}^{n+\frac{1}{2}} = -T_{0,3}^{n+\frac{1}{2}} - T_{1,4}^{n} - T_{1,2}^{n} = -20 - 400 - 90.10 = -510.10$$

At node 2,3

$$T_{3,3}^{n+\frac{1}{2}} + T_{1,3}^{n+\frac{1}{2}} - 4T_{2,3}^{n+\frac{1}{2}} = -T_{2,4}^{n} - T_{2,2}^{n}$$

$$T_{1,3}^{n+\frac{1}{2}} - 4T_{2,3}^{n+\frac{1}{2}} + T_{3,3}^{n+\frac{1}{2}} = -T_{2,4}^{n} - T_{2,2}^{n} = -400 - 113.98 = -513.98$$

At node 3,3

$$T_{4,3}^{n+\frac{1}{2}} + T_{2,3}^{n+\frac{1}{2}} - 4T_{3,3}^{n+\frac{1}{2}} = -T_{3,4}^{n} - T_{3,2}^{n}$$

$$T_{2,3}^{n+\frac{1}{2}} - 4T_{3,3}^{n+\frac{1}{2}} = -T_{4,3}^{n+\frac{1}{2}} - T_{3,4}^{n} - T_{3,2}^{n}$$

Since $T_{4,3}$ is always at 20°C, the above equation becomes

$$T_{2,3}^{n+\frac{1}{2}} - 4T_{3,3}^{n+\frac{1}{2}} = -T_{4,3}^{n+\frac{1}{2}} - T_{3,4}^{n} - T_{3,2}^{n} = -20 - 400 - 90.10 = -510.10$$

The following tridiagonal set of linear algebraic equations is obtained for various i nodes at $j = 3$:

$$\begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_{1,3}^{n+\frac{1}{2}} \\ T_{2,3}^{n+\frac{1}{2}} \\ T_{3,3}^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} -510.10 \\ -513.98 \\ -510.10 \end{bmatrix}$$

The solution by TDMA is: $T_{1,3}^{n+\frac{1}{2}} = 182.46$, $T_{2,3}^{n+\frac{1}{2}} = 219.72$, $T_{3,3}^{n+\frac{1}{2}} = 182.46$°C.

The second half iteration (scanning various j nodes for given i) is performed using the discretized equation

$$\frac{T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1}}{\Delta y^2} = 0$$

Since $\Delta x = \Delta y$, the discretized equation becomes

$$T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1} - 4T_{i,j}^{n+1} = -T_{i+1,j}^{n+\frac{1}{2}} - T_{i-1,j}^{n+\frac{1}{2}}$$

At node 1,1

$$T_{1,2}^{n+1} + T_{1,0}^{n+1} - 4T_{1,1}^{n+1} = -T_{2,1}^{n+\frac{1}{2}} - T_{0,1}^{n+\frac{1}{2}}$$

$$-4T_{1,1}^{n+1} + T_{1,2}^{n+1} = -T_{1,0}^{n+1} - T_{2,1}^{n+\frac{1}{2}} - T_{0,1}^{n+\frac{1}{2}}$$

Since $T_{1,0}$ is always at 20°C, the above equation becomes

$$-4T_{1,1}^{n+1} + T_{1,2}^{n+1} = -T_{1,0}^{n+1} - T_{2,1}^{n+\frac{1}{2}} - T_{0,1}^{n+\frac{1}{2}} = -20 - 55.71 - 20 = -95.71$$

At node 1,2

$$T_{1,3}^{n+1} + T_{1,1}^{n+1} - 4T_{1,2}^{n+1} = -T_{2,2}^{n+\frac{1}{2}} - T_{0,2}^{n+\frac{1}{2}}$$

$$T_{1,1}^{n+1} - 4T_{1,2}^{n+1} + T_{1,3}^{n+1} = -113.98 - 20 = -133.98$$

At node 1,3

$$T_{1,4}^{n+1} + T_{1,2}^{n+1} - 4T_{1,3}^{n+1} = -T_{2,3}^{n+\frac{1}{2}} - T_{0,3}^{n+\frac{1}{2}}$$

Since $T_{1,4}$ is always at 400°C, the above equation becomes

$$T_{1,2}^{n+1} - 4T_{1,3}^{n+1} = -400 - 219.72 - 20 = -639.72$$

The following tridiagonal set of linear algebraic equations is obtained for various j nodes at $i = 1$:

$$\begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_{1,1}^{n+1} \\ T_{1,2}^{n+1} \\ T_{1,3}^{n+1} \end{bmatrix} = \begin{bmatrix} -95.71 \\ -133.98 \\ -639.72 \end{bmatrix}$$

The solution by TDMA is: $T_{1,1}^{n+1}$ = 46.63, $T_{1,2}^{n+1}$ = 90.81, $T_{1,3}^{n+1}$ = 182.63°C.

At node 2,1

$$T_{2,2}^{n+1} + T_{2,0}^{n+1} - 4T_{2,1}^{n+1} = -T_{3,1}^{n+\frac{1}{2}} - T_{1,1}^{n+\frac{1}{2}}$$

$$-4T_{2,1}^{n+1} + T_{2,2}^{n+1} = -T_{2,0}^{n+1} - T_{3,1}^{n+\frac{1}{2}} - T_{1,1}^{n+\frac{1}{2}}$$

Since $T_{2,0}$ is always at 20°C, the above equation becomes

$$-4T_{2,1}^{n+1} + T_{2,2}^{n+1} = -T_{2,0}^{n+1} - T_{3,1}^{n+\frac{1}{2}} - T_{1,1}^{n+\frac{1}{2}} = -20 - 46.43 - 46.63 = -113.06$$

At node 2,2

$$T_{2,3}^{n+1} + T_{2,1}^{n+1} - 4T_{2,2}^{n+1} = -T_{3,2}^{n+\frac{1}{2}} - T_{1,2}^{n+\frac{1}{2}}$$

$$T_{2,1}^{n+1} - 4T_{2,2}^{n+1} + T_{2,3}^{n+1} = -90.10 - 90.81 = -180.91$$

At node 2,3

$$T_{2,4}^{n+1} + T_{2,2}^{n+1} - 4T_{2,3}^{n+1} = -T_{3,3}^{n+\frac{1}{2}} - T_{1,3}^{n+\frac{1}{2}}$$

Since $T_{2,4}$ is always at 400°C, the above equation becomes

$$T_{2,2}^{n+1} - 4T_{2,3}^{n+1} = -400 - 182.46 - 182.63 = -765.09$$

The following tridiagonal set of linear algebraic equations is obtained for various j nodes at i = 2:

$$\begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_{2,1}^{n+1} \\ T_{2,2}^{n+1} \\ T_{2,3}^{n+1} \end{bmatrix} = \begin{bmatrix} -113.06 \\ -180.91 \\ -765.09 \end{bmatrix}$$

The solution by TDMA is: $T_{2,1}^{n+1}$ = 56.87, $T_{2,2}^{n+1}$ = 114.41, $T_{2,3}^{n+1}$ = 219.88°C.

At node 3,1

$$T_{3,2}^{n+1} + T_{3,0}^{n+1} - 4T_{3,1}^{n+1} = -T_{4,1}^{n+\frac{1}{2}} - T_{2,1}^{n+\frac{1}{2}}$$

$$-4T_{3,1}^{n+1} + T_{3,2}^{n+1} = -T_{3,0}^{n+1} - T_{4,1}^{n+\frac{1}{2}} - T_{2,1}^{n+\frac{1}{2}}$$

Since $T_{3,0}$ is always at 20°C, the above equation becomes

$$-4T_{3,1}^{n+1} + T_{3,2}^{n+1} = -T_{3,0}^{n+1} - T_{4,1}^{n+\frac{1}{2}} - T_{2,1}^{n+\frac{1}{2}} = -20 - 20 - 56.87 = -96.87$$

At node 3,2

$$T_{3,3}^{n+1} + T_{3,1}^{n+1} - 4T_{3,2}^{n+1} = -T_{4,2}^{n+\frac{1}{2}} - T_{2,2}^{n+\frac{1}{2}}$$

$$T_{3,1}^{n+1} - 4T_{3,2}^{n+1} + T_{3,3}^{n+1} = -20 - 114.41 = -134.41$$

At node 3,3

$$T_{3,4}^{n+1} + T_{3,2}^{n+1} - 4T_{3,3}^{n+1} = -T_{4,3}^{n+\frac{1}{2}} - T_{2,3}^{n+\frac{1}{2}}$$

Since $T_{3,4}$ is always at 400°C, the above equation becomes

$$T_{3,2}^{n+1} - 4T_{3,3}^{n+1} = -400 - 20 - 219.88 = -639.88$$

The following tridiagonal set of linear algebraic equations is obtained for various j nodes at $i = 3$:

$$\begin{bmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_{3,1}^{n+1} \\ T_{3,2}^{n+1} \\ T_{3,3}^{n+1} \end{bmatrix} = \begin{bmatrix} -96.87 \\ -134.41 \\ -639.88 \end{bmatrix}$$

The solution by TDMA is: $T_{3,1}^{n+1} = 46.97$, $T_{3,2}^{n+1} = 91.03$, $T_{3,3}^{n+1} = 182.73$°C.

Program 10.2 for the solution of the above problem is given in the Appendix. After 25 iterations when convergence is obtained, the results from the computer program are: $T_{1,1} = 47.14$, $T_{1,2} = 91.25$, $T_{1,3} = 182.86$, $T_{2,1} = 57.32$, $T_{2,2} = 115.00$, $T_{2,3} = 220.16$, $T_{3,1} = 47.14$, $T_{3,2} = 91.25$, $T_{3,3} = 182.86$°C.

Similar results are obtained in Example 10.1 in which the problem was solved using the Gauss–Seidel method.

10.6 ADI Method for Transient Heat Conduction

The ADI method can be extended for the solution of two-dimensional transient heat conduction. The explicit schemes are stable only with some constraints on Δx and Δt, whereas implicit schemes are not associated with these constraints. Therefore the ADI method, which is an implicit method shall be used. Transient heat conduction in two-dimensional space is given by [see Eq. (9.26)]

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

Taking the first half-step in time, we get

$$\frac{T_{i,j}^{n+\frac{1}{2}} - T_{i,j}^{n}}{\Delta t/2} = \alpha \left(\frac{T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j+1}^{n} + T_{i,j-1}^{n} - 2T_{i,j}^{n}}{\Delta y^2} \right) \tag{10.14}$$

Letting $\Delta = \Delta x = \Delta y$ and $M = \dfrac{\alpha \Delta t}{\Delta^2}$, we get

$$T_{i,j}^{n+\frac{1}{2}} - T_{i,j}^{n} = \frac{M}{2}\left(T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i,j+1}^{n} + T_{i,j-1}^{n} - 2T_{i,j}^{n}\right) \tag{10.15}$$

Multiplying both sides by $\frac{2}{M}$, we get

$$\frac{2}{M}\left(T_{i,j}^{n+\frac{1}{2}} - T_{i,j}^{n}\right) = T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i,j+1}^{n} + T_{i,j-1}^{n} - 2T_{i,j}^{n} \tag{10.16}$$

$$-T_{i-1,j}^{n+\frac{1}{2}} + \left(2 + \frac{2}{M}\right)T_{i,j}^{n+\frac{1}{2}} - T_{i+1,j}^{n+\frac{1}{2}} = T_{i,j+1}^{n} + T_{i,j-1}^{n} + T_{i,j}^{n}\left(\frac{2}{M} - 2\right) \tag{10.17}$$

Now let us carry out the second half of the iteration

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n+\frac{1}{2}}}{\Delta t/2} = \alpha\left(\frac{T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1}}{\Delta y^2}\right) \tag{10.18}$$

$$T_{i,j}^{n+1} - T_{i,j}^{n+\frac{1}{2}} = \frac{M}{2}\left(T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1} + T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}}\right) \tag{10.19}$$

Multiplying both sides by $\frac{2}{M}$, we get

$$\frac{2}{M}\left(T_{i,j}^{n+1} - T_{i,j}^{n+\frac{1}{2}}\right) = T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1} + T_{i+1,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} \tag{10.20}$$

$$-T_{i,j-1}^{n+1} + \left(2 + \frac{2}{M}\right)T_{i,j}^{n+1} - T_{i,j+1}^{n+1} = T_{i-1,j}^{n+\frac{1}{2}} + T_{i+1,j}^{n+\frac{1}{2}} + T_{i,j}^{n+\frac{1}{2}}\left(\frac{2}{M} - 2\right) \tag{10.21}$$

ADI is an implicit method and is therefore unconditionally stable; moreover, because it is a line-by-line method, TDMA can be used to update the temperature for nodes in a line. Initially Eq. (10.17) is considered for the first half of the iteration. In this equation, T^n is the temperature at time t and $T^{n+\frac{1}{2}}$ are the updated temperatures computed in this first half of iteration. Sweeping of each line along the x-axis is carried out from bottom to top. Then Eq. (10.21) is considered for the second half of the iteration. In this equation, $T^{n+\frac{1}{2}}$ are known and T^{n+1} are computed. The sweeping of each line along the y-axis is carried out from left to right and the temperature profile at time $t + \Delta t$ is computed. This temperature profile at $t + \Delta t$ can be used to obtain the temperature profile at $t + 2\Delta t$ by again carrying out the first half and the second half of the iteration. Thus marching in time is carried out for this parabolic PDE.

EXAMPLE 10.11 A slab of size 2 m × 2 m is initially at 0°C, and at $t = 0$ all the four sides of the slab are made at 400°C. Take $\Delta = \Delta x = \Delta y = 0.1$ m and $\alpha = 1$ m^2/s. Determine the temperature of the slab at various nodes at $t = 0.5$ s. Take $\Delta t = 0.05$ s and for computing consider the upper quadrant of the slab.

Solution The upper quadrant of the slab is shown in Fig. 10.14. The size of the quadrant is 1 m × 1 m and 10 parts along an axis are made; therefore $\Delta = \Delta x = \Delta y = 0.1$ m. Let us take $\Delta t = 0.05$ s; therefore $M = \dfrac{\alpha \Delta t}{\Delta^2} = \dfrac{0.05}{0.1^2} = 5$. Thus $2 + \dfrac{2}{M} = 2.4$ and $\dfrac{2}{M} - 2 = -1.6$.

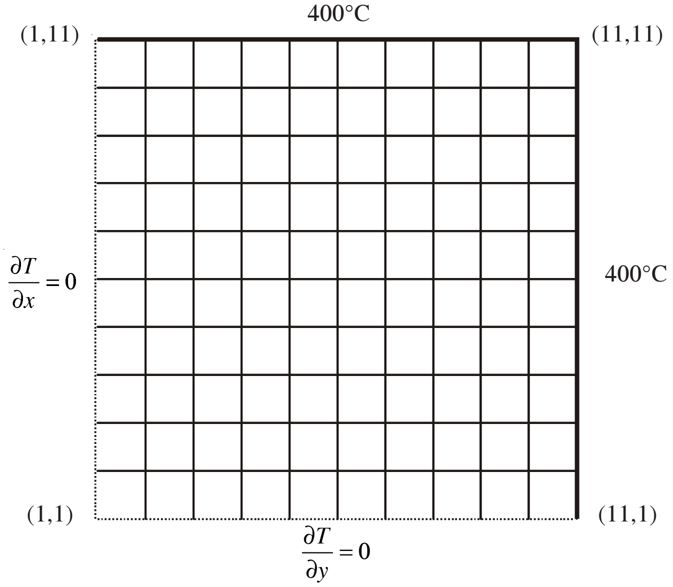


Fig. 10.14 Upper quadrant of slab in Example 10.11.

First half of iteration

Equations for node (1,1) *to node* (10,1)

At node (1,1), using Eq. (10.17) and from symmetry $T_{0,1}^{n+\frac{1}{2}} = T_{2,1}^{n+\frac{1}{2}}$ and $T_{1,0}^{n} = T_{1,2}^{n}$, we get

$$2.4T_{1,1}^{n+\frac{1}{2}} - 2T_{2,1}^{n+\frac{1}{2}} = 2T_{1,2}^{n} - 1.6T_{1,1}^{n}$$

At node (2,1), using Eq. (10.17) and from symmetry $T_{2,0}^{n} = T_{2,2}^{n}$, we get

$$-T_{1,1}^{n+\frac{1}{2}} + 2.4T_{2,1}^{n+\frac{1}{2}} - T_{3,1}^{n+\frac{1}{2}} = 2T_{2,2}^{n} - 1.6T_{2,1}^{n}$$

At node (3,1), using Eq. (10.17) and from symmetry $T_{3,0}^{n} = T_{3,2}^{n}$, we get

$$-T_{2,1}^{n+\frac{1}{2}} + 2.4T_{3,1}^{n+\frac{1}{2}} - T_{4,1}^{n+\frac{1}{2}} = 2T_{3,2}^{n} - 1.6T_{3,1}^{n}$$

At node (10,1), using Eq. (10.17) and from symmetry $T_{10,0}^{n} = T_{10,2}^{n}$, we get

$$-T_{9,1}^{n+\frac{1}{2}} + 2.4T_{10,1}^{n+\frac{1}{2}} = 2T_{10,2}^{n} - 1.6T_{10,1}^{n} + T_{11,1}^{n+\frac{1}{2}}$$

In the above equation on the right hand side, $T_{11,1} = 400$. The above set of 10 equations constitute a tridiagonal matrix and can be solved using TDMA.

Equations for node (1,2) *to node* (10,2)

At node (1,2), using Eq. (10.17) and from symmetry $T_{0,2}^{n+\frac{1}{2}} = T_{2,2}^{n+\frac{1}{2}}$, we get

$$2.4T_{1,2}^{n+\frac{1}{2}} - 2T_{2,2}^{n+\frac{1}{2}} = T_{1,3}^{n} + T_{1,1}^{n} - 1.6T_{1,2}^{n}$$

At node (2,2), using Eq. (10.17), we get

$$-T_{1,2}^{n+\frac{1}{2}} + 2.4T_{2,2}^{n+\frac{1}{2}} - T_{3,2}^{n+\frac{1}{2}} = T_{2,3}^{n} + T_{2,1}^{n} - 1.6T_{2,2}^{n}$$

At node (3,2), using Eq. (10.17), we get

$$-T_{2,2}^{n+\frac{1}{2}} + 2.4T_{3,2}^{n+\frac{1}{2}} - T_{4,2}^{n+\frac{1}{2}} = T_{3,3}^{n} + T_{3,1}^{n} - 1.6T_{3,2}^{n}$$

At node (10,2), using Eq. (10.17), we get

$$-T_{9,2}^{n+\frac{1}{2}} + 2.4T_{10,2}^{n+\frac{1}{2}} = T_{10,3}^{n} + T_{10,1}^{n} - 1.6T_{10,2}^{n} + T_{11,2}^{n+\frac{1}{2}}$$

In the above equation on the right hand side, $T_{11,2} = 400$. The above set of 10 equations constitute a tridiagonal matrix and can be solved using TDMA.

Equations for node (1,10) *to node* (10,10)

At node (1,10), using Eq. (10.17), and from symmetry $T_{0,10}^{n+\frac{1}{2}} = T_{2,10}^{n+\frac{1}{2}}$, we get

$$2.4T_{1,10}^{n+\frac{1}{2}} - 2T_{2,10}^{n+\frac{1}{2}} = T_{1,11}^{n} + T_{1,9}^{n} - 1.6T_{1,10}^{n}$$

At node (2,10), using Eq. (10.17), we get

$$-T_{1,10}^{n+\frac{1}{2}} + 2.4T_{2,10}^{n+\frac{1}{2}} - T_{3,10}^{n+\frac{1}{2}} = T_{2,11}^{n} + T_{2,9}^{n} - 1.6T_{2,10}^{n}$$

At node (3,10), using Eq. (10.17), we get

$$-T_{2,10}^{n+\frac{1}{2}} + 2.4T_{3,10}^{n+\frac{1}{2}} - T_{4,10}^{n+\frac{1}{2}} = T_{3,11}^{n} + T_{3,9}^{n} - 1.6T_{3,10}^{n}$$

At node (10,10) using Eq. (10.17) we get

$$-T_{9,10}^{n+\frac{1}{2}} + 2.4T_{10,10}^{n+\frac{1}{2}} = T_{10,11}^{n} + T_{10,9}^{n} - 1.6T_{10,10}^{n} + T_{11,10}^{n+\frac{1}{2}}$$

In the above set of equations on the right hand side, $T_{i,11} = 400$ and $T_{11,10} = 400$. The above set of 10 equations constitute a tri-diagonal matrix and can be solved using TDMA.

Second half of iteration

Equations for node (1,1) *to node* (1,10)

At node (1,1), using Eq. (10.21) and from symmetries $T_{1,0}^{n+\frac{1}{2}} = T_{1,2}^{n+\frac{1}{2}}$ and $T_{0,1}^{n} = T_{2,1}^{n}$, we get

$$2.4T_{1,1}^{n+1} - 2T_{1,2}^{n+1} = 2T_{2,1}^{n+\frac{1}{2}} - 1.6T_{1,1}^{n+\frac{1}{2}}$$

At node (1,2), using Eq. (10.21) and from symmetry $T_{0,2}^{n} = T_{2,2}^{n}$, we get

$$-T_{1,1}^{n+1} + 2.4T_{1,2}^{n+1} - T_{1,3}^{n+1} = 2T_{2,2}^{n+\frac{1}{2}} - 1.6T_{1,2}^{n+\frac{1}{2}}$$

At node (1,3), using Eq. (10.21) and from symmetry $T_{0,3}^{n} = T_{2,3}^{n}$, we get

$$-T_{1,2}^{n+1} + 2.4T_{1,3}^{n+1} - T_{1,4}^{n+1} = 2T_{2,3}^{n+\frac{1}{2}} - 1.6T_{1,3}^{n+\frac{1}{2}}$$

At node (1,10), using Eq. (10.21) and from symmetry $T_{0,10}^{n} = T_{2,10}^{n}$, we get

$$-T_{1,9}^{n+1} + 2.4T_{1,10}^{n+1} = 2T_{2,10}^{n+\frac{1}{2}} - 1.6T_{1,10}^{n+\frac{1}{2}} + T_{1,11}^{n+1}$$

In the above equation on the right hand side, $T_{1,11} = 400$. The above set of 10 equations constitute a tridiagonal matrix and can be solved using TDMA.

Equations for node (2,1) *to node* (2,10)

At node (2,1), using Eq. (10.21) and from symmetry $T_{2,0}^{n+\frac{1}{2}} = T_{2,2}^{n+\frac{1}{2}}$, we get

$$2.4T_{2,1}^{n+1} - 2T_{2,2}^{n+1} = T_{3,1}^{n+\frac{1}{2}} + T_{1,1}^{n+\frac{1}{2}} - 1.6T_{2,1}^{n+\frac{1}{2}}$$

At node (2,2), using Eq. (10.21), we get

$$-T_{2,1}^{n+1} + 2.4T_{2,2}^{n+1} - T_{2,3}^{n+1} = T_{3,2}^{n+\frac{1}{2}} + T_{1,2}^{n+\frac{1}{2}} - 1.6T_{2,2}^{n+\frac{1}{2}}$$

At node (2,3), using Eq. (10.21), we get

$$-T_{2,2}^{n+1} + 2.4T_{2,3}^{n+1} - T_{2,4}^{n+1} = T_{3,3}^{n+\frac{1}{2}} + T_{1,3}^{n+\frac{1}{2}} - 1.6T_{2,3}^{n+\frac{1}{2}}$$

At node (2,10), using Eq. (10.21), we get

$$-T_{2,9}^{n+1} + 2.4T_{2,10}^{n+1} = T_{3,10}^{n+\frac{1}{2}} + T_{1,10}^{n+\frac{1}{2}} - 1.6T_{2,10}^{n+\frac{1}{2}} + T_{2,11}^{n+1}$$

In the above equation on the right hand side, $T_{2,11}$ = 400. The above set of 10 equations constitute a tridiagonal matrix and can be solved using TDMA.

Equations for node (10,1) *to node* (10,10)

At node (2,1), using Eq. (10.21) and from symmetry $T_{10,0}^{n+\frac{1}{2}} = T_{10,2}^{n+\frac{1}{2}}$, we get

$$2.4T_{10,1}^{n+1} - 2T_{10,2}^{n+1} = T_{11,1}^{n+\frac{1}{2}} + T_{9,1}^{n+\frac{1}{2}} - 1.6T_{10,1}^{n+\frac{1}{2}}$$

At node (2,2), using Eq. (10.21), we get

$$-T_{10,1}^{n+1} + 2.4T_{10,2}^{n+1} - T_{10,3}^{n+1} = T_{11,2}^{n+\frac{1}{2}} + T_{9,2}^{n+\frac{1}{2}} - 1.6T_{10,2}^{n+\frac{1}{2}}$$

At node (2,3), using Eq. (10.21), we get

$$-T_{10,2}^{n+1} + 2.4T_{10,3}^{n+1} - T_{10,4}^{n+1} = T_{11,3}^{n+\frac{1}{2}} + T_{9,3}^{n+\frac{1}{2}} - 1.6T_{10,3}^{n+\frac{1}{2}}$$

At node (2,10), using Eq. (10.21), we get

$$-T_{10,9}^{n+1} + 2.4T_{10,10}^{n+1} = T_{11,10}^{n+\frac{1}{2}} + T_{9,10}^{n+\frac{1}{2}} - 1.6T_{10,10}^{n+\frac{1}{2}} + T_{10,11}^{n+1}$$

In the above set of equations on the right hand side, $T_{11,i}$ = 400 and $T_{10,11}$ = 400. The above set of 10 equations constitute a tridiagonal matrix and can be solved using TDMA. Note that for both the first-half and second-half iterations the tridiagonal matrix that is formed has the following coefficients:

$$a_2 = a_3 = a_4 = a_5 = a_6 = a_7 = a_8 = a_9 = a_{10} = -1$$

$$b_1 = b_2 = b_3 = b_4 = b_5 = b_6 = b_7 = b_8 = b_9 = b_{10} = 2.4$$

$$c_1 = -2, c_2 = c_3 = c_4 = c_5 = c_6 = c_7 = c_8 = c_9 = -1$$

Program 10.3 for the solution of the above problem is given in the Appendix. The temperatures (in °C) at t = 0.5 s are presented in Table 10.2.

Table 10.2 Temperatures in Example 10.11

$T_{1,1}$ = 329.77	$T_{2,1}$ = 331.09	$T_{3,1}$ = 334.21	$T_{4.1}$ = 339.01	$T_{5,1}$ = 345.20
$T_{1,2}$ = 329.83	$T_{2,2}$ = 331.70	$T_{3,2}$ = 334.86	$T_{4,2}$ = 339.65	$T_{5,2}$ = 345.80
$T_{1,3}$ = 330.02	$T_{2,3}$ = 333.54	$T_{3,3}$ = 336.81	$T_{4,3}$ = 341.58	$T_{5,3}$ = 347.61
$T_{1,4}$ = 330.42	$T_{2,4}$ = 336.68	$T_{3,4}$ = 340.10	$T_{4,4}$ = 344.82	$T_{5,4}$ = 350.64
$T_{1,5}$ = 331.19	$T_{2,5}$ = 341.22	$T_{3,5}$ = 344.80	$T_{4,5}$ = 349.39	$T_{5,5}$ = 354.86
$T_{1,6}$ = 332.64	$T_{2,6}$ = 347.31	$T_{3,6}$ = 350.96	$T_{4,6}$ = 355.29	$T_{5,6}$ = 360.25
$T_{1,7}$ = 335.34	$T_{2,7}$ = 355.10	$T_{3,7}$ = 358.61	$T_{4,7}$ = 362.43	$T_{5,7}$ = 366.68
$T_{1,8}$ = 340.39	$T_{2,8}$ = 364.85	$T_{3,8}$ = 367.76	$T_{4,8}$ = 370.77	$T_{5,8}$ = 374.10
$T_{1,9}$ = 349.80	$T_{2,9}$ = 376.94	$T_{3,9}$ = 378.59	$T_{4,9}$ = 380.49	$T_{5,9}$ = 382.71
$T_{1,10}$ = 367.33	$T_{2,10}$ = 389.30	$T_{3,10}$ = 388.85	$T_{4,10}$ = 389.60	$T_{5,10}$ = 390.70

$T_{6,1} = 352.52$	$T_{7,1} = 360.60$	$T_{8,1} = 369.54$	$T_{9,1} = 381.09$	$T_{10,1} = 388.03$
$T_{6,2} = 353.06$	$T_{7,2} = 361.06$	$T_{8,2} = 369.90$	$T_{9,2} = 381.31$	$T_{10,2} = 388.17$
$T_{6,3} = 354.67$	$T_{7,3} = 362.42$	$T_{8,3} = 370.96$	$T_{9,3} = 381.98$	$T_{10,3} = 388.60$
$T_{6,4} = 357.35$	$T_{7,4} = 364.68$	$T_{8,4} = 372.73$	$T_{9,4} = 383.07$	$T_{10,4} = 389.30$
$T_{6,5} = 361.08$	$T_{7,5} = 367.81$	$T_{8,5} = 375.16$	$T_{9,5} = 384.59$	$T_{10,5} = 390.27$
$T_{6,6} = 365.79$	$T_{7,6} = 371.75$	$T_{8,6} = 378.22$	$T_{9,6} = 386.49$	$T_{10,6} = 391.47$
$T_{6,7} = 371.37$	$T_{7,7} = 376.38$	$T_{8,7} = 381.80$	$T_{9,7} = 388.71$	$T_{10,7} = 392.88$
$T_{6,8} = 377.76$	$T_{7,8} = 381.65$	$T_{8,8} = 385.87$	$T_{9,8} = 391.25$	$T_{10,8} = 394.47$
$T_{6,9} = 385.18$	$T_{7,9} = 387.81$	$T_{8,9} = 390.63$	$T_{9,9} = 394.16$	$T_{10,9} = 396.38$
$T_{6,10} = 391.98$	$T_{7,10} = 393.37$	$T_{8,10} = 394.88$	$T_{9,10} = 396.86$	$T_{10,10} = 397.96$

Exercises

10.1 Using the Gauss-Seidel method, determine the temperatures at positions 1, 2, 3 and 4 shown in Fig. 10.15.

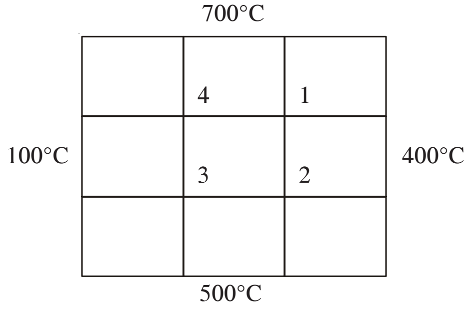


Fig. 10.15 Exercise 10.1.

(**Ans:** $T_1 = 487.5$, $T_2 = 437.5$, $T_3 = 362.5$, $T_4 = 412.5$°C)

10.2 Using the Gauss-Seidel method, determine the temperature of the heated plate shown in Fig. 10.16. The dimension of the plate is 40 cm × 40 cm and is made of aluminium. The thermal conductivity of aluminium is 0.5 W/m-K.

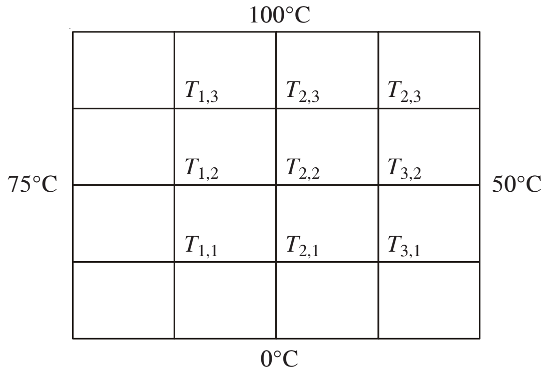


Fig. 10.16 Exercise 10.2.

(**Ans:** $T_{1,1}$ = 42.86, $T_{1,2}$ = 63.17, $T_{1,3}$ = 78.57, $T_{2,1}$ = 33.26, $T_{2,2}$ = 56.25, $T_{2,3}$ = 76.12, $T_{3,1}$ = 33.93, $T_{3,2}$ = 52.46, $T_{3,3}$ = 69.64°C)

10.3 Using the Gauss-Seidel method, determine the steady state temperatures for nodes 1 to 6 shown in Fig. 10.17. The thermal conductivity of the body is 1.5 W/m-K. $\Delta x = \Delta y$ = 25 cm.

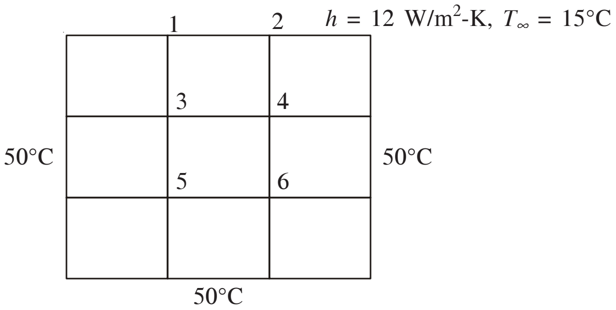


Fig. 10.17 Exercise 10.3.

(**Ans:** T_1 = 27.6, T_2 = 27.6, T_3 = 41.6, T_4 = 41.6, T_5 = 47.2, T_6 = 47.2°C)

10.4 Calculate the steady state temperatures for nodes 1 to 16 shown in Fig. 10.18. Take $\Delta x = \Delta y$ = 20 cm and k = 2.3 W/m-K.

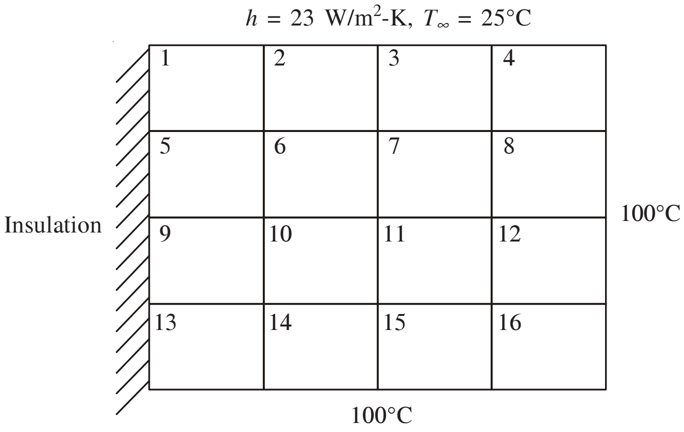


Fig. 10.18 Exercise 10.4.

(**Ans:** T_1 = 35.28, T_2 = 35.89, T_3 = 38.49, T_4 = 48.36, T_5 = 55.24, T_6 = 56.66, T_7 = 61.84, T_8 = 74.20, T_9 = 72.37, T_{10} = 73.67, T_{11} = 78.01, T_{12} = 86.58, T_{13} = 86.91, T_{14} = 87.63, T_{15} = 89.94, T_{16} = 94.13°C)

10.5 A slab of size 2 m × 2 m shown in Fig. 10.19 is initially at 0°C. At t = 0 s, all the four sides of the slab are made at 600°C. Take $\Delta x = \Delta y$ = 0.1 m. Take α = 1 m^2/s. Determine the temperature of the slab at various nodes at t = 0.25 s. Take Δt = 0.05 s, and for computing, consider the upper quadrant of the slab as shown in Fig. 10.19.

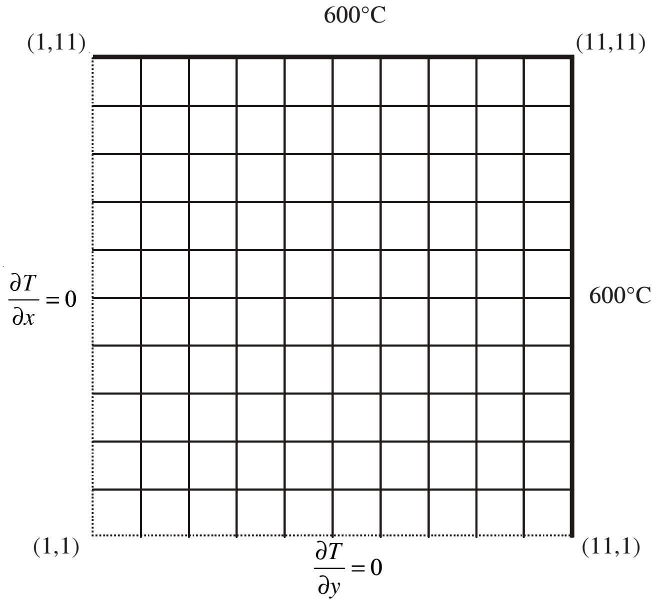


Fig. 10.19 Exercise 10.5.

(**Ans:** Program 10.3 can be modified and the temperatures (in °C) at t = 0.25 s are presented in Table 10.3.

Table 10.3 Temperatures in Exercise 10.5

$T_{1,1}$ = 290.10	$T_{2,1}$ = 294.61	$T_{3,1}$ = 308.63	$T_{4.1}$ = 329.39	$T_{5,1}$ = 356.77
$T_{1,2}$ = 290.34	$T_{2,2}$ = 297.26	$T_{3,2}$ = 311.43	$T_{4.2}$ = 332.19	$T_{5,2}$ = 359.39
$T_{1,3}$ = 291.18	$T_{2,3}$ = 305.32	$T_{3,3}$ = 319.95	$T_{4.3}$ = 340.64	$T_{5,3}$ = 367.31
$T_{1,4}$ = 292.95	$T_{2,4}$ = 319.18	$T_{3,4}$ = 334.48	$T_{4.4}$ = 354.95	$T_{5,4}$ = 380.66
$T_{1,5}$ = 296.35	$T_{2,5}$ = 339.47	$T_{3,5}$ = 355.48	$T_{4.5}$ = 375.40	$T_{5,5}$ = 399.59
$T_{1,6}$ = 302.74	$T_{2,6}$ = 366.94	$T_{3,6}$ = 383.30	$T_{4.6}$ = 402.10	$T_{5,6}$ = 424.03
$T_{1,7}$ = 314.69	$T_{2,7}$ = 401.84	$T_{3,7}$ = 417.53	$T_{4.7}$ = 434.20	$T_{5,7}$ = 452.99
$T_{1,8}$ = 336.96	$T_{2,8}$ = 443.29	$T_{3,8}$ = 456.10	$T_{4.8}$ = 469.16	$T_{5,8}$ = 483.88
$T_{1,9}$ = 378.48	$T_{2,9}$ = 491.07	$T_{3,9}$ = 497.67	$T_{4.9}$ = 505.61	$T_{5,9}$ = 515.51
$T_{1,10}$ = 455.84	$T_{2,10}$ = 563.32	$T_{3,10}$ = 562.67	$T_{4.10}$ = 566.37	$T_{5,10}$ = 571.09
$T_{6,1}$ = 390.11	$T_{7,1}$ = 427.17	$T_{8,1}$ = 462.90	$T_{9,1}$ = 496.07	$T_{10,1}$ = 576.63
$T_{6,2}$ = 392.45	$T_{7,2}$ = 429.12	$T_{8,2}$ = 464.48	$T_{9,2}$ = 497.27	$T_{10,2}$ = 576.89
$T_{6,3}$ = 399.47	$T_{7,3}$ = 435.00	$T_{8,3}$ = 469.20	$T_{9,3}$ = 500.88	$T_{10,3}$ = 577.69
$T_{6,4}$ = 411.25	$T_{7,4}$ = 444.85	$T_{8,4}$ = 477.09	$T_{9,4}$ = 506.92	$T_{10,4}$ = 579.01
$T_{6,5}$ = 427.88	$T_{7,5}$ = 458.70	$T_{8,5}$ = 488.17	$T_{9,5}$ = 515.38	$T_{10,5}$ = 580.87
$T_{6,6}$ = 449.20	$T_{7,6}$ = 476.39	$T_{8,6}$ = 502.28	$T_{9,6}$ = 526.13	$T_{10,6}$ = 583.23
$T_{6,7}$ = 474.24	$T_{7,7}$ = 497.03	$T_{8,7}$ = 518.67	$T_{9,7}$ = 538.58	$T_{10,7}$ = 586.01
$T_{6,8}$ = 500.60	$T_{7,8}$ = 518.57	$T_{8,8}$ = 535.63	$T_{9,8}$ = 551.33	$T_{10,8}$ = 589.01
$T_{6,9}$ = 527.28	$T_{7,9}$ = 540.20	$T_{8,9}$ = 552.54	$T_{9,9}$ = 563.91	$T_{10,9}$ = 592.14
$T_{6,10}$ = 576.02	$T_{7,10}$ = 580.89	$T_{8,10}$ = 585.36	$T_{9,10}$ = 589.41	$T_{10,10}$ = 596.94

10.6 Solve Exercise 10.5 to determine the temperature profile at 0.5 s.
(**Ans:** Program 10.3 can be modified and the temperatures (in °C) at $t = 0.5$ s are presented in Table 10.4.

Table 10.4 Temperatures in Exercise 10.6

$T_{1,1} = 494.66$	$T_{2,1} = 496.64$	$T_{3,1} = 501.32$	$T_{4,1} = 508.51$	$T_{5,1} = 517.80$
$T_{1,2} = 494.74$	$T_{2,2} = 497.55$	$T_{3,2} = 502.29$	$T_{4,2} = 509.48$	$T_{5,2} = 518.71$
$T_{1,3} = 495.03$	$T_{2,3} = 500.31$	$T_{3,3} = 505.21$	$T_{4,3} = 512.37$	$T_{5,3} = 521.42$
$T_{1,4} = 495.63$	$T_{2,4} = 505.01$	$T_{3,4} = 510.15$	$T_{4,4} = 517.23$	$T_{5,4} = 525.95$
$T_{1,5} = 496.78$	$T_{2,5} = 511.83$	$T_{3,5} = 517.20$	$T_{4,5} = 524.09$	$T_{5,5} = 532.29$
$T_{1,6} = 498.96$	$T_{2,6} = 520.96$	$T_{3,6} = 526.45$	$T_{4,6} = 532.93$	$T_{5,6} = 540.37$
$T_{1,7} = 503.02$	$T_{2,7} = 532.65$	$T_{3,7} = 537.91$	$T_{4,7} = 543.65$	$T_{5,7} = 550.03$
$T_{1,8} = 510.59$	$T_{2,8} = 547.27$	$T_{3,8} = 551.64$	$T_{4,8} = 556.16$	$T_{5,8} = 561.14$
$T_{1,9} = 524.71$	$T_{2,9} = 565.42$	$T_{3,9} = 567.89$	$T_{4,9} = 570.73$	$T_{5,9} = 574.06$
$T_{1,10} = 551.00$	$T_{2,10} = 583.95$	$T_{3,10} = 583.27$	$T_{4,10} = 584.40$	$T_{5,10} = 586.05$
$T_{6,1} = 528.78$	$T_{7,1} = 540.91$	$T_{8,1} = 554.31$	$T_{9,1} = 571.64$	$T_{10,1} = 582.04$
$T_{6,2} = 529.59$	$T_{7,2} = 541.59$	$T_{8,2} = 554.84$	$T_{9,2} = 571.97$	$T_{10,2} = 582.26$
$T_{6,3} = 532.01$	$T_{7,3} = 543.63$	$T_{8,3} = 556.44$	$T_{9,3} = 572.97$	$T_{10,3} = 582.90$
$T_{6,4} = 536.03$	$T_{7,4} = 547.02$	$T_{8,4} = 559.09$	$T_{9,4} = 574.61$	$T_{10,4} = 583.95$
$T_{6,5} = 541.62$	$T_{7,5} = 551.72$	$T_{8,5} = 562.75$	$T_{9,5} = 576.89$	$T_{10,5} = 585.40$
$T_{6,6} = 548.69$	$T_{7,6} = 557.62$	$T_{8,6} = 567.33$	$T_{9,6} = 579.73$	$T_{10,6} = 587.21$
$T_{6,7} = 557.06$	$T_{7,7} = 564.57$	$T_{8,7} = 572.70$	$T_{9,7} = 583.08$	$T_{10,7} = 589.32$
$T_{6,8} = 566.64$	$T_{7,8} = 572.48$	$T_{8,8} = 578.81$	$T_{9,8} = 586.87$	$T_{10,8} = 591.71$
$T_{6,9} = 577.77$	$T_{7,9} = 581.71$	$T_{8,9} = 585.94$	$T_{9,9} = 591.24$	$T_{10,9} = 594.56$
$T_{6,10} = 587.97$	$T_{7,10} = 590.05$	$T_{8,10} = 592.32$	$T_{9,10} = 595.29$	$T_{10,10} = 596.94$

Appendix

Programs in C++

Program	*Title*
1.1	Program for the solution of tridiagonal equations
1.2	Program for the solution of linear algebraic equations by the Gauss Elimination method
1.3	Program for the solution of linear algebraic equations by the Gauss–Seidel method
2.1	Program to solve for pressure drop in a pipe (nonlaminar case)
2.2	Program to solve for minimum fluidization velocity
2.3	Program to solve for terminal velocity
2.4	Program for the solution of two simultaneous nonlinear equations
3.1	Program to calculate the molar volume in the liquid and vapour phases at the given temperature and pressure
3.2	Program to calculate the bubble point temperature and the dew point temperature of a mixture of given composition, assuming Raoult's law to be true
3.3	Program to calculate the compositions of the vapour and liquid phases at the given temperature and pressure under flash conditions, assuming Raoult's law to be true
3.4	Program to calculate the bubble point pressure, bubble point temperature, dew point pressure and dew point temperature of a mixture of given composition, assuming the modified Raoult's law to be true
3.5	Program to calculate the compositions of the vapour and liquid phases at the given temperature and pressure under flash conditions, assuming the modified Raoult's law to be true
3.6	Program to calculate the vapour pressure at the given temperature using the Peng–Robinson equation of state by comparing the fugacities of the liquid and vapour phases
3.7	Program to calculate the bubble point pressure using the gamma–phi approach
3.8	Program to calculate the bubble point pressure using the Peng–Robinson equation of state
3.9	Program for the solution of two simultaneous chemical reactions in chemical equilibrium
3.10	Program to calculate the adiabatic flame temperature (AFT) for a fuel
4.1	Program to solve an ordinary differential equation by the Runge–Kutta method
4.2	Program to determine the velocity of a particle in a pneumatic conveyor

4.3 Program to solve two simultaneous ordinary differential equations by the Runge–Kutta method

4.4 Program to solve three simultaneous ordinary differential equations by the Runge–Kutta method

4.5 Program to solve three simultaneous ordinary differential equations for the reaction $A \to B \to C$ by the Runge–Kutta fourth order method

4.6 Program to solve four simultaneous ordinary differential equations for the reactions $A + B \to C$ and $B + C \to D$ by the Runge–Kutta method

4.7 Program to solve ordinary differential equations in a non-isothermal tubular reactor by the Runge–Kutta method

7.1 Program to calculate the concentration profile in a tubular reactor with axial dispersion (second order reaction)

7.2 Program to calculate the concentration profile in a tubular reactor with axial dispersion in which two parallel reactions take place

8.1 Program to calculate the concentration profile along the radius for reaction–diffusion in a spherical catalyst pellet (second order isothermal reaction)

8.2 Program to calculate the concentration profile along the radius for reaction-diffusion in a spherical catalyst pellet (non-isothermal, beta = 1)

9.1 Program to calculate the temperature profile in a rectangular slab during transient heat conduction

9.2 Program to calculate the concentration profile in a sphere during transient diffusion of drug from spherical pellet

10.1 Program to calculate the temperature profile in a two-dimensional body during steady heat conduction using the Gauss-Seidel method

10.2 Program to calculate the temperature profile in a two-dimensional body during steady heat conduction using the ADI method

10.3 Program to calculate the temperature profile in a two-dimensional body during transient heat conduction using the ADI method

PROGRAM 1.1

```
//PROGRAM 1.1
//program for the solution of tridiagonal equations
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,n,i1,n1,k;
float a[21],b[21],c[21],d[21],x[21],beta[21],gamma[21];
//a is subdiagonal, b is diagonal and c is superdiagonal
for(i=2;i<=7;++i)
{
```

```
a[i]=1.0;
}
for(i=1;i<=7;++i)
{
b[i]=-2.0;
}
for(i=1;i<=6;++i)
{
c[i]=1.0;
}
d[1]=-240.0;
for(i=2;i<=6;++i)
{
d[i]=-40.0;
}
d[7]=-60.0;
i=1;
n=7;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
cout<<"\t\t\t THE SOLUTION BY TDMA"<<endl;
for(i=1;i<=7;++i)
{
cout<<x[i]<<endl;
}
getch();
}
```

PROGRAM 1.2

```
//PROGRAM 1.2
//program for the solution of linear algebraic equations
//by the Gauss Elimination method
#include<iostream.h>
```

```
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int n,m,l,i,j,k,jj,kp1,nn,ip1;
float a[10][11],x[10],sum,big,ab,quot,t;
n=4;
cout<<n<<endl;
m=n+1;
l=n-1;
cout<<"Input the elements of A rowwise and elements of B"<<endl;
for(i=1;i<=n;i++)
{
for(j=1;j<=m;j++)
{
cin>>a[i][j];
}
}
for(i=1;i<=n;i++)
{
for(j=1;j<=m;j++)
{
cout<<a[i][j]<<endl;
}
}
for(k=1;k<=l;k++)
{
big=fabs(a[k][k]);
jj=k;
kp1=k+1;
for(i=kp1;i<=n;i++)
{
ab=fabs(a[i][k]);
if((big-ab)<0.0)
{
big=ab;
jj=i;
}
}
if((jj-k)>0)
{
for(j=k;j<=m;j++)
{
t=a[jj][j];
a[jj][j]=a[k][j];
```

```
a[k][j]=t;
}
}
for(i=kp1;i<=n;i++)
{
quot=a[i][k]/a[k][k];
for(j=kp1;j<=m;j++)
{
a[i][j]=a[i][j]-quot*a[k][j];
}
}
for(i=kp1;i<=n;i++)
{
a[i][k]=0.0;
}
}
x[n]=a[n][m]/a[n][n];
for(nn=1;nn<=l;nn++)
{
sum=0.0;
i=n-nn;
ip1=i+1;
for(j=ip1;j<=n;j++)
{
sum=sum+a[i][j]*x[j];
}
x[i]=(a[i][m]-sum)/a[i][i];
}
for(i=1;i<=n;i++)
{cout<<x[i]<<endl;}
getch();
}
```

PROGRAM 1.3

```
//PROGRAM 1.3
//program for the solution of linear algebraic equations
//by the Gauss-Seidel method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float x1old,x2old,x3old,x1new,x2new,x3new;
x1new=2.0;
```

```
x2new=3.0;
x3new=4.0;
do
{
x1old=x1new;
x2old=x2new;
x3old=x3new;
x1new=(44.0-x2old-2*x3old)/10.0;
x2new=(51.0-2*x1new-x3old)/10.0;
x3new=(61.0-x1new-2*x2new)/10.0;
}while(fabs(x1new-x1old)>1e-6&&fabs(x2new-x2old)>1e-6&&fabs(x3new-
    x3old)>1e-6);
cout<<x1new<<" "<<x2new<<" "<<x3new<<endl;
getch();
}
```

PROGRAM 2.1

```
//PROGRAM 2.1
//program to solve for pressure drop in a pipe (nonlaminar case)
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float fricf,epsilon,d,mu,rho,v,fricfnew,f,fdash,Re,deltap,length,a1,a2,a3;
int n;
d=0.004,v=50.0,rho=1.23,mu=1.79e-5,epsilon=0.0015e-3,length=1.0;
cout<<"\t\t\t OUTPUT"<<endl;
cout<<"\nEnter the initial value of fricfact";
cin>>fricf;
a1=epsilon/d;
Re=rho*v*d/mu;
a2=2.51/Re;
n=0;
fricfnew=0.01;
do
{
fricf=fricfnew;
f=(1.0/sqrt(fricf))+2.0*log10((a1/3.7)+(a2/sqrt(fricf)));
a3=-0.5*pow(fricf,-1.5);
fdash=a3+2.0*a2*a3/((a1/3.7)+(a2/sqrt(fricf)));
fricfnew=fricf-f/fdash;
n=n+1;
```

```
}while(fabs(fricfnew-fricf)>1e-6);
deltap=fricfnew*length*v*v*rho/(2.0*d);
cout<<“\t Friction factor is “<<fricfnew<<endl;
cout<<“Pressure drop is “<<deltap<<endl;
cout<<“Number of iterations performed “<<n<<endl;
getch();
}
```

PROGRAM 2.2

```
//PROGRAM 2.2
//program to solve for minimum fluidization velocity
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float epsilon,mu,vmf,phis,dp,rhop,rhog,a1,a2,a3,v,vnew,f,fdash;
const g=9.81;
int n;
dp=0.00012, phis=0.88, rhog=2.374, rhop=1000.0, mu=1.845e-5,
   epsilon=0.42;
cout<<“\t\t\t OUTPUT”<<endl;
cout<<“\nEnter the initial value of vmf in m/s “;
cin>>vmf;
a1=1.75*rhog*(1.0-epsilon)/(phis*dp*pow(epsilon,3.0));
a2=150.0*mu*(1.0-epsilon)*(1.0-epsilon)/(phis*phis*dp*dp*pow(epsilon,3));
a3=(1.0-epsilon)*(rhop-rhog)*g;
n=0;
vnew=0.01;
do
{
v=vnew;
f=a1*v*v+a2*v-a3;
fdash=2.0*a1*v+a2;
vnew=v-f/fdash;
n=n+1;
}while(fabs(vnew-v)>1e-6);
cout<<“\t Velocity at minimum fluidization is “<<vnew<< “ m/s “<<endl;
cout<<“Number of iterations performed were “<<n<<endl;
getch();
}
```

PROGRAM 2.3

```
//PROGRAM 2.3
//program to solve for terminal velocity
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float vt,vtnew,rhop,rhog,dp,cd,rep,mu,a1;
float g=9.81;
int n;
rhog=1.18,rhop=900.0,dp=0.002,mu=1.85e-5;
cout<<"\nEnter the value of initial value of terminal velocity in m/
s ";
cin>>vtnew;
do
{
vt=vtnew;
rep=rhog*vt*dp/mu;
cd=24.0*(1.0+0.15*pow(rep,0.687))/rep;
a1=4.0*(rhop-rhog)*g*dp/(3.0*cd*rhog);
vtnew=sqrt(a1);
n=n+1;
}while(fabs(vtnew-vt)>1e-6);
cout<<"\t Value of terminal velocity is "<<vtnew<<endl;
cout<<"number of iterations performed is "<<n<<endl;
getch();
}
```

PROGRAM 2.4

```
//PROGRAM 2.4
//program for the solution of two simultaneous nonlinear equations
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float x1,x2,x1new,x2new,f1,f2,df1dx1,df1dx2,df2dx1,df2dx2;
float d,deltax1,deltax2;
int n;
x1new=0.1;
```

```
x2new=0.5;
n=0;
do
{
x1=x1new;
x2=x2new;
f1=pow(2.71828,x1)+x1*x2-1.0;
f2=sin(x1*x2)+x1+x2-1.0;
df1dx1=pow(2.71828,x1)+x2;
df1dx2=x1;
df2dx1=x2*cos(x1*x2)+1.0;
df2dx2=x1*cos(x1*x2)+1.0;
d=df1dx1*df2dx2-df1dx2*df2dx1;
deltax1=(f2*df1dx2-f1*df2dx2)/d;
deltax2=(f1*df2dx1-f2*df1dx1)/d;
x1new=x1+deltax1;
x2new=x2+deltax2;
n=n+1;
}while(fabs(x1new-x1)>1e-6&&fabs(x2new-x2)>1e-6);
cout<<"The number of iterations performed is "<<n<<endl;
cout<<x1new<<" "<<x2new<<endl;
getch();
}
```

PROGRAM 3.1

```
//PROGRAM 3.1
//program to calculate the molar volume in the liquid and vapour phases at the
//given temperature and pressure
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float w,s,t,tc,k,a,b,r=8.314,lpha,sol[2],vold,vnew,B,tr,b0,b1;
float p,pc,f,f1;
cout<<"Enter the value of temperature in deg K and pressure in Pa";
cin>>t>>p;
cout<<"Enter the value of critical temperature in deg K and critical
   pressure in Pa";
cin>>tc>>pc;
cout<<"Enter the value of acentric factor";
cin>>w;
//
//VIRIAL GAS EQUATION OF STATE Z(T,P)
//
```

```
tr=t/tc;
b0=.083-0.422*pow(tr,-1.6);
b1=.139-0.172*pow(tr,-4.2);
B=(b0+w*b1)*r*tc/pc;
vnew=r*t/p+B;
cout<<"Volume of vapour by virial eos Z(T,P) "<<vnew<<"m3/mol"<<endl;
//
//VIRIAL GAS EQUATION OF STATE Z(T,V)
//
vnew=r*t/p;
do
 {
  vold=vnew;
  f=p*vold/(r*t)-1-B/vold;
  f1=p/(r*t)+B/(vold*vold);
  vnew=vold-f/f1;
 }
while(fabs(vnew-vold)>1e-6);
cout<<"Volume of vapour by virial eos Z(T,V) "<<vnew<<"m3/mol"<<endl;
//
//PENG-ROBINSON CUBIC EQUATION OF STATE
//
int i=0;
k=.37464+1.54226*w-.26992*w*w;
s=1+k*(1-pow(t/tc,.5));
lpha=pow(s,2);
a=.45724*r*r*tc*tc*lpha/pc;
b=.07780*r*tc/pc;
vnew=b;
for(i=0;i<=1;++i)
 {
 do
 {
  vold=vnew;
  f=pow(vold,3)*p+vold*vold*(p*b-r*t)-vold*(3*p*b*b+2*b*r*t-a);
  f=f+(p*b*b*b+b*b*r*t-a*b);
  f1=pow(vold,2)*3*p+vold*2*(b*p-t*r)+(a-3*b*b*p-2*r*t*b);
  vnew=vold-f/f1;
 }
  while(fabs(vnew-vold)>1e-6);
  sol[i]=vnew;
  vnew=r*t/p;
 }
cout<<"Volume of saturated liquid by Peng-Robinson "<<sol[0]<<"m3/
mol"<<endl<<
```

```
"Volume of saturated vapour by Peng-Robinson "<<sol[1]<<"m3/mol\n";
//
//REDLICH-KWONG CUBIC EQUATION OF STATE
//
i=0;
a=.42748*r*r*pow(tc,2.5)/pc;
b=.08664*r*tc/pc;
vnew=b;
for(i=0;i<=1;++i)
 {
 do
 {
  vold=vnew;
     f=pow(vold,3)*p-r*t*vold*vold-vold*(p*b*b+b*r*t-a/sqrt(t))-a*b/
sqrt(t);
  f1=pow(vold,2)*3*p-vold*2*r*t-(p*b*b+b*r*t-a/sqrt(t));
  vnew=vold-f/f1;
  }
  while(fabs(vnew-vold)>1e-6);
  sol[i]=vnew;
  vnew=r*t/p;
  }
cout<<"Volume of saturated liquid by Redlich-Kwong "<<sol[0]<<"m3/
mol"<<endl<<
"Volume of saturated vapour by Redlich-Kwong "<<sol[1]<<"m3/mol\n";
//
//VAN DER WAALS CUBIC EQUATION OF STATE
//
i=0;
a=27*r*r*tc*tc/(64*pc);
b=r*tc/(8*pc);
vnew=b;
for(i=0;i<=1;++i)
 {
 do
 {
  vold=vnew;
  f=pow(vold,3)*p-vold*vold*(p*b+r*t)+a*vold-a*b;
  f1=pow(vold,2)*3*p-vold*2*(b*p+t*r)+a;
  vnew=vold-f/f1;
  }
  while(fabs(vnew-vold)>1e-6);
  sol[i]=vnew;
  vnew=r*t/p;
  }
```

```
cout<<"Volume of saturated liquid by van der Waals "<<sol[0]<<"m3/
mol"<<endl<<
"Volume of saturated vapour by van der Waals "<<sol[1]<<"m3/mol\n";
getch();
}
```

PROGRAM 3.2

```
//PROGRAM 3.2
//program to calculate the BPT and DPT
//of a mixture of given composition, assuming Raoult's law to be true
//BPT is calculated by taking the given composition to be in liquid phase
//DPT is calculated by taking the given composition to be in vapour phase
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float p,p1sat,p2sat,p1satn,t1sat,t2sat;
float told,tnew,x1,x2,y1,y2,z1,a1,b1,c1,a2,b2,c2;
float f,f1;
cout<<"\nEnter the mole fraction of component 1";
cin>>z1;
cout<<"\nEnter the pressure in kPa";
cin>>p;
// the Antoine constants are for acetone (1) and water (2). For use of
// these constants temperature is in deg C and pressure in kPa.
a1=14.39155;
b1=2795.317;
c1=230.002;
a2=16.26205;
b2=3799.887;
c2=226.346;
//CALCULATION OF BUBBLE POINT TEMPERATURE
x1=z1;
x2=1-z1;
t1sat=b1/(a1-log(p))-c1;
t2sat=b2/(a2-log(p))-c2;
tnew=x1*t1sat+x2*t2sat;
do
 {
 told=tnew;
 p1sat=exp(a1-b1/(told+c1));
```

```
 p2sat=exp(a2-b2/(told+c2));
 f=p-x1*p1sat-x2*p2sat;
                 f1=-x1*p1sat*b1/((told+c1)*(told+c1))-x2*p2sat*b2/
((told+c2)*(told+c2));
 tnew=told-f/f1;
 }while(fabs(tnew-told)>1e-6);
cout<<“\nThe bubble point temperature is:”<<tnew;
//CALCULATION OF DEW POINT TEMPERATURE
y1=z1;
y2=1-z1;
t1sat=b1/(a1-log(p))-c1;
t2sat=b2/(a2-log(p))-c2;
tnew=y1*t1sat+y2*t2sat;
do
 {
 told=tnew;
 p1sat=exp(a1-b1/(told+c1));
 p2sat=exp(a2-b2/(told+c2));
 f=(1/p)-(y1/p1sat)-(y2/p2sat);
                   f1=(y1*b1/((told+c1)*(told+c1)))/(p1sat)+(y2*b2/
((told+c2)*(told+c2)))/(p2sat);
 tnew=told-f/f1;
 }while(fabs(tnew-told)>1e-6);
cout<<“\nThe dew point temperature is ”<<tnew;
getch();
}
```

PROGRAM 3.3

```
//PROGRAM 3.3
//program to calculate the compositions of the vapour and liquid phases
//at the given
//temperature and pressure under flash conditions, assuming Raoult’s law
//to be true
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i;
float psat[4],k[4],z[4],x[4],y[4],dpp,bpp,V,p,Vo,f,f1;
// dpp is the dew point pressure, bpp is bubble point pressure and
// V is the number of moles in the vapour phase.
psat[1]=195.75,psat[2]=97.84,psat[3]=50.32;
```

```
cout<<“Enter the composition of acetone (1), acetonitrile (2),
nitromethane (3)”;
cin>>z[1]>>z[2]>>z[3];
bpp=z[1]*psat[1]+z[2]*psat[2]+z[3]*psat[3];
dpp=1/(z[1]/psat[1]+z[2]/psat[2]+z[3]/psat[3]);
cout<<“Bubble point pressure of the mixture is “<<bpp<<“ kPa”<<endl;
cout<<“Dew point pressure of the mixture is “<<dpp<<“ kPa”<<endl;
cout<<“\nEnter the pressure in kPa in between DPP and BPP \n”;
cin>>p;
for(i=1;i<4;i++)
 {
 k[i]=psat[i]/p;
 }
cout<<“\n Enter an assumed value for the vapour fraction V”;
cin>>V;
f = f1 = 0.0;
do
 {
 Vo=V;
  for(i=1;i<4;i++)
 {
  f=f+z[i]*(k[i]-1)/(1-Vo+Vo*k[i]);
  f1=f1-z[i]*(k[i]-1)*(k[i]-1)/pow((1-Vo+Vo*k[i]),2);
 }
  V=Vo-f/f1;
 }
while(fabs(V-Vo)>1e-6);
for(i=1;i<4;i++)
 {
  x[i]=z[i]/(1-V+V*k[i]);
  y[i]=x[i]*k[i];
 }
cout<<“Mole fraction of acetone in the liquid phase is “<<x[1]<<endl;
cout<<“Mole fraction of acetone in the vapour phase is “<<y[1]<<endl;
cout<<“Mole fraction of acetonitrile in the liquid phase is “<<x[2]<<endl;
cout<<“Mole fraction of acetonitrile in the vapour phase is “<<y[2]<<endl;
cout<<“Mole fraction of nitromethane in liquid phase is “<<x[3]<<endl;
cout<<“Mole fraction of nitromethane in vapour phase is “<<y[3]<<endl;
cout<<“Number of moles in vapour phase is “<<V<<endl;
cout<<“x[1]+x[2]+x[3]=”<<x[1]+x[2]+x[3]<<endl;
cout<<“y[1]+y[2]+y[3]=”<<y[1]+y[2]+y[3]<<endl;
getch();
}
```

PROGRAM 3.4

```
//PROGRAM 3.4
//program to calculate the bubble point pressure, bubble point temperature,
//dew point pressure and dew point temperature, assuming the modified
//Raoult’s law to be true
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float p,t,a1,b1,c1,a2,b2,c2,p1sat,p2sat,r=8.314,pold,pnew,g11,g22,t1sat,t2sat;
float tnew,told,x1,x2,y1,y2,h12,h21,g1,g2,m,a12=437.98*4.186,a21=1238*4.186;
float V1=76.92,V2=18.07;
a1=16.678;
b1=3640.2;
c1=219.61;
a2=16.2887;
b2=3816.44;
c2=227.02;
//the component 1 is acetone and 2 is water. The pressure in Antoine equation
//is in kPa and temperature in deg C. a12 and a21 are in cal/mol.
//
//CALCULATION OF BPP (temperature and liquid phase composition are given)
cout<<“Calculation of BPP”<<endl;
cout<<“Enter the value of temperature in deg C and mole fraction x1”;
cin>>t>>x1;
x2=1-x1;
p1sat=exp(a1-b1/(c1+t));
p2sat=exp(a2-b2/(c2+t));
h12=V2*exp(-a12/(r*(t+273.15)))/V1;
h21=V1*exp(-a21/(r*(t+273.15)))/V2;
m=h12/(x1+x2*h12)-h21/(x2+x1*h21);
g1=exp(-log(x1+x2*h12)+x2*m);
g2=exp(-log(x2+x1*h21)-x1*m);
p=x1*g1*p1sat+x2*g2*p2sat;
cout<<“BPP=”<<p<<“kPa\n”;
//
//CALCULATION OF BPT (pressure and liquid phase composition are given)
cout<<“Calculation of BPT”<<endl;
cout<<“Enter the value of pressure in kPa and x1\n”;
cin>>p>>x1;
x2=1-x1;
t1sat=b1/(a1-log(p))-c1;
t2sat=b2/(a2-log(p))-c2;
```

```
tnew=x1*t1sat+x2*t2sat;
do
 {
 told=tnew;
 p1sat=exp(a1-b1/(c1+told));
 p2sat=exp(a2-b2/(c2+told));
 h12=V2*exp(-a12/(r*(told+273.15)))/V1;
 h21=V1*exp(-a21/(r*(told+273.15)))/V2;
 m=h12/(x1+x2*h12)-h21/(x2+x1*h21);
 g1=exp(-log(x1+x2*h12)+x2*m);
 g2=exp(-log(x2+x1*h21)-x1*m);
 p1sat=p/(g1*x1+g2*x2*(p2sat/p1sat));
 tnew=b1/(a1-log(p1sat))-c1;
 }
while(fabs(tnew-told)>.0001);
cout<<“BPT=”<<tnew<<“deg C\n”;
//
//CALCULATION OF DPP (temperature and vapour phase composition are given)
cout<<“Calculation of DPP”<<endl;
cout<<“Enter the temperature in deg C and y1\n”;
cin>>t>>y1;
y2=1-y1;
p1sat=exp(a1-b1/(c1+t));
p2sat=exp(a2-b2/(c2+t));
g1=g2=1;
g11=g22=1;
pnew=1/(y1/(g1*p1sat)+y2/(g2*p2sat));
do
 {
 pold=pnew;
 do
 {
 g1=g11;
 g2=g22;
 x1=y1*pold/(g1*p1sat);
 x2=y2*pold/(g2*p2sat);
 x1=x1/(x1+x2);
 x2=1-x1;
 h12=V2*exp(-a12/(r*(t+273.15)))/V1;
 h21=V1*exp(-a21/(r*(t+273.15)))/V2;
 m=h12/(x1+x2*h12)-h21/(x2+x1*h21);
 g11=exp(-log(x1+x2*h12)+x2*m);
 g22=exp(-log(x2+x1*h21)-x1*m);
 }
 while((fabs(g11-g1)>.001)&&(fabs(g22-g2)>.001));
 pnew=1/(y1/(g1*p1sat)+y2/(g2*p2sat));
 }
```

```
while(fabs(pnew-pold)>.0001);
cout<<“DPP=”<<pnew<<“kPa\n”;
//
//CALCULATION OF DPT (pressure and vapour phase composition are given)
cout<<“Calculation of DPT”<<endl;
cout<<“Enter the pressure in kPa and y1\n”;
cin>>p>>y1;
y2=1-y1;
t1sat=b1/(a1-log(p))-c1;
t2sat=b2/(a2-log(p))-c2;
tnew=y1*t1sat+y2*t2sat;
g11=g22=1;
do
 {
 told=tnew;
 p1sat=exp(a1-b1/(c1+told));
 p2sat=exp(a2-b2/(c2+told));
 do
 {
 g1=g11;
 g2=g22;
 x1=y1*p/(g1*p1sat);
 x2=y2*p/(g2*p2sat);
 x1=x1/(x1+x2);
 x2=1-x1;
 h12=V2*exp(-a12/(r*(told+273.15)))/V1;
 h21=V1*exp(-a21/(r*(told+273.15)))/V2;
 m=h12/(x1+x2*h12)-h21/(x2+x1*h21);
 g11=exp(-log(x1+x2*h12)+x2*m);
 g22=exp(-log(x2+x1*h21)-x1*m);
 }
 while((fabs(g11-g1)>.0001)&&(fabs(g22-g2)>.0001));
 p1sat=p*(y1/g1+y2*p1sat/(g2*p2sat));
 tnew=b1/(a1-log(p1sat))-c1;
 }
while(fabs(tnew-told)>.0001);
cout<<“DPT=”<<tnew<<“deg C\n”;
getch();
}
```

PROGRAM 3.5

```
//PROGRAM 3.5
//program to calculate the compositions of the liquid and vapour phases under
//flash conditions, assuming the modified Raoult’s law to be true
#include<iostream.h>
```

```
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
// the component 1 is acetone and 2 is water. The pressure in Antoine equation
// is in kPa and temperature in deg C. a12 and a21 are in cal/mol.
float t,p,z1,z2,a12=292.66,a21=1445.26,V1=74.05,V2=18.07,h12,h21;
float r=1.987,m,g1,g2,g1n,g2n,gb1,gb2,gd1,gd2;
float p1sat,p2sat,k1,k2,V,Vnew,bpp,dpp,pnew,pold;
float A1,A2,B1,B2,C1,C2;
float x1,x2,y1,y2,f,f1;
cout<<“Enter the temperature in deg C”;
cin>>t;
cout<<“Enter the overall composition of species 1”;
cin>>z1;
z2=1-z1;
//Listing the values of the Antoine parameters
A1=14.39155;
A2=16.26205;
B1=2795.817;
B2=3799.887;
C1=230.002;
C2=226.346;
//Calculation of BPP
x1=z1;
x2=z2;
p1sat=exp(A1-(B1/(t+C1)));
p2sat=exp(A2-(B2/(t+C2)));
h12=V2*exp(-a12/(r*(t+273.15)))/V1;
h21=V1*exp(-a21/(r*(t+273.15)))/V2;
m=(h12/(x1+x2*h12))-(h21/(x2+x1*h21));
g1=exp(-log(x1+x2*h12)+x2*m);
g2=exp(-log(x2+x1*h21)-x1*m);
p=x1*g1*p1sat+x2*g2*p2sat;
cout<<“BPP=”<<p<<“kPa\n”;
bpp=p;
gb1=g1;
gb2=g2;
//Calculation of DPP
y1=z1;
y2=z2;
p1sat=exp(A1-(B1/(t+C1)));
p2sat=exp(A2-(B2/(t+C2)));
g1=g2=1;
pnew=1/(y1/(g1*p1sat)+y2/(g2*p2sat));
```

```
g1n=g1;g2n=g2;
do
 {
 pold=pnew;
 do
 {
 g1=g1n;
 g2=g2n;
 x1=y1*pold/(g1*p1sat);
 x2=y2*pold/(g2*p2sat);
 x1=x1/(x1+x2);
 x2=1-x1;
 h12=V2*exp(-a12/(r*(t+273.15)))/V1;
 h21=V1*exp(-a21/(r*(t+273.15)))/V2;
 m=(h12/(x1+x2*h12))-(h21/(x2+x1*h21));
 g1n=exp(-log(x1+x2*h12)+x2*m);
 g2n=exp(-log(x2+x1*h21)-x1*m);
 }
 while(fabs(g1n-g1)>.0001&&fabs(g2n-g2)>.0001);
 pnew=1/(y1/(g1n*p1sat)+y2/(g2n*p2sat));
 }
while(fabs(pnew-pold)>.0001);
cout<<"DPP="<<pnew<<"\n";
dpp=pnew;
gd1=g1n;
gd2=g2n;
cout<<"Enter a pressure between "<<dpp<<" and "<<bpp<<"\n";
cin>>p;
V=(bpp-p)/(bpp-dpp);
g1=((p-dpp)*(gb1-gd1))/(bpp-dpp)+gd1;
g2=((p-dpp)*(gb2-gd2))/(bpp-dpp)+gd2;
//Calculation of distribution coefficients
do
 {
 g1n=g1;
 g2n=g2;
 k1=g1n*p1sat/p;
 k2=g2n*p2sat/p;
 do
 {
 V=Vnew;
 y1=(k1*z1)/(1-V+V*k1);
 y2=(k2*z2)/(1-V+V*k2);
 x1=y1/k1;
 x2=y2/k2;
 f=y1-x1+y2-x2;
```

```
  f1=-(z1*(k1-1)*(k1-1)/((1-V+V*k1)*(1-V+V*k1))+
  z2*(k2-1)*(k2-1)/((1-V+V*k2)*(1-V+V*k2)));
  Vnew=V-f/f1;
 }
  while(fabs(Vnew-V)>.00001);
  h12=V2*exp(-a12/(r*(t+273.15)))/V1;
  h21=V1*exp(-a21/(r*(t+273.15)))/V2;
  m=(h12/(x1+x2*h12))-(h21/(x2+x1*h21));
  g1=exp(-log(x1+x2*h12)+x2*m);
  g2=exp(-log(x2+x1*h21)-x1*m);
 }
while(fabs(g1-g1n)>.0001&&fabs(g2-g2n)>.0001);
cout<<"The number of moles in vapour phase is"<<Vnew<<"\n";
cout<<"x1+x2="<<(x1+x2)<<"\n";
cout<<"y1+y2="<<(y1+y2)<<"\n";
cout<<"x1="<<x1<<"\n";
cout<<"y1="<<y1<<"\n";
getch();
}
```

PROGRAM 3.6

```
//PROGRAM 3.6
//program to calculate the vapour pressure at the given
//temperature using the Peng–Robinson eos by comparing the fugacities of the
//liquid and vapour phases
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float w,s,t,tc,k,a,b,r=8.314,lpha,vold,vnew;
float vliq,vvap,zliq,zvap,c,d,fl,fv,pnew,p,pc,f,f1;
cout<<"Enter the temperature in deg K and assumed pressure in Pa";
cin>>t>>pnew;
cout<<"Enter the value of the critical temperature in deg K and the
critical pressure in Pa";
cin>>tc>>pc;
cout<<"Enter the value of the acentric factor";
cin>>w;
k=.37464+1.54226*w-.26992*w*w;
s=1+k*(1-pow(t/tc,.5));
lpha=pow(s,2);
a=.45724*r*r*tc*tc*lpha/pc;
b=.07780*r*tc/pc;
```

```
do
 {
  p=pnew;
  vnew=b;
 do
 {
  vold=vnew;
  f=pow(vold,3.0)*p+vold*vold*(p*b-r*t)-vold*(3.0*p*b*b+2.0*b*r*t-a);
  f=f+(p*b*b*b+b*b*r*t-a*b);
  f1=pow(vold,2.0)*3.0*p+vold*2.0*(b*p-t*r)+(a-3.0*b*b*p-2.0*r*t*b);
  vnew=vold-f/f1;
 }
  while(fabs(vnew-vold)>1e-6);
  vliq=vnew;
  zliq=p*vliq/(r*t);
  c=(a/(2.0*sqrt(2.0)*b*r*t))*(log((zliq+(1.0+sqrt(2.0))*b*p/(r*t))/
(zliq+(1.0-sqrt(2.0))*b*p/(r*t))));
  fl=p*exp(zliq-1-log(zliq-p*b/(r*t))-c);
  vnew=r*t/p;
 do
 {
  vold=vnew;
  f=pow(vold,3.0)*p+vold*vold*(p*b-r*t)-vold*(3.0*p*b*b+2.0*b*r*t-a);
  f=f+(p*b*b*b+b*b*r*t-a*b);
  f1=pow(vold,2.0)*3.0*p+vold*2.0*(b*p-t*r)+(a-3.0*b*b*p-2.0*r*t*b);
  vnew=vold-f/f1;
 }
  while(fabs(vnew-vold)>1e-6);
  vvap=vnew;
  zvap=p*vvap/(r*t);
  d=(a/(2.0*sqrt(2.0)*b*r*t))*(log((zvap+(1.0+sqrt(2.0))*b*p/(r*t))/
    (zvap+(1.0-sqrt(2.0))*b*p/(r*t))));
  fv=p*exp(zvap-1.0-log(zvap-b)-d);
  pnew=p*fl/fv;
 }
while(fabs(pnew-p)>1e-6);
cout<<“The saturated vapour pressure at “<<t<<“ deg K is “<<pnew<<“
  Pa”<<endl;
getch();
}
```

PROGRAM 3.7

```
//PROGRAM 3.7
//program to calculate the bubble point pressure using the gamma-phi approach
#include<iostream.h>
```

```
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float p,t,p1sat,p2sat,r=8.314,pnew,vc1,vc2,x1,x2,y1,y2,h12,h21,b11;
float b22,b12,vc12,pc1,pc2,pc12,w1,w2,w12,tc1,tc2,tc12,zc1,zc2,zc12;
float fc1,fc2,snew=0.0,g1,g2,f1,f2,b0,b1,tr1,tr2,tr12,k1,k2,sold,v1;
float v2,a12,a21,z,d12,A1,A2,B1,B2,C1,C2;
// read the values of tc1,tc2,pc1,pc2,w1,w2,zc1,zc2
// the data given are for the methanol (1) - water (2) system
// A1, B1, C1, A2, B2, C2 denote the Antoine constants in this program
a12=107.38*4.186;a21=469.55*4.186;
tc1=512.6;tc2=647.1;pc1=80.97*pow(10,5);pc2=220.55*pow(10,5);
w1=0.564;w2=0.345;zc1=0.224;zc2=0.229;v1=40.73*pow(10,-6);
v2=18.07*pow(10,-6);
//feed the temperature in degree C
t=100.0;x1=0.958;x2=1-x1;
A1=16.5938;
A2=16.2620;
B1=3644.3;
B2=3799.89;
C1=239.76;
C2=226.35;
p1sat=exp(A1-B1/(C1+t));
p2sat=exp(A2-B2/(C2+t));
p1sat=p1sat*1000; // converting kPa to Pa
p2sat=p2sat*1000;
t=t+273.15;
h12=(v2/v1)*exp(-a12/(r*t));
h21=(v1/v2)*exp(-a21/(r*t));
z=h12/(x1+x2*h12)-h21/(x2+x1*h21);
g1=exp(-log(x1+x2*h12)+x2*z);
g2=exp(-log(x2+x1*h21)-x1*z);
tr1=t/tc1;
b0=.083-0.422*pow(tr1,-1.6);
b1=.139-0.172*pow(tr1,-4.2);
b11=(r*tc1/pc1)*(b0+w1*b1);
tr2=t/tc2;
b0=.083-0.422*pow(tr2,-1.6);
b1=.139-0.172*pow(tr2,-4.2);
b22=(r*tc2/pc2)*(b0+w2*b1);
w12=(w1+w2)*0.5;
tc12=pow((tc1*tc2),0.5);
zc12=(zc1+zc2)*0.5;
vc1=zc1*r*tc1/pc1;vc2=zc2*r*tc2/pc2;
```

```
vc12=pow((pow(vc1,0.333333)+pow(vc2,0.33333))*0.5,3);
pc12=zc12*r*tc12/vc12;
tr12=t/tc12;
b0=.083-0.422*pow(tr12,-1.6);
b1=.139-0.172*pow(tr12,-4.2);
b12=(r*tc12/pc12)*(b0+w12*b1);
d12=2*b12-b11-b22;
p=x1*g1*p1sat+x2*g2*p2sat;
y1=x1*g1*p1sat/p;y2=x2*g2*p2sat/p;
pnew = p;
do
 {
 p=pnew;
 f1=p1sat*(exp(b11*p1sat/(r*t)))*(exp((v1*(p-p1sat)/(r*t))));
 f2=p2sat*(exp(b22*p2sat/(r*t)))*(exp((v2*(p-p2sat)/(r*t))));
 do
 {
 sold=snew;
 fc1=exp((p/(r*t))*(b11+y2*y2*d12));
 fc2=exp((p/(r*t))*(b22+y1*y1*d12));
 k1=g1*f1/(fc1*p);
 k2=g2*f2/(fc2*p);
 snew=x1*k1+x2*k2;
 y1=x1*k1/snew;
 y2=x2*k2/snew;
 }
 while(fabs(snew-sold)>1e-6);
 pnew=(x1*g1*f1/fc1)+(x2*g2*f2/fc2);
 y1=x1*g1*f1/(fc1*pnew);y2=x2*g2*f2/(fc2*pnew);
 }
while(fabs(pnew-p)>1e-6);
cout<<“fc1=”<<fc1<<endl<<“fc2=”<<fc2<<endl;
cout<<“g1=”<<g1<<endl<<“g2=”<<g2<<endl;
cout<<“k1=”<<k1<<endl<<“k2=”<<k2<<endl;
cout<<“p=”<<p<<endl<<“y1=”<<y1<<endl;
getch();
}
```

PROGRAM 3.8

```
//PROGRAM 3.8
//program to calculate the bubble point pressure using the Peng-Robinson eos
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
```

```
float t,x1,x2,y1,y2,tc1,tc2,v,vnew,pnew,p,zliq,zvap,avap,bvap;
float fc1l,fc2l,fc1v,fc2v,y1n,y2n;
float k1,k2,w1,w2,f,f1,lpha1,lpha2,r,snew,sold,pc1,pc2;
float aliq,bliq,b1,b2,a11,a22,a12,m1,m2;
clrscr();
//the data are for the CO2 (1) - n-pentane (2) system
t=377.65;x1=0.5;
cout<<“The value of x1=”<<x1<<endl;
cout<<“Enter an assumed value of y1 greater than x1 \n”;
cin>>y1;
tc1=304.2;tc2=469.7;pc1=73.83e5;pc2=33.70e5;w1=0.224;w2=0.252;
r=8.314;x2=1-x1;y2=1-y1;
k1=0.37464+1.54226*w1-0.26992*w1*w1;
k2=0.37464+1.54226*w2-0.26992*w2*w2;
m1=1+k1*(1-pow(t/tc1,0.5));
m2=1+k2*(1-pow(t/tc2,0.5));
lpha1=m1*m1;
lpha2=m2*m2;
a11=0.455724*r*r*tc1*tc1*lpha1/pc1;
a22=0.455724*r*r*tc2*tc2*lpha2/pc2;
a12=(pow(a11*a22,0.5));
b1=0.07780*r*tc1/pc1;
b2=0.07780*r*tc2/pc2;
aliq=(x1*x1*a11+x2*x2*a22+2*x1*x2*a12);
bliq=x1*b1+x2*b2;
pnew=50e5; // assumed value for pressure in Pa
snew=0.0;
do
 {
 p=pnew;
 vnew=bliq;
 do
 {
 v=vnew;
 f=pow(v,3)*p+v*v*(p*bliq-r*t)-v*(3*p*bliq*bliq+2*bliq*r*t-aliq);
 f=f+(p*bliq*bliq*bliq+bliq*bliq*r*t-aliq*bliq);
 f1=pow(v,2)*3*p+v*2*(bliq*p-r*t)+(aliq-3*bliq*bliq*p-2*r*t*bliq);
 vnew=v-(f/f1);
 }
 while(fabs(vnew-v)>1e-6);
 zliq=p*vnew/(r*t);
 fc1l=exp((b1/bliq)*(zliq-1)-log(zliq-bliq*p/(r*t))-(aliq/
(2*sqrt(2)*r*t*bliq))*
 ((2*(x1*a11+x2*a12)/aliq)-(b1/bliq))*log((zliq+(2.414*bliq*p/
(r*t)))/(zliq-
 (.414*bliq*p/(r*t)))));
```

```
  fc2l=exp((b2/bliq)*(zliq-1)-log(zliq-bliq*p/(r*t))-(aliq/
(2*sqrt(2)*r*t*bliq))*
  ((2*(x1*a12+x2*a22)/aliq)-(b2/bliq))*log((zliq+(2.414*bliq*p/
(r*t)))/(zliq-
  (.414*bliq*p/(r*t)))));
 do
 {
  sold=snew;
  avap=(y1*y1*a11+y2*y2*a22+2*y1*y2*a12);
  bvap=y1*b1+y2*b2;
  vnew=r*t/p;
 do
 {
  v=vnew;
  f=pow(v,3)*p+v*v*(p*bvap-r*t)-v*(3*p*bvap*bvap+2*bvap*r*t-avap);
  f=f+(p*bvap*bvap*bvap+bvap*bvap*r*t-avap*bvap);
  f1=pow(v,2)*3*p+v*2*(bvap*p-r*t)+(avap-3*bvap*bvap*p-2*r*t*bvap);
  vnew=v-(f/f1);
 }
  while(fabs(vnew-v)>1e-6);
  zvap=p*vnew/(r*t);
  fc1v=exp((b1/bvap)*(zvap-1)-log(zvap-bvap*p/(r*t))-(avap/
(2*sqrt(2)*r*t*bvap))*
  ((2*(y1*a11+y2*a12)/avap)-(b1/bvap))*log((zvap+(2.414*bvap*p/
(r*t)))/(zvap-
  (.414*bvap*p/(r*t)))));
  fc2v=exp((b2/bvap)*(zvap-1)-log(zvap-bvap*p/(r*t))-(avap/
(2*sqrt(2)*r*t*bvap))*
  ((2*(y1*a12+y2*a22)/avap)-(b2/bvap))*log((zvap+(2.414*bvap*p/
(r*t)))/(zvap-
  (.414*bvap*p/(r*t)))));
  k1=fc1l/fc1v;k2=fc2l/fc2v;cout<<“k1=”<<k1<<endl<<“k2=”<<k2<<endl;
  snew=k1*x1+k2*x2;
  y1=k1*x1/snew;
  y2=k2*x2/snew;
 }
  while(fabs(snew-sold)>1e-6);
  pnew=p*snew;
 }
while(fabs(pnew-p)>1e-6);
cout<<“k1=”<<k1<<endl<<“k2=”<<k2<<endl<<“bpp=”<<pnew<<endl<<“y1=”<<y1<<endl;
getch();
}
```

PROGRAM 3.9

```
//PROGRAM 3.9
//program for the solution of two simultaneous chemical reactions
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float x1,x2,x1new,x2new,f1,f2,df1dx1,df1dx2,df2dx1,df2dx2;
float d1,d2,d3,d4,d5,d6,d7,d8,d9,d10,d11,d,deltax1,deltax2;
int n;
x1new=0.9;
x2new=0.5;
n=0;
do
{
x1=x1new;
x2=x2new;
d1=(x1-x2)*pow((3*x1+x2),3);
d2=(1-x1)*(5-x1-x2)*pow((6+2*x1),2);
f1=(d1/d2)-0.575;
f2=(x2*(3*x1+x2)/((x1-x2)*(5-x1-x2)))-2.21;
d3=pow((3*x1+x2),2)*(12.0*x1-8.0*x2)/((1-x1)*(5-x1 x2)
  *(6+2*x1)*(6+2*x1));
d4=pow((3*x1+x2),3)*(x1-x2)*(8*x1*x1+6*x1*x2-24*x1+2*x2-16);
d5=pow((1-x1),2)*pow((5-x1-x2),2)*pow((6+2*x1),3);
df1dx1=d3-(d4/d5);
d6=3*(x1-x2)*(3*x1+x2)*(3*x1+x2)-pow((3*x1+x2),3);
d7=(1-x1)*(5-x1-x2)*(6+2*x1)*(6+2*x1);
d8=((x1-x2)*(pow((3*x1+x2),3)))/((1-x1)*(5-x1-x2)*(5-x1-x2)
  *(6+2*x1)*(6+2*x1));
df1dx2=(d6/d7)+d8;
d9=(x1-x2)*(x1-x2)*(5-x1-x2)*(5-x1-x2);
df2dx1=3*x2/((x1-x2)*(5-x1-x2))-(x2*(3*x1+x2)*(5-2*x1))/d9;
d10=(3*x1+2*x2)/((x1-x2)*(5-x1-x2));
d11=x2*(3*x1+x2)*(2*x2-5)/((pow((x1-x2),2))*pow((5-x1-x2),2));
df2dx2=d10-d11;
d=df1dx1*df2dx2-df1dx2*df2dx1;
deltax1=(f2*df1dx2-f1*df2dx2)/d;
deltax2=(f1*df2dx1-f2*df1dx1)/d;
x1new=x1+deltax1;
x2new=x2+deltax2;
n=n+1;
```

```
}while(fabs(x1new-x1)>1e-6&&fabs(x2new-x2)>1e-6);
cout<<"The number of iterations performed is "<<n<<endl;
cout<<x1new<<" "<<x2new<<endl;
getch();
}
```

PROGRAM 3.10

```
//PROGRAM 3.10
//program to calculate the adiabatic flame temperature (AFT) for a fuel
//case of complete conversion
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float sa,sb,sc,sd,da,db,dc,dd,t,tnew,t0=298.15,t1,n1,n2,n3,n4,f,f1,h0;
float u1=1,u2=3.5,u3=2,u4=3;
// n1, n2, n3, n4 are the number of moles entering of species
// 1, 2, 3, 4 respectively and u1, u2, u3, and u4 are their stoichiometric
// coefficients. The data is given for the reaction
// C2H6 + 3.5O2 = 2CO2 + 3H2O
// C2H6 is 1, O2 is 2, CO2 is 3 and H2O is 4
float a1=1.648,a2=6.085,a3=5.316,a4=7.700;
float b1=4.124e-2,b2=.3631e-2,b3=1.4285e-2,b4=.04594e-2;
float c1=-1.530e-5,c2=-.1709e-5,c3=-.8362e-5,c4=.2521e-5;
float d1=1.740e-9,d2=.3133e-9,d3=1.784e-9,d4=-.8587e-9;
cout<<"Enter the value of n1,n2,n3,n4\n";
cin>>n1>>n2>>n3>>n4;
cout<<"\nEnter the inlet temperature in deg C";
cin>>t1;
t1=t1+273.15;
sa=n1*a1+n2*a2+n3*a3+n4*a4;
sb=n1*b1+n2*b2+n3*b3+n4*b4;
sc=n1*c1+n2*c2+n3*c3+n4*c4;
sd=n1*d1+n2*d2+n3*d3+n4*d4;
da=u4*a4+u3*a3-u2*a2-u1*a1;
db=u4*b4+u3*b3-u2*b2-u1*b1;
dc=u4*c4+u3*c3-u2*c2-u1*c1;
dd=u4*d4+u3*d3-u2*d2-u1*d1;
h0=(u4*(-57.7979)+u3*(-94.052)-u2*0-u1*(-20.236))*1000;
tnew=1000;
//for various old values of tnew the final answer is the same
do
 {
```

```
  t=tnew;
  f=sa*(t-t1)+(sb/2)*(t*t-t1*t1)+(sc/3)*(t*t*t-t1*t1*t1)+(sd/4)
    *(t*t*t*t-t1*t1*t1*t1);
  f=f+h0+da*(t-t0)+(db/2)*(t*t-t0*t0)+(dc/3)*(t*t*t-t0*t0*t0)+(dd/4)
    *(t*t*t*t-t0*t0*t0*t0);
  f1=sa+sb*t+sc*t*t+sd*t*t*t+da+db*t+dc*t*t+dd*t*t*t;
  tnew=t-f/f1;
  }while(fabs((tnew-t)/tnew)>1e-6);
cout<<"AFT="<<tnew;
getch();
}
```

PROGRAM 4.1

```
//PROGRAM 4.1
//program to solve an ordinary differential equation by the Runge-Kutta method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float h,x0,xf,y,k1,k2,k3,k4;
int n;
x0=0.00000,y=2.00000;
float func(float,float);
cout<<"\t\t\t OUTPUT"<<endl;
cout<<"\nEnter the value of x at which y is required: ";
cin>>xf;
cout<<"\tEnter the value of step length (h): ";
cin>>h;
n=(xf-x0)/h;
for(int i=0;i<=n-1;i++)
{
k1=h*func(x0,y);
k2=h*func(x0+0.5*h,y+0.5*k1);
k3=h*func(x0+0.5*h,y+0.5*k2);
k4=h*func(x0+h,y+k3);
y=y+((k1+2.0*k2+2.0*k3+k4)/6.0);
x0=x0+h;
}
cout<<"\t Value found by Runge-Kutta method at given x: "<<y;
cout<<endl;
getch();
}
float func(float x, float y)
{
```

```
float f=-y/(1.0+x);
return(f);
}
```

PROGRAM 4.2

```
//PROGRAM 4.2
//program to determine the velocity of a particle in a pneumatic conveyor
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float h,z0,z,zf,y0,y,vp,k1,k2,k3,k4;
int n;
z0=0.00000,y0=0.00000;
float func(float,float);
cout<<"\t\t\t OUTPUT"<<endl;
cout<<"\nEnter the value of z in m at which vp is required: ";
cin>>zf;
cout<<"\tEnter the value of step length (h): ";
cin>>h;
n=(zf-z0)/h;
for(int i=0;i<=n-1;i++)
{
k1=h*func(z0,y0);
k2=h*func(z0+0.5*h,y0+0.5*k1);
k3=h*func(z0+0.5*h,y0+0.5*k2);
k4=h*func(z0+h,y0+k3);
y=y0+((k1+2.0*k2+2.0*k3+k4)/6.0);
z0=z0+h;
y0=y;
vp=sqrt(y);
cout<<"\t Value found at z = "<<z0<< " = "<<vp<<endl;
}
cout<<"\t Value found by Runge-Kutta method at given z: "<<vp;
cout<<endl;
getch();
}
float func(float a, float b)
{
float rep=19.648*(12.0-sqrt(b));
float cd=24.0*(1.0+0.15*pow(rep,0.687))/rep;
float f=6.55*cd*(12.0-sqrt(b))*(12.0-sqrt(b))-19.594;
return(f);
}
```

PROGRAM 4.3

```
//PROGRAM 4.3
//program to solve two simultaneous ordinary differential equations
//by Runge-Kutta method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float h,x0,xf,y,z,k1,k2,k3,k4,l1,l2,l3,l4;
int n;
x0=0.00000,y=2.00000,z=1.00000;
float func1(float,float,float);
float func2(float,float,float);
cout<<"\t\t\t OUTPUT"<<endl;
cout<<"\nEnter the value of x at which y and z are required: ";
cin>>xf;
cout<<"\tEnter the value of step length (h): ";
cin>>h;
n=(xf-x0)/h;
for(int i=0;i<=n-1;i++)
{
k1=h*func1(x0,y,z);
l1=h*func2(x0,y,z);
k2=h*func1(x0+0.5*h,y+0.5*k1,z+0.5*l1);
l2=h*func2(x0+0.5*h,y+0.5*k1,z+0.5*l1);
k3=h*func1(x0+0.5*h,y+0.5*k2,z+0.5*l2);
l3=h*func2(x0+0.5*h,y+0.5*k2,z+0.5*l2);
k4=h*func1(x0+h,y+k3,z+l3);
l4=h*func2(x0+h,y+k3,z+l3);
y=y+((k1+2.0*k2+2.0*k3+k4)/6.0);
z=z+((l1+2.0*l2+2.0*l3+l4)/6.0);
x0=x0+h;
}
cout<<"\t Value at given x: "<<y<<" "<<z;
cout<<endl;
getch();
}
float func1(float x, float y, float z)
{
float f=z;
return(f);
}
float func2(float x, float y, float z)
{
```

```
float f=-y;
return(f);
}
```

PROGRAM 4.4

```
//PROGRAM 4.4
//program to solve three simultaneous ordinary differential equations
//by the Runge-Kutta method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
double h,t0,tf,temp1,temp2,temp3,k1,k2,k3,k4;
double l1,l2,l3,l4,m1,m2,m3,m4;
long n;
t0=0.00000,temp1=20.00000,temp2=20.00000,temp3=20.00000;
double func1(double,double,double,double);
double func2(double,double,double,double);
double func3(double,double,double,double);
cout<<"\t\t\t OUTPUT"<<endl;
cout<<"\nEnter the value of t in sec at which temperatures are required: ";
cin>>tf;
cout<<"\tEnter the value of the step length (h): ";
cin>>h;
n=(tf-t0)/h;
cout<<"The number n is = "<<n<<endl;
for(long i=0;i<=n-1;i++)
{
k1=h*func1(t0,temp1,temp2,temp3);
l1=h*func2(t0,temp1,temp2,temp3);
m1=h*func3(t0,temp1,temp2,temp3);
k2=h*func1(t0+0.5*h,temp1+0.5*k1,temp2+0.5*l1,temp3+0.5*m1);
l2=h*func2(t0+0.5*h,temp1+0.5*k1,temp2+0.5*l1,temp3+0.5*m1);
m2=h*func3(t0+0.5*h,temp1+0.5*k1,temp2+0.5*l1,temp3+0.5*m1);
k3=h*func1(t0+0.5*h,temp1+0.5*k2,temp2+0.5*l2,temp3+0.5*m2);
l3=h*func2(t0+0.5*h,temp1+0.5*k2,temp2+0.5*l2,temp3+0.5*m2);
m3=h*func3(t0+0.5*h,temp1+0.5*k2,temp2+0.5*l2,temp3+0.5*m2);
k4=h*func1(t0+h,temp1+k3,temp2+l3,temp3+m3);
l4=h*func2(t0+h,temp1+k3,temp2+l3,temp3+m3);
m4=h*func3(t0+h,temp1+k3,temp2+l3,temp3+m3);
temp1=temp1+((k1+2.0*k2+2.0*k3+k4)/6.0);
temp2=temp2+((l1+2.0*l2+2.0*l3+l4)/6.0);
temp3=temp3+((m1+2.0*m2+2.0*m3+m4)/6.0);
```

```
t0=t0+h;
}
cout<<"\t Value at given t: "<<temp1<<" "<<temp2<<" "<<temp3;
cout<<endl;
getch();
}
double func1(double t, double temp1, double temp2, double temp3)
{
double f=0.065-0.0021*temp1;
return(f);
}
double func2(double t, double temp1, double temp2, double temp3)
{
double f=0.002*temp1-0.0021*temp2+0.025;
return(f);
}
double func3(double t, double temp1, double temp2, double temp3)
{
double f=0.002*temp2-0.0021*temp3+0.025;
return(f);
}
```

PROGRAM 4.5

```
//PROGRAM 4.5
//program to solve three simultaneous ordinary differential equations
//for the reaction a -> b -> c by the Runge-Kutta fourth order method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float h,t0,tf,a,b,c,k1,k2,k3,k4;
float l1,l2,l3,l4,m1,m2,m3,m4;
int n;
t0=0.00000,a=1.00000,b=0.00000,c=0.00000;
float func1(float,float,float,float);
float func2(float,float,float,float);
float func3(float,float,float,float);
cout<<"\t\t\t OUTPUT"<<endl;
cout<<"\nEnter the value of t in sec at which concentrations are required: ";
cin>>tf;
cout<<"\tEnter the value of step length (h): ";
cin>>h;
n=(tf-t0)/h;
```

```
cout<<"The number n is "<<n<<endl;
for(int i=0;i<=n-1;i++)
{
k1=h*func1(t0,a,b,c);
l1=h*func2(t0,a,b,c);
m1=h*func3(t0,a,b,c);
k2=h*func1(t0+0.5*h,a+0.5*k1,b+0.5*l1,c+0.5*m1);
l2=h*func2(t0+0.5*h,a+0.5*k1,b+0.5*l1,c+0.5*m1);
m2=h*func3(t0+0.5*h,a+0.5*k1,b+0.5*l1,c+0.5*m1);
k3=h*func1(t0+0.5*h,a+0.5*k2,b+0.5*l2,c+0.5*m2);
l3=h*func2(t0+0.5*h,a+0.5*k2,b+0.5*l2,c+0.5*m2);
m3=h*func3(t0+0.5*h,a+0.5*k2,b+0.5*l2,c+0.5*m2);
k4=h*func1(t0+h,a+k3,b+l3,c+m3);
l4=h*func2(t0+h,a+k3,b+l3,c+m3);
m4=h*func3(t0+h,a+k3,b+l3,c+m3);
a=a+((k1+2.0*k2+2.0*k3+k4)/6.0);
b=b+((l1+2.0*l2+2.0*l3+l4)/6.0);
c=c+((m1+2.0*m2+2.0*m3+m4)/6.0);
t0=t0+h;
}
cout<<"\t Value at given t: "<<a<<" "<<b<<" "<<c<<endl;
getch();
}
float func1(float t, float a, float b, float c)
{
float f=-a;
return(f);
}
float func2(float t, float a, float b, float c)
{
float f=a-b;
return(f);
}
float func3(float t, float a, float b, float c)
{
float f=b;
return(f);
}
```

PROGRAM 4.6

```
//PROGRAM 4.6
//program to solve four simultaneous ordinary differential equations
//for the reactions a + b -> c and b + c -> d by the Runge-Kutta method
#include<iostream.h>
#include<conio.h>
```

```
#include<math.h>
void main()
{
clrscr();
double h,t0,tf,a,b,c,d,k1,k2,k3,k4;
double l1,l2,l3,l4,m1,m2,m3,m4,n1,n2,n3,n4;
long n;
t0=0.00000,a=1.00000,b=1.00000,c=0.00000,d=0.00000;
double func1(double,double,double,double,double);
double func2(double,double,double,double,double);
double func3(double,double,double,double,double);
double func4(double,double,double,double,double);
cout<<“\t\t\t OUTPUT”<<endl;
cout<<“\nEnter the value of t in sec at which concentrations are required: “;
cin>>tf;
cout<<“\tEnter the value of step length (h): “;
cin>>h;
n=(tf-t0)/h;
cout<<“The number n is = “<<n<<endl;
for(long i=0;i<=n-1;i++)
{
k1=h*func1(t0,a,b,c,d);
l1=h*func2(t0,a,b,c,d);
m1=h*func3(t0,a,b,c,d);
n1=h*func4(t0,a,b,c,d);
k2=h*func1(t0+0.5*h,a+0.5*k1,b+0.5*l1,c+0.5*m1,d+0.5*n1);
l2=h*func2(t0+0.5*h,a+0.5*k1,b+0.5*l1,c+0.5*m1,d+0.5*n1);
m2=h*func3(t0+0.5*h,a+0.5*k1,b+0.5*l1,c+0.5*m1,d+0.5*n1);
n2=h*func4(t0+0.5*h,a+0.5*k1,b+0.5*l1,c+0.5*m1,d+0.5*n1);
k3=h*func1(t0+0.5*h,a+0.5*k2,b+0.5*l2,c+0.5*m2,d+0.5*n2);
l3=h*func2(t0+0.5*h,a+0.5*k2,b+0.5*l2,c+0.5*m2,d+0.5*n2);
m3=h*func3(t0+0.5*h,a+0.5*k2,b+0.5*l2,c+0.5*m2,d+0.5*n2);
n3=h*func4(t0+0.5*h,a+0.5*k2,b+0.5*l2,c+0.5*m2,d+0.5*n2);
k4=h*func1(t0+h,a+k3,b+l3,c+m3,d+n3);
l4=h*func2(t0+h,a+k3,b+l3,c+m3,d+n3);
m4=h*func3(t0+h,a+k3,b+l3,c+m3,d+n3);
n4=h*func4(t0+h,a+k3,b+l3,c+m3,d+n3);
a=a+((k1+2.0*k2+2.0*k3+k4)/6.0);
b=b+((l1+2.0*l2+2.0*l3+l4)/6.0);
c=c+((m1+2.0*m2+2.0*m3+m4)/6.0);
d=d+((n1+2.0*n2+2.0*n3+n4)/6.0);
t0=t0+h;
}
cout<<“\t Value at given t: “<<a<<“ “<<b<<“ “<<c<<“ “<<d<<endl;
getch();
}
```

```
double func1(double t, double a, double b, double c, double d)
{
double f=-a*b;
return(f);
}
double func2(double t, double a, double b, double c, double d)
{
double f=-a*b-b*c;
return(f);
}
double func3(double t, double a, double b, double c, double d)
{
double f=a*b-b*c;
return(f);
}
double func4(double t, double a, double b, double c, double d)
{
double f=b*c;
return(f);
}
```

PROGRAM 4.7

```
//PROGRAM 4.7
//program to solve ordinary differential equations in a non-isothermal
//tubular reactor by the Runge-Kutta method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float h,z0,zf,x,t,k1,k2,k3,k4,l1,l2,l3,l4;
int n;
z0=0.00000,x=0.00000,t=294.15;
float func1(float,float,float);
float func2(float,float,float);
cout<<"\t\t\t OUTPUT"<<endl;
cout<<"\nEnter the value of z in m at which x and t are required: ";
cin>>zf;
cout<<"\tEnter the value of step length (h): ";
cin>>h;
n=(zf-z0)/h;
for(int i=0;i<=n-1;i++)
{
```

```
k1=h*func1(z0,x,t);
l1=h*func2(z0,x,t);
k2=h*func1(z0+0.5*h,x+0.5*k1,t+0.5*l1);
l2=h*func2(z0+0.5*h,x+0.5*k1,t+0.5*l1);
k3=h*func1(z0+0.5*h,x+0.5*k2,t+0.5*l2);
l3=h*func2(z0+0.5*h,x+0.5*k2,t+0.5*l2);
k4=h*func1(z0+h,x+k3,t+l3);
l4=h*func2(z0+h,x+k3,t+l3);
x=x+((k1+2.0*k2+2.0*k3+k4)/6.0);
t=t+((l1+2.0*l2+2.0*l3+l4)/6.0);
z0=z0+h;
}
cout<<"\t Value at given z: "<<x<<" "<<t<<endl;
cout<<endl;
getch();
}
float func1(float z, float x, float t)
{
float f=0.0527*(1-x)*exp(33.68*(1-388.71/t));
return(f);
}
float func2(float z, float x, float t)
{
float f=7.665*(388.71-t)-29554.1*0.0527*(1-x)*exp(33.68*(1-388.71/t));
return(f);
}
```

PROGRAM 7.1

```
//PROGRAM 7.1
//program to calculate the concentration profile in a
//tubular reactor with axial dispersion (second order reaction)
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,n,i1,n1,k,iter;
float a[101],b[101],c[101],d[101],x[101],x1[101],beta[101],gamma[101];
for(i=2;i<=20;++i)
{a[i]=2.0004;
}
a[21]=2.0008;
c[1]=2.0008;
for(i=2;i<=20;++i)
```

```
{c[i]=0.0004;
}
d[1]=-20004.0;
for(i=2;i<=21;++i)
{d[i]=0.0;
}
for(i=1;i<=21;++i)
{x[i]=0.0;
}
iter=0;
do
{
iter=iter+1;
for(i=1;i<=21;++i)
{x1[i]=x[i];}
b[1]=-20005.9992-x1[1];
for(i=2;i<=21;++i)
{b[i]=-2.0008-x1[i];
}
i=1;
n=21;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
}while(fabs(x[12]-x1[12])>1e-6&&fabs(x[18]-x1[18])>1e-6);
cout<<“\t\t\t THE SOLUTION BY TDMA”<<endl;
for(i=1;i<=21;++i)
{
cout<<“x[“<<i<<“] = “<<x[i]<<endl;
}
cout<<“Number of iterations is “<<iter;
getch();
}
```

PROGRAM 7.2

```
//PROGRAM 7.2
//program to calculate the concentration profile in a tubular reactor
//with axial dispersion in which two parallel reactions take place
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int n,m,l,i,j,k,jj,kp1,nn,ip1;
float a[90][91],x[90],x1[90],sum,big,ab,quot,t;
n=84;
cout<<n<<endl;
m=n+1;
l=n-1;
for(i=1;i<=n;i++)
{
for(j=1;j<=m;j++)
{
a[i][j]=0.0;
}
}
for(i=1;i<=84;i++)
{x[i]=0.01;}
do
{
for(i=1;i<=84;i++)
{x1[i]=x[i];}
a[1][1]=-20005.9992-x1[2];
a[1][5]=2.0008;
a[2][2]=-20005.9992-x1[1]-x1[3];
a[2][6]=2.0008;
a[3][3]=-20005.9992-x1[2];
a[3][7]=2.0008;
a[4][4]=-20005.9992;
a[4][8]=2.0008;
a[5][1]=2.0004;
a[5][5]=-2.0008-x1[6];
a[5][9]=0.0004;
a[6][2]=2.0004;
a[6][6]=-2.0008-x1[5]-x1[7];
a[6][10]=0.0004;
a[7][3]=2.0004;
a[7][7]=-2.0008-x1[6];
```

```
a[7][11]=0.0004;
a[8][4]=2.0004;
a[8][8]=-2.0008;
a[8][12]=0.0004;
a[9][5]=2.0004;
a[9][9]=-2.0008-x1[10];
a[9][13]=0.0004;
a[10][6]=2.0004;
a[10][10]=-2.0008-x1[9]-x1[11];
a[10][14]=0.0004;
a[11][7]=2.0004;
a[11][11]=-2.0008-x1[10];
a[11][15]=0.0004;
a[12][8]=2.0004;
a[12][12]=-2.0008;
a[12][16]=0.0004;
a[13][9]=2.0004;
a[13][13]=-2.0008-x1[14];
a[13][17]=0.0004;
a[14][10]=2.0004;
a[14][14]=-2.0008-x1[13]-x1[15];
a[14][18]=0.0004;
a[15][11]=2.0004;
a[15][15]=-2.0008-x1[14];
a[15][19]=0.0004;
a[16][12]=2.0004;
a[16][16]=-2.0008;
a[16][20]=0.0004;
a[17][13]=2.0004;
a[17][17]=-2.0008-x1[18];
a[17][21]=0.0004;
a[18][14]=2.0004;
a[18][18]=-2.0008-x1[17]-x1[19];
a[18][22]=0.0004;
a[19][15]=2.0004;
a[19][19]=-2.0008-x1[18];
a[19][23]=0.0004;
a[20][16]=2.0004;
a[20][20]=-2.0008;
a[20][24]=0.0004;
a[21][17]=2.0004;
a[21][21]=-2.0008-x1[22];
a[21][25]=0.0004;
a[22][18]=2.0004;
a[22][22]=-2.0008-x1[21]-x1[23];
a[22][26]=0.0004;
```

```
a[23][19]=2.0004;
a[23][23]=-2.0008-x1[22];
a[23][27]=0.0004;
a[24][20]=2.0004;
a[24][24]=-2.0008;
a[24][28]=0.0004;
a[25][21]=2.0004;
a[25][25]=-2.0008-x1[26];
a[25][29]=0.0004;
a[26][22]=2.0004;
a[26][26]=-2.0008-x1[25]-x1[27];
a[26][30]=0.0004;
a[27][23]=2.0004;
a[27][27]=-2.0008-x1[26];
a[27][31]=0.0004;
a[28][24]=2.0004;
a[28][28]=-2.0008;
a[28][32]=0.0004;
a[29][25]=2.0004;
a[29][29]=-2.0008-x1[30];
a[29][33]=0.0004;
a[30][26]=2.0004;
a[30][30]=-2.0008-x1[29]-x1[31];
a[30][34]=0.0004;
a[31][27]=2.0004;
a[31][31]=-2.0008-x1[30];
a[31][35]=0.0004;
a[32][28]=2.0004;
a[32][32]=-2.0008;
a[32][36]=0.0004;
a[33][29]=2.0004;
a[33][33]=-2.0008-x1[34];
a[33][37]=0.0004;
a[34][30]=2.0004;
a[34][34]=-2.0008-x1[33]-x1[35];
a[34][38]=0.0004;
a[35][31]=2.0004;
a[35][35]=-2.0008-x1[34];
a[35][39]=0.0004;
a[36][32]=2.0004;
a[36][36]=-2.0008;
a[36][40]=0.0004;
a[37][33]=2.0004;
a[37][37]=-2.0008-x1[38];
a[37][41]=0.0004;
a[38][34]=2.0004;
```

```
a[38][38]=-2.0008-x1[37]-x1[39];
a[38][42]=0.0004;
a[39][35]=2.0004;
a[39][39]=-2.0008-x1[38];
a[39][43]=0.0004;
a[40][36]=2.0004;
a[40][40]=-2.0008;
a[40][44]=0.0004;
a[41][37]=2.0004;
a[41][41]=-2.0008-x1[42];
a[41][45]=0.0004;
a[42][38]=2.0004;
a[42][42]=-2.0008-x1[41]-x1[43];
a[42][46]=0.0004;
a[43][39]=2.0004;
a[43][43]=-2.0008-x1[42];
a[43][47]=0.0004;
a[44][40]=2.0004;
a[44][44]=-2.0008;
a[44][48]=0.0004;
a[45][41]=2.0004;
a[45][45]=-2.0008-x1[46];
a[45][49]=0.0004;
a[46][42]=2.0004;
a[46][46]=-2.0008-x1[45]-x1[47];
a[46][50]=0.0004;
a[47][43]=2.0004;
a[47][47]=-2.0008-x1[46];
a[47][51]=0.0004;
a[48][44]=2.0004;
a[48][48]=-2.0008;
a[48][52]=0.0004;
a[49][45]=2.0004;
a[49][49]=-2.0008-x1[50];
a[49][53]=0.0004;
a[50][46]=2.0004;
a[50][50]=-2.0008-x1[49]-x1[51];
a[50][54]=0.0004;
a[51][47]=2.0004;
a[51][51]=-2.0008-x1[50];
a[51][55]=0.0004;
a[52][48]=2.0004;
a[52][52]=-2.0008;
a[52][56]=0.0004;
a[53][49]=2.0004;
a[53][53]=-2.0008-x1[54];
```

```
a[53][57]=0.0004;
a[54][50]=2.0004;
a[54][54]=-2.0008-x1[53]-x1[55];
a[54][58]=0.0004;
a[55][51]=2.0004;
a[55][55]=-2.0008-x1[54];
a[55][59]=0.0004;
a[56][52]=2.0004;
a[56][56]=-2.0008;
a[56][60]=0.0004;
a[57][53]=2.0004;
a[57][57]=-2.0008-x1[58];
a[57][61]=0.0004;
a[58][54]=2.0004;
a[58][58]=-2.0008-x1[57]-x1[59];
a[58][62]=0.0004;
a[59][55]=2.0004;
a[59][59]=-2.0008-x1[58];
a[59][63]=0.0004;
a[60][56]=2.0004;
a[60][60]=-2.0008;
a[60][64]=0.0004;
a[61][57]=2.0004;
a[61][61]=-2.0008-x1[62];
a[61][65]=0.0004;
a[62][58]=2.0004;
a[62][62]=-2.0008-x1[61]-x1[63];
a[62][66]=0.0004;
a[63][59]=2.0004;
a[63][63]=-2.0008-x1[62];
a[63][67]=0.0004;
a[64][60]=2.0004;
a[64][64]=-2.0008;
a[64][68]=0.0004;
a[65][61]=2.0004;
a[65][65]=-2.0008-x1[66];
a[65][69]=0.0004;
a[66][62]=2.0004;
a[66][66]=-2.0008-x1[65]-x1[67];
a[66][70]=0.0004;
a[67][63]=2.0004;
a[67][67]=-2.0008-x1[66];
a[67][71]=0.0004;
a[68][64]=2.0004;
a[68][68]=-2.0008;
a[68][72]=0.0004;
```

```
a[69][65]=2.0004;
a[69][69]=-2.0008-x1[70];
a[69][73]=0.0004;
a[70][66]=2.0004;
a[70][70]=-2.0008-x1[69]-x1[71];
a[70][74]=0.0004;
a[71][67]=2.0004;
a[71][71]=-2.0008-x1[70];
a[71][75]=0.0004;
a[72][68]=2.0004;
a[72][72]=-2.0008;
a[72][76]=0.0004;
a[73][69]=2.0004;
a[73][73]=-2.0008-x1[74];
a[73][77]=0.0004;
a[74][70]=2.0004;
a[74][74]=-2.0008-x1[73]-x1[75];
a[74][78]=0.0004;
a[75][71]=2.0004;
a[75][75]=-2.0008-x1[74];
a[75][79]=0.0004;
a[76][72]=2.0004;
a[76][76]=-2.0008;
a[76][80]=0.0004;
a[77][73]=2.0004;
a[77][77]=-2.0008-x1[78];
a[77][81]=0.0004;
a[78][74]=2.0004;
a[78][78]=-2.0008-x1[77]-x1[79];
a[78][82]=0.0004;
a[79][75]=2.0004;
a[79][79]=-2.0008-x1[78];
a[79][83]=0.0004;
a[80][76]=2.0004;
a[80][80]=-2.0008;
a[80][84]=0.0004;
a[81][77]=2.0008;
a[81][81]=-2.0008-x1[82];
a[82][78]=2.0008;
a[82][82]=-2.0008-x1[81]-x1[83];
a[83][79]=2.0008;
a[83][83]=-2.0008-x1[82];
a[84][80]=2.0008;
a[84][84]=-2.0008;
a[1][85]=-20004.0;
a[2][85]=-20004.0;
```

```
a[3][85]=-x1[1]*x1[2];
a[4][85]=-x1[2]*x1[3];
a[5][85]=0.0;
a[6][85]=0.0;
a[7][85]=-x1[5]*x1[6];
a[8][85]=-x1[6]*x1[7];
a[9][85]=0.0;
a[10][85]=0.0;
a[11][85]=-x1[9]*x1[10];
a[12][85]=-x1[10]*x1[11];
a[13][85]=0.0;
a[14][85]=0.0;
a[15][85]=-x1[13]*x1[14];
a[16][85]=-x1[14]*x1[15];
a[17][85]=0.0;
a[18][85]=0.0;
a[19][85]=-x1[17]*x1[18];
a[20][85]=-x1[18]*x1[19];
a[21][85]=0.0;
a[22][85]=0.0;
a[23][85]=-x1[21]*x1[22];
a[24][85]=-x1[22]*x1[23];
a[25][85]=0.0;
a[26][85]=0.0;
a[27][85]=-x1[25]*x1[26];
a[28][85]=-x1[26]*x1[27];
a[29][85]=0.0;
a[30][85]=0.0;
a[31][85]=-x1[29]*x1[30];
a[32][85]=-x1[30]*x1[31];
a[33][85]=0.0;
a[34][85]=0.0;
a[35][85]=-x1[33]*x1[34];
a[36][85]=-x1[34]*x1[35];
a[37][85]=0.0;
a[38][85]=0.0;
a[39][85]=-x1[37]*x1[38];
a[40][85]=-x1[38]*x1[39];
a[41][85]=0.0;
a[42][85]=0.0;
a[43][85]=-x1[41]*x1[42];
a[44][85]=-x1[42]*x1[43];
a[45][85]=0.0;
a[46][85]=0.0;
a[47][85]=-x1[45]*x1[46];
a[48][85]=-x1[46]*x1[47];
```

```
a[49][85]=0.0;
a[50][85]=0.0;
a[51][85]=-x1[49]*x1[50];
a[52][85]=-x1[50]*x1[51];
a[53][85]=0.0;
a[54][85]=0.0;
a[55][85]=-x1[53]*x1[54];
a[56][85]=-x1[54]*x1[55];
a[57][85]=0.0;
a[58][85]=0.0;
a[59][85]=-x1[57]*x1[58];
a[60][85]=-x1[58]*x1[59];
a[61][85]=0.0;
a[62][85]=0.0;
a[63][85]=-x1[61]*x1[62];
a[64][85]=-x1[62]*x1[63];
a[65][85]=0.0;
a[66][85]=0.0;
a[67][85]=-x1[65]*x1[66];
a[68][85]=-x1[66]*x1[67];
a[69][85]=0.0;
a[70][85]=0.0;
a[71][85]=-x1[69]*x1[70];
a[72][85]=-x1[70]*x1[71];
a[73][85]=0.0;
a[74][85]=0.0;
a[75][85]=-x1[73]*x1[74];
a[76][85]=-x1[74]*x1[75];
a[77][85]=0.0;
a[78][85]=0.0;
a[79][85]=-x1[77]*x1[78];
a[80][85]=-x1[78]*x1[79];
a[81][85]=0.0;
a[82][85]=0.0;
a[83][85]=-x1[81]*x1[82];
a[84][85]=-x1[82]*x1[83];
for(k=1;k<=l;k++)
{
big=fabs(a[k][k]);
jj=k;
kp1=k+1;
for(i=kp1;i<=n;i++)
{
ab=fabs(a[i][k]);
if((big-ab)<0.0)
{
```

```
big=ab;
jj=i;
}
}
if((jj-k)>0)
{
for(j=k;j<=m;j++)
{
t=a[jj][j];
a[jj][j]=a[k][j];
a[k][j]=t;
}
}
for(i=kp1;i<=n;i++)
{
quot=a[i][k]/a[k][k];
for(j=kp1;j<=m;j++)
{
a[i][j]=a[i][j]-quot*a[k][j];
}
}
for(i=kp1;i<=n;i++)
{
a[i][k]=0.0;
}
}
x[n]=a[n][m]/a[n][n];
for(nn=1;nn<=l;nn++)
{
sum=0.0;
i=n-nn;
ip1=i+1;
for(j=ip1;j<=n;j++)
{
sum=sum+a[i][j]*x[j];
}
x[i]=(a[i][m]-sum)/a[i][i];
}
}while(fabs(x[21]-x1[21])>1e-6&&fabs(x[84]-x1[84])>1e-6);
for(i=1;i<=n;i++)
{cout<<x[i]<<endl;}
getch();
}
```

PROGRAM 8.1

```
//PROGRAM 8.1
//program to calculate the concentration profile along the radius for
//reaction-diffusion in a spherical catalyst pellet (second order
//isothermal reaction)
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,n,i1,n1,k,iter;
float a[105],b[105],x1[105],c[105],d[105],x[105],beta[105],gamma[105];
for(i=1;i<=100;++i)
{x[i]=0.0;
}
//loop starts from here
iter=0;
do
{
iter=iter+1;
for(i=1;i<=100;++i)
{x1[i]=x[i];
}
for(i=2;i<=100;++i)
{a[i]=1.0-(1.0/(i-1.0));
}
b[1]=-6.0-0.01*x1[1];
for(i=2;i<=100;++i)
{b[i]=-2.0-0.01*x1[i];
}
c[1]=6.0;
for(i=2;i<=99;++i)
{c[i]=1.0+(1.0/(i-1.0));;
}
for(i=1;i<=99;++i)
{d[i]=0.0;
}
d[100]=-100.0/99.0;
i=1;
n=100;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
```

```
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
}while(fabs(x[1]-x1[1])>1e-6&&fabs(x[100]-x1[100])>1e-6);
cout<<"\t\t\t THE SOLUTION BY TDMA"<<endl;
for(i=1;i<=100;++i)
{
cout<<"x["<<i<<"] = "<<x[i]<<endl;
}
cout<<"Number of iterations is "<<iter;
getch();
}
```

PROGRAM 8.2

```
//PROGRAM 8.2
//program to calculate the concentration profile along the radius for
//reaction-diffusion in a spherical catalyst pellet (non-isothermal, beta=1)
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,n,i1,n1,k,iter;
float a[105],b[105],x1[105],c[105],d[105],x[105],beta[105],gamma[105];
for(i=1;i<=100;++i)
{x[i]=0.0;
}
iter=0;
//loop starts from here
do
{
iter=iter+1;
for(i=1;i<=100;++i)
{x1[i]=x[i];
}
for(i=2;i<=100;++i)
```

```
{a[i]=1.0-(1.0/(i-1.0));
}
b[1]=-6.0-0.01*exp((1.0-x1[1])/(2.0-x1[1]));
for(i=2;i<=100;++i)
{b[i]=-2.0-0.01*exp((1.0-x1[i])/(2.0-x1[i]));
}
c[1]=6.0;
for(i=2;i<=99;++i)
{c[i]=1.0+(1.0/(i-1.0));;
}
for(i=1;i<=99;++i)
{d[i]=0.0;
}
d[100]=-100.0/99.0;
i=1;
n=100;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
}while(fabs(x[1]-x1[1])>1e-6&&fabs(x[100]-x1[100])>1e-6);
cout<<"\t\t\t THE SOLUTION BY TDMA"<<endl;
for(i=1;i<=100;++i)
{
cout<<"x["<<i<<"] = "<<x[i]<<endl;
}
cout<<"Number of iterations is "<<iter;
getch();
}
```

PROGRAM 9.1

```
//PROGRAM 9.1
//program to calculate the temperature profile in a rectangular
//slab during transient heat conduction
```

```
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,n,i1,n1,k;
float a[21],b[21],c[21],d[21],x[21],beta[21],gamma[21];
float x1old,x2old,x3old,x4old,time,timef;
x[1]=20.0;
x[2]=20.0;
x[3]=20.0;
x[4]=20.0;
time=0.0;
timef=3.0;
//a is subdiagonal, b is diagonal and c is superdiagonal
a[2]=1.0;
a[3]=1.0;
a[4]=1.0;
b[1]=-1.5;
b[2]=-3.0;
b[3]=-3.0;
b[4]=-3.0;
c[1]=1.0;
c[2]=1.0;
c[3]=1.0;
for(time=0.1;time<timef;time=time+0.1)
{
x1old=x[1];
x2old=x[2];
x3old=x[3];
x4old=x[4];
d[1]=-0.5*x1old;
d[2]=-x2old;
d[3]=-x3old;
d[4]=-x4old-300.0;
i=1;
n=4;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
```

```
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
cout<<“\t\t\t THE SOLUTION BY TDMA AT TIME = “<<time<<“ seconds”<<endl;
cout<<x[1]<<“ “<<x[2]<<“ “<<x[3]<<“ “<<x[4]<<endl;
}
getch();
}
```

PROGRAM 9.2

```
//PROGRAM 9.2
//program to calculate the concentration profile in a sphere
//during transient diffusion of drug from spherical pellet
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,n,i1,n1,k;
float a[21],b[21],c[21],d[21],x[21],beta[21],gamma[21];
float x1old,x2old,x3old,x4old,x5old,x6old,x7old,x8old,x9old,x10old,time,timef;
for(i=1;i<=10;++i)
{
x[i]=68.9;
}
time=0.0;
timef=10800.0;
//a is subdiagonal, b is diagonal and c is superdiagonal
for(i=2;i<=10;++i)
{
a[i]=-(1.0-1.0/(i-1.0));
}
for(i=2;i<=10;++i)
{
b[i]=3544.5;
}
b[1]=591.4;
for(i=2;i<=9;++i)
{
```

```
c[i]=-(1.0+1.0/(i-1.0));
}
c[1]=-1.0;
for(time=0.0;time<timef;time=time+1.0)
{
x1old=x[1];
x2old=x[2];
x3old=x[3];
x4old=x[4];
x5old=x[5];
x6old=x[6];
x7old=x[7];
x8old=x[8];
x9old=x[9];
x10old=x[10];
d[1]=x1old*590.4;
d[2]=x2old*3542.5;
d[3]=x3old*3542.5;
d[4]=x4old*3542.5;
d[5]=x5old*3542.5;
d[6]=x6old*3542.5;
d[7]=x7old*3542.5;
d[8]=x8old*3542.5;
d[9]=x9old*3542.5;
d[10]=x10old*3542.5;
i=1;
n=10;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
}
cout<<“\t\t\t THE SOLUTION BY TDMA AT TIME = “<<time<<“ seconds”<<endl;
for(i=1;i<=10;++i)
```

```
{
cout<<x[i]<<endl;
}
getch();
}
```

PROGRAM 10.1

```
//PROGRAM 10.1
//program to calculate the temperature profile in a 2-D body
//during steady heat conduction using the Gauss-Seidel method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
float t11old,t12old,t13old,t11new,t12new,t13new;
float t21old,t22old,t23old,t21new,t22new,t23new;
float t31old,t32old,t33old,t31new,t32new,t33new;
t11new=t12new=t13new=101.0;
t21new=t22new=t23new=101.0;
t31new=t32new=t33new=101.0;
do
{
t11old=t11new;
t12old=t12new;
t13old=t13new;
t21old=t21new;
t22old=t22new;
t23old=t23new;
t31old=t31new;
t32old=t32new;
t33old=t33new;
t11new=(t12old+50+0.5*t21old+100.0/3.0)*3/7;
t12new=(t11new+t13old+t22old+100)/4.0;
t13new=(t12new+t23old+600)/4;
t21new=(t22old+0.5*t11new+0.5*t31old+100/3)*3/7;
t22new=(t12new+t32old+t23old+t21new)/4;
t23new=(t13new+t22new+t33old+500)/4;
t31new=(0.5*t21new+0.5*t32old+100/3)*3/4;
t32new=(t22new+0.5*t31new+0.5*t33old+100/3)*3/7;
t33new=(t23new+250+0.5*t32new+100/3)*3/7;
}while(fabs(t11new-t11old)>1e-6&&fabs(t12new-t12old)>1e-
6&&fabs(t13new-t13old)>1e-6
```

```
&&fabs(t21new-t21old)>1e-6&&fabs(t22new-t22old)>1e-6&&fabs(t23new-
t23old)>1e-6
&&fabs(t31new-t31old)>1e-6&&fabs(t32new-t32old)>1e-6&&fabs(t33new-
t33old)>1e-6);
cout<<t11new<<" "<<t12new<<" "<<t13new<<endl;
cout<<t21new<<" "<<t22new<<" "<<t23new<<endl;
cout<<t31new<<" "<<t32new<<" "<<t33new<<endl;
getch();
}
```

PROGRAM 10.2

```
//PROGRAM 10.2
//program to calculate the temperature profile in a 2-D body
//during steady heat conduction using the ADI method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,ii,jj,n,nn,nmax,i1,n1,k;
float a[21],b[21],c[21],d[21],x[21],beta[21],gamma[21], t[21][21];
float tstar[21][21];
a[2]=1.0;
a[3]=1.0;
b[1]=-4.0;
b[2]=-4.0;
b[3]=-4.0;
c[1]=1.0;
c[2]=1.0;
cout<<"Enter the maximum number of iterations ";
cin>>nmax;
t[0][1]=tstar[0][1]=20.0;
t[0][2]=tstar[0][2]=20.0;
t[0][3]=tstar[0][3]=20.0;
t[1][0]=tstar[1][0]=20.0;
t[2][0]=tstar[2][0]=20.0;
t[3][0]=tstar[3][0]=20.0;
t[4][1]=tstar[4][1]=20.0;
t[4][2]=tstar[4][2]=20.0;
t[4][3]=tstar[4][3]=20.0;
t[1][4]=tstar[1][4]=400.0;
t[2][4]=tstar[2][4]=400.0;
t[3][4]=tstar[3][4]=400.0;
```

```
for(i=1;i<=3;i++)
{
for(j=1;j<=3;j++)
{
t[i][j]=20.0;
}
}
for(nn=1;nn<=nmax;nn++)
{
for(jj=1;jj<=3;jj++)
{
d[1]=-t[0][jj]-t[1][jj+1]-tstar[1][jj-1];
d[2]=-t[2][jj+1]-tstar[2][jj-1];
d[3]=-t[4][jj]-t[3][jj+1]-tstar[3][jj-1];
i=1;
n=3;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
tstar[1][jj]=x[1];
tstar[2][jj]=x[2];
tstar[3][jj]=x[3];
}
for(ii=1;ii<=3;ii++)
{
d[1]=-t[ii][0]-tstar[ii+1][1]-tstar[ii-1][1];
d[2]=-tstar[ii+1][2]-tstar[ii-1][2];
d[3]=-t[ii][4]-tstar[ii+1][3]-tstar[ii-1][3];
i=1;
n=3;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
```

```
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
t[ii][1]=x[1];
t[ii][2]=x[2];
t[ii][3]=x[3];
}
}
cout<<“\t\t\t THE SOLUTION BY ADI”<<endl;
cout<<t[1][1]<<“ “<<t[1][2]<<“ “<<t[1][3]<<endl;
cout<<t[2][1]<<“ “<<t[2][2]<<“ “<<t[2][3]<<endl;
cout<<t[3][1]<<“ “<<t[3][2]<<“ “<<t[3][3]<<endl;
getch();
}
```

PROGRAM 10.3

```
//PROGRAM 10.3
//program to calculate the temperature profile in a 2-D body
//during transient heat conduction using the ADI method
#include<iostream.h>
#include<conio.h>
#include<math.h>
void main()
{
clrscr();
int i,j,ii,jj,n,nn,nmax,i1,n1,k,kk,count;
float a[21],b[21],c[21],d[21],x[21],beta[21],gamma[21],t[21][21];
float tstar[21][21],time,timef;
timef=0.5;
for(k=1;k<=10;k++)
{
a[k]=-1.0;
b[k]=2.4;
c[k]=-1.0;
}
```

```
c[1]=-2.0;
for(k=1;k<=11;k++)
{
t[11][k]=400.0;
tstar[11][k]=400.0;
t[k][11]=400.0;
tstar[k][11]=400.0;
}
for(i=1;i<=10;i++)
{
for(j=1;j<=10;j++)
{
t[i][j]=0.0;
tstar[i][j]=0.0;
}
}
for(time=0.0;time<=timef;time=time+0.05)
{
for(jj=1;jj<=10;jj++)
{
if(jj==1)
{
for(ii=1;ii<=10;ii++)
{
d[ii]=2*t[ii][2]-1.6*t[ii][1];
}
d[10]=d[10]+400.0;
}
else
{
for(ii=1;ii<=10;ii++)
{
d[ii]=t[ii][jj+1]+t[ii][jj-1]-1.6*t[ii][jj];
}
d[10]=d[10]+400.0;
}
i=1;
n=10;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
```

```
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
for(count=1;count<=10;count=count+1)
{
tstar[count][jj]=x[count];
}
}
for(ii=1;ii<=10;ii++)
{
if(ii==1)
{
for(jj=1;jj<=10;jj++)
{
d[jj]=2*tstar[ii+1][1]-1.6*tstar[ii][1];
}
d[10]=d[10]+400.0;
}
else
{
for(jj=1;jj<=10;jj++)
{
d[jj]=tstar[ii-1][jj]+tstar[ii+1][jj]-1.6*tstar[ii][jj];
}
d[10]=d[10]+400.0;
}
i=1;
n=10;
beta[i]=b[i];
gamma[i]=d[i]/beta[i];
i1=i+1;
for(j=i1;j<=n;++j)
{
beta[j]=b[j]-a[j]*c[j-1]/beta[j-1];
gamma[j]=(d[j]-a[j]*gamma[j-1])/beta[j];
}
x[n]=gamma[n];
n1=n-i;
for(k=1;k<=n1;++k)
{
```

```
j=n-k;
x[j]=gamma[j]-c[j]*x[j+1]/beta[j];
}
for(count=1;count<=10;count=count+1)
{
t[ii][count]=x[count];
}
}
}
cout<<"\t\t\t THE SOLUTION BY ADI AT TIME = "<<time<<" s"<<endl;
for(i=1;i<=10;i++)
{
for(j=1;j<=10;j++)
{
cout<<"t["<<i<<"]["<<j<<"] = "<<t[i][j]<<"\t";
}
}
getch();
}
```

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Index

INTRODUCTION TO
NUMERICAL METHODS IN CHEMICAL ENGINEERING

Pradeep Ahuja

This book is an exhaustive presentation of the numerical methods used in chemical engineering. Intended primarily as a textbook for BE/BTech students of chemical engineering, the book will also be useful to research and development/process professionals in the fields of chemical, biochemical, mechanical and biomedical engineering.

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