Scilab Textbook Companion for Introduction To Numerical Methods In Chemical Engineering by P. Ahuja¹

Created by
Chandra Prakash Sipani
B.TECH Part-2
Chemical Engineering
IIT-BHU
College Teacher
Ahuja, Pradeep
Cross-Checked by
Pradeep Ahuja

May 21, 2016

¹Funded by a grant from the National Mission on Education through ICT, http://spoken-tutorial.org/NMEICT-Intro. This Textbook Companion and Scilab codes written in it can be downloaded from the "Textbook Companion Project" section at the website http://scilab.in

Book Description

Title: Introduction To Numerical Methods In Chemical Engineering

Author: P. Ahuja

Publisher: PHI Learning, New Delhi

Edition: 1

Year: 2010

ISBN: 8120340183

Scilab numbering policy used in this document and the relation to the above book.

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

AP Appendix to Example(Scilab Code that is an Appednix to a particular Example of the above book)

For example, Exa 3.51 means solved example 3.51 of this book. Sec 2.3 means a scilab code whose theory is explained in Section 2.3 of the book.

Contents

Lis	st of Scilab Codes	4
1	linear algebraic equations	5
2	NONLINEAR ALGEBRAIC EQUATIONS	12
3	CHEMICAL ENGINEERING THERMODYNAMICS	17
4	INITIAL VALUE PROBLEMS	35
5	BOUNDARY VALUE PROBLEMS	56
6	CONVECTION DIFFUSION PROBLEMS	66
7	TUBULAR REACTOR WITH AXIAL DISPERSION	72
8	CHEMICAL REACTION AND DIFFUSION IN SPHERI- CAL CATALYST PELLET	7 6
9	ONE DIMENSIONAL TRANSIENT HEAT CONDUCTION	81
10	TWO DIMENSIONAL STEADY AND TRANSIENT HEAT CONDUCTION	88

List of Scilab Codes

Exa 1.1	TDMA method	5
Exa 1.2	gauss elimination method	6
Exa 1.3	gauss elimination method	7
Exa 1.4	gauss elimination method	8
Exa 1.5	gauss seidel method	10
Exa 1.6	gauss seidel method	10
Exa 2.1	algebraic equations	12
Exa 2.2	algebraic equations	13
Exa 2.3	algebraic equations	13
Exa 2.4	algebraic equations	14
Exa 2.5	algebraic equations	15
Exa 2.6	algebraic equations	16
Exa 3.1	thermodynamics	17
Exa 3.2	thermodynamics	19
Exa 3.3	flash calculations using Raoult law	21
Exa 3.4	BPT and DPT calculation using modified raoult law .	22
Exa 3.5	flash calculations using modified Raoult law	25
Exa 3.6	vapour pressure calculation using cubic equation of state	27
Exa 3.7	pressure x y diagram using gamma phi approach	29
Exa 3.9	chemical reaction engineering 2 simultaneous reactions	31
Exa 3.10	adiabatic flame temperature	33
Exa 4.1	solution of ordinary differential equation	35
Exa 4.2	solution of ordinary differential equation	36
Exa 4.3	double pipe heat exchanger	37
Exa 4.4	stirred tank with coil heater	38
Exa 4.5	stirred tank with coil heater	39
Exa 4.6	pneumatic conveying	40
Exa 4.7	simultaneous ordinary differential equations	41

Exa 4.8	simultaneous ordinary differential equations 42
Exa 4.9	simultaneous ordinary differential equations
Exa 4.10	series of stirred tank with coil heater
Exa 4.11	batch and stirred tank reactor
Exa 4.12	batch and stirred tank reactor
Exa 4.13	batch and stirred tank reactor
Exa 4.14	batch and stirred tank reactor
Exa 4.15	plug flow reactor
Exa 4.16	plug flow reactor
Exa 4.17	plug flow reactor
Exa 4.18	non isothermal plug flow reactor
Exa 5.1	discretization in 1 D space
Exa 5.2	discretization in 1 D space
Exa 5.3	discretization in 1 D space
Exa 5.4	discretization in 1 D space
Exa 5.5	discretization in 1 D space
Exa 5.6	1 D steady state heat conduction 61
Exa 5.7	1 D steady state heat conduction
Exa 5.8	chemical reaction and diffusion in pore
Exa 6.1	upwind scheme
Exa 6.2	upwind scheme
Exa 7.1	boundary value problem in chemical reaction engineering 72
Exa 7.2	boundary value problem in chemical reaction engineer-
	ing second order
Exa 8.1	first order reaction
Exa 8.2	second order reaction
Exa 8.3	non isothermal condition
Exa 8.4	non isothermal condition
Exa 9.1	transient conduction in rectangular slab 81
Exa 9.2	transient conduction in rectangular slab 82
Exa 9.3	transient conduction in cylinder
Exa 9.4	transient conduction in sphere
Exa 9.5	transient diffusion in sphere
Exa 10.1	discretization in 2 D space gauss seidel method 88
Exa 10.2	discretization in 2 D space gauss seidel method 89
Exa 10.3	discretization in 2 D space
Exa 10.8	discretization in 2 D space
Exa. 10.9	discretization in 2 D space 92

Exa 10.10	ADI method	93
Exa 10.11	ADI method for transient heat conduction	94

Chapter 1

linear algebraic equations

Scilab code Exa 1.1 TDMA method

```
1 / \text{ch } 1 \text{ ex } 1.1 - \text{ solving set of algebraic equations by}
       Tri diagonal Matrix Algorithm Method.
3 disp("the soln of eg 1.1-->");
4 for i=2:7, a(i)=1;
                                      //sub diagonal
      assignment
6 for j=1:7, b(j)=-2;
                                     //main diagonal
      assignment
7 end
8 \text{ for } k=1:6, c(k)=1;
                                     //super diagonal
      assignment
9 end
                                      //given values
10 d(1) = -240
      assignment
11 for l=2:6, d(1)=-40;
12 end
13 d(7) = -60
14
15 i=1;
16 n = 7;
```

```
17 beta1(i)=b(i);
                                     //initial b is equal
      to beta since a1=0
18 gamma1(i)=d(i)/beta1(i);
                                     //\sin ce c7=0
19 m = i + 1;
20 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
21 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
22 \text{ end}
23 x(n) = gamma1(n);
                                     //\sin ce c7=0
24 n1=n-i;
25 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
      j);
26 \, \text{end}
27
28 disp("the solution of ex 1.1 by TDMA method is");
29 for i=1:7, disp(x(i));
30 \, \text{end}
```

Scilab code Exa 1.2 gauss elimination method

```
1 / ch 1 ex 1.2
2 clc
3 disp("the soln of eg 1.2-->");
4 \text{ a1=10}, \text{ a2=1}, \text{ a3=2},
                                      //1 st row
                                      //2nd row
5 b1=2, b2=10, b3=1,
                                      //3rd row
6 c1=1, c2=2, c3=10,
7 d1=44, d2=51, d3=61,
                                      //given values
9 b3=b3-(b1/a1)*a3
                                      // for making b1=0
10 b2=b2-(b1/a1)*a2
11 d2=d2-(b1/a1)*d1
12 b1=b1-(b1/a1)*a1
13
14 c3=c3-(c1/a1)*a3
                                     // for making c1=0
15 c2=c2-(c1/a1)*a2
16 d3=d3-(c1/a1)*d1
```

Scilab code Exa 1.3 gauss elimination method

```
1 / \cosh 1 ex 1.3
2 clc
3 disp("the soln of eg 1.3-->");
4 \text{ a1=3}, \text{ a2=1}, \text{ a3=-2},
                                        //1 st row
                                        //2nd row
5 b1=-1, b2=4, b3=-3,
6 \text{ c1=1}, \text{ c2=-1}, \text{ c3=4},
                                        //3rd row
7 d1=9, d2=-8, d3=1,
                                     //given values
9 b3=b3-(b1/a1)*a3
                                        // for making b1=0
10 b2=b2-(b1/a1)*a2
11 d2=d2-(b1/a1)*d1
12 b1=b1-(b1/a1)*a1
13
14 c3=c3-(c1/a1)*a3
                                       // for making c1=0
15 c2=c2-(c1/a1)*a2
16 d3=d3-(c1/a1)*d1
17 c1=c1-(c1/a1)*a1
18
                                      // for making c2=0
19 c3=c3-(c2/b2)*b3
20 d3=d3-(c2/b2)*d2
21 c2=c2-(c2/b2)*b2
```

Scilab code Exa 1.4 gauss elimination method

```
1 // \text{ ch } 1 \text{ ex } 1.4
2 clc
3 disp("the solution of eg 1.4-->");
4 a1=.35, a2=.16, a3=.21, a4=.01
                                                      //1 st
      row
5 b1=.54, b2=.42, b3=.54, b4=.1
                                                     //2nd row
6 c1=.04, c2=.24, c3=.1, c4=.65
                                                     //3rd row
7 d1=.07, d2=.18, d3=.15, d4=.24
                                                     //4th row
8 \text{ r1}=14, \text{ r2}=28, \text{ r3}=17.5, \text{ r4}=10.5
                                                    //given
      values
9
10 b4=b4-(b1/a1)*a4
                                                   // for
      making b1=0
11 b3=b3-(b1/a1)*a3
12 b2=b2-(b1/a1)*a2
13 r2=r2-(b1/a1)*r1
14 b1=b1-(b1/a1)*a1
15
                                                  // for
16 c4=c4-(c1/a1)*a4
      making c1=0
17 c3=c3-(c1/a1)*a3
18 c2=c2-(c1/a1)*a2
19 r3=r3-(c1/a1)*r1
20 c1=c1-(c1/a1)*a1
21
                                                  // for
22 d4=d4-(d1/a1)*a4
```

```
making d1=0
23 d3=d3-(d1/a1)*a3
24 d2=d2-(d1/a1)*a2
25 \quad r4=r4-(d1/a1)*r1
26 d1=d1-(d1/a1)*a1
27
                                                  // for
28 c4=c4-(c2/b2)*b4
      making c2=0
29 c3=c3-(c2/b2)*b3
30 \text{ r3=r3-(c2/b2)*r2}
31 c2=c2-(c2/b2)*b2
32
33 d4=d4-(d2/b2)*b4
                                                 // for making
       d2 = 0
34 d3=d3-(d2/b2)*b3
35 \quad r4=r4-(d2/b2)*r2
36 d2=d2-(d2/b2)*b2
37
38 d4=d4-(d3/c3)*c4
                                                //for making
      d3 = 0
39 \text{ r4=r4-(d3/c3)*r3}
40 d3=d3-(d3/c3)*c3
41
42 B2=r4/d4;
43 D2=(r3-(c4*B2))/c3;
44 B1=(r2-(D2*b3)-(B2*b4))/b2;
45 D1=(r1-(B2*a4)-(D2*a3)-(B1*a2))/a1;
46 disp (B2, D2, B1, D1," the values of MOLAR FLOW RATES of
      D1, B1, D2, B2 respectively are");
47
48 B = D2 + B2;
49 \times 1B = (.21 \times D2 + .01 \times B2)/B;
50 \text{ x2B} = (.54*D2 + .1*B2)/B;
51 \times 3B = (.1*D2 + .65*B2)/B;
52 \times 4B = (.15*D2 + .24*B2)/B;
53 disp(x4B, x3B, x2B, x1B," the composition of stream B
       is");
54
```

```
55  D=D1+B1;
56  x1D=(.35*D1 + .16*B1)/D;
57  x2D=(.54*D1 + .42*B1)/D;
58  x3D=(.04*D1 + .24*B1)/D;
59  x4D=(.07*D1 + .18*B1)/D;
60  disp(x4D, x2D, x2D, x1D,"the composition of stream D is");
```

Scilab code Exa 1.5 gauss seidel method

```
1 clc
2 disp("the soln of eg 1.5--> Gauss Seidel Method");
3 \text{ for } i=1:3, xnew(i)=2, e(i)=1
4 end
5 x = 1e - 6
6 while e(1) > x & e(2) > x & e(3) > x do
        for i=1:3, xold(i)=xnew(i),end
        xnew(1) = (44 - xold(2) - 2 * xold(3)) / 10
8
        xnew(2) = (-2*xnew(1)+51-xold(3))/10
10
        xnew(3) = (-2*xnew(2) - xnew(1) + 61) / 10
        for i=1:3,e(i)=abs(xnew(i)-xold(i))
11
12
        end
13 end
14 disp("the values of x1,x2,x3 respectively is");
15 for i=1:3, disp(xnew(i));
16 \text{ end}
```

Scilab code Exa 1.6 gauss seidel method

```
1 clc
2 disp("the soln of eg 1.6--> Gauss Seidel Method");
3 for i=1:3,xnew(i)=2,e(i)=1
4 end
```

```
5 x = 1e - 6
6 while e(1) > x & e(2) > x & e(3) > x do
        for i=1:3, xold(i)=xnew(i),end
        xnew(1) = (9 - xold(2) + 2 * xold(3))/3
8
9
        xnew(2) = (xnew(1) - 8 + 3 * xold(3))/4
        xnew(3) = (xnew(2) - xnew(1) + 1)/4
10
        for i=1:3,e(i)=abs(xnew(i)-xold(i))
11
12
        end
13 end
14 disp("the values of x1,x2,x3 respectively is");
15 for i=1:3,disp(xnew(i));
16 \text{ end}
```

Chapter 2

NONLINEAR ALGEBRAIC EQUATIONS

Scilab code Exa 2.1 algebraic equations

```
1 //ch 2 ex 2.1 solving using newton's method.
3 disp("the soln of eqn 2.1--> Newton Method");
                                //initial value
4 x = .5
5 \text{ xnew=0}
6 e = 1
7 while e>10^-4 do x=xnew, function y=Fa(x),
             y = x^3 - 5 * x + 1;
                                                //defining
                fn
9 endfunction
                                            //
10 der=derivative(Fa,x),
      differentiating the fn
11 xnew=x-Fa(x)/der,
12 e = abs(xnew - x),
14 disp(xnew, "the root of the eqn is");
```

Scilab code Exa 2.2 algebraic equations

```
1 clc
2 disp("the solution of ex 2.2 --> Pressure Drop in
      Pipe");
3 \text{ meu} = 1.79 * 10^{-5}
4 rough = .0000015
                       //roughness
5 \text{ dia} = .004
6 e_by_D=rough/dia
7 \text{ rho} = 1.23
8 v = 50
                       //velocity of air
9 1 = 1
10 Re=(rho*v*dia)/meu
                                 //Reynold's number
11 \text{ ffnew=0.01}
12 e = 1
13 t1=e_by_D/3.7
                                 //term 1 of eqn.
14 t2=2.51/Re
                                 //term 2 of eqn.
15 disp(Re, "the Reynolds no. is");
16 funcprot(0)
17 while e>1e-6 do ff=ffnew, function y=Fh(ff),
            t3=sqrt(ff),
18
       y=1/t3+2*log(t1+t2/t3)/2.3,
19
          //divide by 2.3 since log is base 'e' instead
           of 10
20 endfunction;
21 fdash=derivative(Fh,ff);
                                            //f '(ff)
22 ffnew=ff-Fh(ff)/fdash;
23 e=abs(ff-ffnew)
24 end
25 disp(ff," the fanning friction factor is")
26 delta_p = (ff*l*v^2*rho)/(2*dia)
                                                         //
      pressure drop
27 disp(delta_p, "the pressure drop in pascals is");
```

Scilab code Exa 2.3 algebraic equations

```
1 clc
2 disp("the solution of eg 2.3 --> minimum
      fluidization velocity");
3 P=2*101325
                     //given data
4 T=298.15
5 M = 28.97 * 10^{-3}
6 R=8.314
7 rho = (P*M)/(R*T)
8 rho_p=1000
9 \text{ dia=}1.2*10^-4
                            //void fraction
10 \text{ ep} = .42
11 sph=.88
12 \text{ meu}=1.845*10^-5
13 t1=1.75*rho*(1-ep)/(sph*dia*ep^3)
                              //these are the terms of the
       function.
14 t2=150*meu*(1-ep)^2/(sph^2*dia^2*ep^3)
15 t3=(1-ep)*(rho_p-rho)*9.8
16 \text{ vnew=0.1}
17 e1=1
18 while e1>1e-6 do v=vnew, function y=Fb(v);
       y=t1*v^2+t2*v-t3,
                                                 //defining
           fn
       endfunction,
20
21 vdash=derivative(Fb,v),
                                                //
      differentiating the fn
22 \text{ vnew=v-Fb(v)/vdash,}
23 \text{ eleabs}(\text{vnew-v}),
25 disp(v," the minimum fluidisation velocity in m/s is"
      );
```

Scilab code Exa 2.4 algebraic equations

```
1 clc
```

```
2 disp("the soln of eg 2.4--> Terminal Velocity");
3 \text{ dia}=2*10^{-3}
4 P=101325
                   //given data
5 T = 298.15
6 M = 28.89 * 10^{-3}
7 R=8.314
8 \text{ rho} = (P*M)/(R*T)
9 rho_oil=900
10 meu=1.85*10^-5
11 Re_oil_by_v=rho*dia/meu
12 \text{ vnew=0.1, e=1}
13 while e>1e-6 do v=vnew, Re_oil=Re_oil_by_v*v,
14
        Cd=24*(1+.15*Re_oil^.687)/Re_oil,
        vnew=sqrt(4*(rho_oil-rho)*9.81*dia/(3*Cd*rho)),
15
16 \text{ e=abs}(\text{vnew-v}),
17 end
18 disp(v,"the terminal velocity in m/s is");
```

Scilab code Exa 2.5 algebraic equations

```
1 clc
2 disp("the soln of eg 2.5--> non linear equations");
3 xnew=0.1, ynew=0.5, e1=1, e2=1
4 while e1>1e-6 & e2>1e-6 do x=xnew, y=ynew,
5 y1=exp(x)+x*y-1,
6 d_fx=exp(x)+y
7 d_fy=x
8 y2=sin(x*y)+x+y-1,
9 d_gx=y*cos(x*y)+1
10 d_gy=x*cos(x*y)+1
11 t1=(y2*d_fy), t2=(y1*d_gy),
12 D1=d_fx*d_gy-d_fy*d_gx
13 delta_x=(t1-t2)/D1
14 t3=(y1*d_gx),t4=(y2*d_fx)
15 delta_y=(t3-t4)/D1
```

Scilab code Exa 2.6 algebraic equations

```
1 clc
2 disp("the soln of eg 2.6-->");
3 \text{ xnew=0.1, ynew=0.5, e1=1, e2=1}
4 while e1>10^-6 & e2>10^-6 do x=xnew, y=ynew,
5 y1=3*x^3+4*y^2-145,
6 d_fx=9*x^2
7 d_f y = 8 * y
8 y2=4*x^2-y^3+28,
9 d_gx=8*x
10 d_gy = -3*y^2
11 D2=d_fx*d_gy-d_gx*d_fy
12 delta_x=(y2*d_fy-y1*d_gy)/D2
13 delta_y = (y1*d_gx-y2*d_fx)/D2
14 \text{ xnew=x+delta_x}
15 ynew=y+delta_y
16 \text{ e1} = abs(xnew-x)
17 e2=abs(ynew-y)
18 end
19 disp(y,x,"the values of x and y are respectively");
```

Chapter 3

CHEMICAL ENGINEERING THERMODYNAMICS

Scilab code Exa 3.1 thermodynamics

```
1 clc
2 disp("the soln of eg 3.1-->Cubic eqn. of state");
3 disp("all values in m3/mol");
4 T=373.15, P=101325, Tc=647.1, Pc=220.55*10^5, w
      =.345, R=8.314
                                         //reduced
5 Tr=T/Tc, Pr=P/Pc,
      pressure & reduced temperature
6 b0 = .083 - .422 * Tr^- - 1.6
7 b1 = .139 - .172 * Tr^- - 4.2
8 B = (b0 + w * b1) * R * Tc/Pc
9 \text{ vnew=1}
10 e1=1, vold=R*T/P+B
11 disp(vold," the soln by virial gas eqn. of volume in
     m3/mol by Z(T,P) is");
12 while e1>1e-6 do vold=vnew, function y=Fh(vold),
           y=P*vold/(R*T)-1-B/vold
13
14 endfunction;
15 ydash=derivative(Fh, vold);
16 vnew=vold-Fh(vold)/ydash;
```

```
17 e1=abs (vold-vnew)
18 end
19 disp(vold," the soln by virial gas eqn. of volume in
                 m3/mol by Z(T,V) is");
20 //by peng robinson method
21 k = .37464 + 1.54226 * w - .26992 * w^2
22 s=1+k*(1-Tr^{.5})
23 \quad lpha=s^2
24 a = .45724 * R^2 * Tc^2 * lpha/Pc
25 b = .0778 * R * Tc/Pc
26 \text{ vnew=b, e2=1,}
27 \text{ vol=b, fe=0, fd=0}
28 disp("the volume of saturated liq. and saturated
                  vapour by peng-robinson method respectively is")
29 for i=0:2 do
30
                                  vol=vnew
                                  v2 = vol^3 + P + vol^2 + (P + b - R + T) - vol + (3 + P + b^2 + 2 + b + P + b^2 + P 
31
                                           R*T-a)+P*b^3+b^2*R*T-a*b
32 \text{ ydash2} = 3*P*vol^2 + (P*b-R*T)*2*vol-(3*P*b^2+2*b*R*T-a)
33 vnew=vol-y2/ydash2,
34 e2=abs(vol-vnew)
35 if i==1 & e2<1e-6 then fd=vnew, vnew=R*T/P,
36 end
37 end
38 disp(vol,fd);
39 funcprot(0)
40 //by redlich-kwong method
41 i = 0
42 a = .42748*R^2*Tc^2.5/Pc
43 \text{ b} = .08664 * R * Tc/Pc
44 \quad Vnew=b, e3=1
45 disp("the vol of saturated liq. and vapour by
                  redlich kwong method respectively are");
46 for i=0:2 do V=Vnew, function y3=gh(V),
                                               v3=V^3*P-R*T*V^2-V*(P*b^2+b*R*T-a/sqrt(T))
47
                                                        ))-a*b/sqrt(T)
48
                                  endfunction,
                                  deriv=derivative(gh,V);
49
```

```
Vnew=V-gh(V)/deriv;
50
            e3 = abs (Vnew - V)
51
            if i==1 & e3<1e-6 then de=Vnew, Vnew=R*T/P</pre>
52
                         //for saturated liq.
53
            end
54
          end
       disp(V,de);
55
56 //vander waals method
57 i = 0
58 a=27*R^2*Tc^2/(64*Pc)
59 b=R*Tc/(8*Pc)
60 \text{ vnew=b, v=b,e=1}
61 for i=0:2 do v=vnew, function v3=bh(v),
            v3=v^3*P-v^2*(P*b+R*T)+a*v-a*b,
62
63
       endfunction
64
       deriva=derivative(bh, v),
       vnew=v-bh(v)/deriva
65
       e4 = abs(v - vnew),
66
       if i==1 \& e4<10^-6 then sol=vnew, vnew=R*T/P
67
68
       end
69 end
70 disp("the vol of saturated liq. and vapour by vander
       waal method respectively are");
71 disp(vnew, sol);
```

Scilab code Exa 3.2 thermodynamics

```
8 T2sat=b2/(a2-log(P))-c2
9 Told=273,e=1
10 \text{ Tnew=x1*T1sat+x2*T2sat}
11 while e>1e-6 do Told=Tnew, function y1=fw(Told),
12
            P1sat = exp(a1-b1/(Told+c1)),
13
            P2sat = exp(a2-b2/(Told+c2)),
            y1=P-x1*P1sat-x2*P2sat
14
            endfunction
15
            ydashd=derivative(fw, Told)
16
            Tnew=Told-fw(Told)/ydashd
17
            e=abs (Told-Tnew)
18
19
20
        disp(Tnew," the bubble point temp. in Celsius is"
           );
21
                                                                   calc
                                                                   of
                                                                  dew
                                                                   point
22 \text{ y1=z1}, \text{ y2=1-z1}, \text{e=1}
23 \text{ Tnew=y1*T1sat+y2*T2sat}
24 while e>1e-6 do Told=Tnew, function y11=fw1(Told),
             P1sat = exp(a1-b1/(Told+c1)),
25
             P2sat = exp(a2-b2/(Told+c2)),
26
27
            y11=1/P-y1/P1sat-y2/P2sat
            endfunction
28
            ydashd=derivative(fw1, Told)
29
            Tnew=Told-fw1(Told)/ydashd
30
            e=abs(Told-Tnew)
31
32
        end
        disp(Tnew, "the dew point temp. in Celsius is");
33
```

Scilab code Exa 3.3 flash calculations using Raoult law

```
1 clc
2 disp("the soln of eg 3.3-->Flash Calc. using Raoults
       Law")
3 \text{ psat}(1) = 195.75, \text{psat}(2) = 97.84, \text{psat}(3) = 50.32
                  //given data
4 z(1) = .3, z(2) = .3, z(3) = .4
5 bpp=z(1)*psat(1)+z(2)*psat(2)+z(3)*psat(3)
                  //Bubble point pressure
6 dpp=1/(z(1)/psat(1)+z(2)/psat(2)+z(3)/psat(3))
             //dew point pressure
7 disp(dpp,bpp,"the bubble point pressure and dew
      point pressure respectively are");
8 P=100, v=1, vnew=1, e=1, y2=0, der=0
                                                          //
      given pressure is between BPP & DPP
9 for i=1:3 k(i)=psat(i)/P
10 \text{ end}
11 while e>1e-6 do v=vnew, for i=1:3,
12
            t1=(1-v+v*k(i)), y2=y2+z(i)*(k(i)-1)/t1,
13
            der=der-z(i)*(k(i)-1)^2/t1^2,
14
            end
       vnew=v-y2/der,e=abs(vnew-v),
15
16
17
       for i=1:3, x(i)=z(i)/(1-v+v*k(i)), y(i)=x(i)*k(i)
18
       end
       disp(x(1), "mol fretn of acetone in liq. phase is
19
       disp(y(1), "mol frctn of acetone in vapour phase
20
          is");
       disp(x(2), "mol fretn of acetonitrile in liq.
21
          phase is");
22
       disp(y(2)," mol frctn of acetonitrile in vapour.
```

```
phase is");

disp(x(3),"mol frctn of nitromethane in liq.
phase is");

disp(y(3),"mol frctn of nitromethane in vapour
phase is");
```

Scilab code Exa 3.4 BPT and DPT calculation using modified raoult law

c a

o f

BP

```
1 a12=437.98*4.186, a21=1238*4.186, v1=76.92, v2=18.07
3 clc
4 disp("the soln of eg 3.4-->");
5 t = 100
6 \text{ x1}=.5, R=8.314
7 a1=16.678, b1=3640.2, c1=219.61
8 \quad a2=16.2887, b2=3816.44, c2=227.02
9 x2=1-x1
10 p1sat = exp(a1-b1/(c1+t))
11 p2sat = exp(a2-b2/(c2+t))
12 h12=v2*exp(-a12/(R*(t+273.15)))/v1
13 h21=v1*exp(-a21/(R*(t+273.15)))/v2
14 m=h12/(x1+x2*h12)-h21/(x2+x1*h21)
15 g1 = \exp(-\log(x1+x2*h12)+x2*m)
16 g2 = \exp(-\log(x2 + x1 + h21) - x1 + m)
17 p=x1*g1*p1sat+x2*g2*p2sat
18 disp(p, "boiling point pressure in kPa is");
```

19

```
20 p=101.325, x1=.5, e=1
21 \times 2 = 1 - \times 1
22 t1sat=b1/(a1-log(p))-c1
23 t2sat=b2/(a2-log(p))-c2
24 \quad tnew=x1*t1sat+x2*t2sat
25 while e>10^-4 do told=tnew,
        p1sat = exp(a1-b1/(c1+told)), p2sat = exp(a2-b2/(c2+told))
26
           told)),
27
        p1sat=p/(g1*x1+g2*x2*(p2sat/p1sat))
        tnew=b1/(a1-log(p1sat))-c1,
28
        e=abs(tnew-told)
29
30 \, \text{end}
31 disp(tnew, "boiling point temperature in Celsius is")
32
33 \text{ e1=1, e2=1, e3=1, pold=1}
34 t = 100, y1 = .5
35 \quad y2 = 1 - y1
36 \text{ p1sat} = \exp(a1-b1/(c1+t))
37 p2sat = exp(a2-b2/(c2+t))
38 g1=1, g2=1, g11=1, g22=1
39 pnew=1/(y1/(g1*p1sat)+y2/(g2*p2sat))
40 while e1>.0001 do pold=pnew, while e2>.0001& e3
      >.0001 do g1=g11,g2=g22,
                                      x1=y1*pold/(g1*p1sat)
41
42
                                      x2=y2*pold/(g2*p2sat)
43
                                      x1=x1/(x1+x2)
                                      x2 = 1 - x1
44
```

o f

BP'

dpp

```
h12=v2*exp(-a12/(R*(t
45
                                        +273.15)))/v1
                                     h21 = v1 * exp(-a21/(R*(t)))
46
                                        +273.15)))/v2
47
                                     m=h12/(x1+x2*h12)-h21
                                        /(x2+x1*h21)
48
                                     g11 = exp(-log(x1+x2*h12))
                                        ) + x2 * m)
                                     g22 = exp(-log(x2+x1*h21))
49
                                        )-x1*m)
                                     e2=abs(g11-g1), e3=abs
50
                                        (g22-g2)
51
                                 end
           pnew=1/(y1/(g1*p1sat)+y2/(g2*p2sat))
52
           e1=abs(pnew-pold)
53
54
        end
      disp(pnew, "dew point pressure in kPa is");
55
56
57 p=101.325, y1=.5, e4=1, e5=1, e6=1
58 y2=1-y1
59 t1sat=b1/(a1-log(p))-c1
60 t2sat=b2/(a2-log(p))-c2
61 \quad tnew=y1*t1sat+y2*t2sat
62 \text{ g11=1}, \text{ g22=1}
63 while e4 > .0001 do told=tnew,
        p1sat = exp(a1-b1/(c1+told))
64
        p2sat = exp(a2-b2/(c2+told)), while e5>.0001 & e6
65
           >.0001 do g1=g11, g2=g22,
66
        x1=y1*p/(g1*p1sat)
        x2=y2*p/(g2*p2sat)
67
        x1=x1/(x1+x2)
68
       x2 = 1 - x1
69
70
       h12=v2*exp(-a12/(R*(t+273.15)))/v1
       h21=v1*exp(-a21/(R*(t+273.15)))/v2
71
```

calc

dpt

```
m=h12/(x1+x2*h12)-h21
72
                                        /(x2+x1*h21)
                                     g11 = exp(-log(x1+x2*h12))
73
                                        ) + x2 * m)
74
                                     g22 = exp(-log(x2+x1*h21))
                                        )-x1*m)
                                     e5=abs(g11-g1), e6=abs
75
                                        (g22-g2)
76
                                end
77
78
           p1sat=p*(y1/g1+y2*p1sat/(g2*p2sat))
79
           tnew=b1/(a1-log(p1sat))-c1
80
           e4=abs(tnew-told)
81
       end
      disp(tnew, "dew point temperature in Celsius is")
82
```

Scilab code Exa 3.5 flash calculations using modified Raoult law

```
1 clc
2 disp("the soln of eg 3.5-->Flash calc. using
      Modified Raoult law");
3 \quad a12=292.66*4.18, \quad a21=1445.26*4.18, \quad v1=74.05*10^-6,
      v2=18.07*10^-6, R=8.314
4 t=100, z1=.3,
5 z2=1-z1
6 \text{ a1}=14.39155, a2=16.262, b1=2795.82, b2=3799.89, c1
      =230.002, c2=226.35
7 e1=1, e2=1, e3=1, e4=1, e5=1, e6=1, vnew=0
                                                       //calc
                                                          o f
                                                         BPP
9 x1=z1, x2=z2
10 p1sat = exp(a1 - (b1/(t+c1)))
11 p2sat = exp(a2 - (b2/(t+c2)))
```

```
12 h12=v2*exp(-a12/(R*(t+273.15)))/v1
13 h21=v1*exp(-a21/(R*(t+273.15)))/v2
14 m=(h12/(x1+x2*h12))-(h21/(x2+x1*h21))
15 g1 = \exp(-\log(x1+x2*h12)+x2*m)
16 g2 = \exp(-\log(x2 + x1 + h21) - x1 + m)
17 p=x1*g1*p1sat+x2*g2*p2sat
18 disp(p,"the bubble point pressure is");
                                                       //g1
19 bpp=p, gb1=g1, gb2=g2
      & g2 are activity co-efficients
20
                                                           calc
                                                           o f
                                                          DPP
21 y1=z1, y2=z2
22 g1=1, g2=1
23 pnew=1/(y1/(g1*p1sat)+y2/(g2*p2sat))
24 \text{ g1n=g1, g2n=g2}
25 while e1>.0001 do pold=pnew, while e2>.0001& e3>.0001
       do g1=g1n, g2=g2n,
26
       x1=y1*pold/(g1*p1sat)
27
       x2=y2*pold/(g2*p2sat)
       x1=x1/(x1+x2)
28
29
       x2=1-x1
30
       g1n = exp(-log(x1+x2*h12)+x2*m)
31
       g2n = exp(-log(x2+x1*h21)-x1*m)
32
       e2=abs(g1n-g1), e3=abs(g2n-g2)
33 end
34 \text{ pnew=1/(y1/(g1n*p1sat)+y2/(g2n*p2sat))}
35 e1=abs(pnew-pold)
36 end
37 disp(pnew, "the dew point pressure is");
38 \text{ dpp=pnew, } gd1=g1n, gd2=g2n
39 p = 200
40 \quad v = (bpp - p) / (bpp - dpp)
41 g1 = ((p-dpp)*(gb1-gd1))/(bpp-dpp)+gd1
```

```
42 g2 = ((p-dpp)*(gb2-gd2))/(bpp-dpp)+gd2
43
44 //calc of distribution co-efficients
45 while e4>.0001 & e5>.0001 do g1n=g1, g2n=g2,
46
       k1=g1n*p1sat/p
47
       k2=g2n*p2sat/p
       while e6>.00001 do v=vnew,
48
            function f=fv(v),
49
            v1 = (k1*z1)/(1-v+v*k1)
50
            y2=(k2*z2)/(1-v+v*k2)
51
52
            x1=y1/k1
53
            x2=y2/k2
54
            f = y1 - x1 + y2 - x2
55
            endfunction
56
            derv=derivative(fv,v)
            vnew=v-fv(v)/derv
57
            e6 = abs (vnew - v)
58
59
       end
       h12=v2*exp(-a12/(R*(t+273.15)))/v1
60
       h21=v1*exp(-a21/(R*(t+273.15)))/v2
61
       m = (h12/(x1+x2*h12)) - (h21/(x2+x1*h21))
62
       g1 = \exp(-\log(x1+x2*h12)+x2*m)
63
       g2 = exp(-log(x2+x1*h21)-x1*m)
64
       e4 = abs(g1 - g1n), e5 = abs(g2 - g2n)
65
66 end
67 disp(v," the no. of moles in vapour phase is");
68 disp(y1,x1,"x1 and y1 respectively are");
```

Scilab code Exa 3.6 vapour pressure calculation using cubic equation of state

```
//given
 4 f1=1, e1=1, e2=1, vnew=1, pnew=1
                                                                                                                                                      //
                 assumed values
  5 k = .37464 + 1.54226 * w - .26992 * w * 2
  6 s=(1+k*(1-(t/tc)^{.5}))^{2},
  7 a = .45724 * R * R * tc * tc * s/pc
 8 b = .0778 * R * tc/pc
  9 //calc of vol. of liq.
10 while f1>10^-4 do p=pnew, vnew=b,
11 t1 = (p*b-R*t)
                                                                                                                       //co-efficients
                 of vol. in the eqn.
12 t2=3*p*b^2+2*b*R*t-a
13 t3=p*b^3+b^2*R*t-a*b
14
                     while e1>1e-6 & vnew>0 do vold=vnew,
15
                                        y1 = vold^3 * p + vold^2 * t1 - vold * t2 + t3,
                                        der=3*vold^2*p+2*vold*t1-t2
16
                                        vnew=vold-y1/der
17
                                        e1=abs (vnew-vold)
18
19 end
20 vliq=vold,
21 //fugacity of liq.
22 zliq=p*vliq/(R*t)
23 c=(a/(2*1.414*b*R*t))*(log((vliq+(1+sqrt(2))*b)/(
                 vliq+(1-sqrt(2))*b))),
24 t5=zliq-p*b/(R*t)
25 fl2=p*exp(zliq-1-log(t5)-c),
26 \text{ vvnew=R*t/p},
                                                                                                    //assumed value close
                 to the ideal value
27 //calc of vol. of vapour
28 while e2>1e-6 do vvold=vvnew,
                                              x2=vvold^3*p+vvold^2*t1-vvold*t2+t3,
29
30
                                        der1=3*vvold^2*p+2*vvold*t1-t2,
31
                      vvnew=vvold-x2/der1
32 e2=abs(vvnew-vvold)
33 end
34 //fugacity of vapour
35 vvap=vvold,zvap=p*vvap/(R*t),
d=(a/(2*sqrt(2)*b*R*t))*(log((zvap+(1+sqrt(2))*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(2)*b*p/(
```

Scilab code Exa 3.7 pressure x y diagram using gamma phi approach

```
1 clc
2 disp("the soln of eg 3.7-->P-x-y calc. using Gamma-
      Phi approach");
                                           //assumed
3 \text{ et=1,er=1,sold=0, snew=0}
      values
4 R=8.314, t=100, x1=.958, a12=107.38*4.18, a21
      =469.55*4.18,
5 tc1=512.6, tc2=647.1, pc1=80.97*10^5, pc2=220.55*10^5,
      w1 = .564, w2 = .345, zc1 = .224, zc2 = .229, v1 = 40.73*10^-6,
       v2=18.07*10^-6
                                             //given data
6 x2=1-x1,
7 a1=16.5938, a2=16.262, b1=3644.3, b2=3799.89, c1
      =239.76, c2=226.35
8 p1sat=\exp(a1-b1/(c1+t))*1000
                                //Saturation Pressure
9 p2sat = exp(a2-b2/(c2+t))*1000
10 t=t+273.15
                                                    //Temp
      in Kelvin req.
11 h12=(v2/v1)*exp(-a12/(R*t))
12 h21 = (v1/v2) * exp(-a21/(R*t))
13 z=h12/(x1+x2*h12)-h21/(x2+x1*h21)
14 g1 = \exp(-\log(x1+x2*h12)+x2*z)
                                 //Activity Co-efficients
```

```
15 g2 = \exp(-\log(x2 + x1 + h21) - x1 + z)
16 \text{ tr1=t/tc1}
                                                          //Reduced
       Temp.
17 b0 = .083 - .422 * tr1^-1.6
18 b1 = .139 - .172 * tr1^-4.2
19 b11 = (R*tc1/pc1)*(b0+b1*w1)
20 \text{ tr}2=t/\text{tc}2
21 b0 = .083 - .422 * tr2^-1.6
22 b1 = .139 - .172 * tr2^-4.2
23 b22 = (R*tc2/pc2)*(b0+b1*w2)
24 \text{ w}12 = (\text{w}1 + \text{w}2)^{2}.5
25 \text{ tc12=(tc1*tc2)^.5}
26 \text{ zc12} = (\text{zc1} + \text{zc2})^{.5}
27 vc1=zc1*R*tc1/pc1, vc2=zc2*R*tc2/pc2
28 \text{ vc}12=((\text{vc}1^{3}.33+\text{vc}2^{3}.33)/2)^{3}
29 pc12=zc12*R*tc12/vc12
30 \text{ tr12=t/tc12}
31 b0=.083-.422*tr12^-1.6
32 b1 = .139 - .172 * tr12^-4.2
33 b12 = (R*tc12/pc12)*(b0+b1*w12)
34 d12 = 2*b12 - b11 - b22
35 p=x1*g1*p1sat+x2*p2sat*g2
36 \text{ y1=x1*g1*p1sat/p}, \text{ y2=x2*g2*p2sat/p}
37 \text{ pnew=p},
38 //calc of Pressure
39 while et>1e-6 do p=pnew,
40
         f1=p1sat*(exp(b11*p1sat/(R*t)))*(exp((v1*(p-t))))
            p1sat)/(R*t))))
41 f2=p2sat*(exp(b22*p2sat/(R*t)))*(exp((v2*(p-p2sat)/(R*t)))
       R*t))))
42 while er>1e-6 do sold=snew,
         fc1=exp((p/(R*t))*(b11+y2^2*d12))
43
     fc2=exp((p/(R*t))*(b22+y1^2*d12))
44
45
        k1=g1*f1/(fc1*p)
46 \text{ k2=g2*f2/(fc2*p)}
47 \text{ snew} = x1*k1+x2*k2
48 \quad y1=x1*k1/snew
49 \quad y2=x2*k2/snew
```

```
50 er=abs(snew-sold)
51 end
52 pnew=(x1*g1*f1/fc1)+(x2*g2*f2/fc2)
53 y1=x1*g1*f1/(fc1*pnew)
54 y2=x2*g2*f2/(fc2*pnew)
55 et=abs(pnew-p)
66 end
57 disp(p,y1,"the amt. of methanol in vapour phase and system pressure in Pa respectively are")
```

Scilab code Exa 3.9 chemical reaction engineering 2 simultaneous reactions

```
1 clc
2 disp("the soln of eg 3.9-->Chemical Reaction
      Equilibrium -2 Simultaneous Reactions")
3 //let x1 and x2 be the reaction co-ordinate for 1st
      and 2nd reactions
                                                   //assumed
4 x1new=.9, x2new=.6,r1=1,r2=1
       values
5 \text{ Kp}=1
                      // since P=1 atm
6 \text{ K1} = .574, \text{ K2} = 2.21
                                     //given
7 Kye1=K1, Kye2=K2
                                     //at eqm.
8 while r1>1e-6 & r2>1e-6, x1=x1new,x2=x2new,
9 m_CH4=1-x1, m_H20=5-x1-x2, m_C0=x1-x2, m_H2=3*x1+x2,
                     //moles of reactants and products
      m_C02=x2
      at eqm.
10 total=m_CO2+m_H2+m_CO+m_H2O+m_CH4
11 Ky1=m_C0*m_H2^3/(m_CH4*m_H20*total^2)
12 Ky2=m_C02*m_H2/(m_C0*m_H20)
                                                    //1st
13
       f1 = Ky1 - .574
          function in x1 and x2
       f2 = Ky2 - 2.21
                                                    //2nd
14
          function in x1 and x2
15
       d3 = ((3*x1+x2)^2*(12*x1-8*x2))/((1-x1)*(5-x1-x2)
```

```
*(6+2*x1)^2
                           d4 = (3 \times x1 + x2)^3 \times (x1 - x2) \times (8 \times x1^2 + 6 \times x1 \times x2 - 24 \times x1 + 2 
16
                                     x2-16)
17
                           d5 = ((1-x1)^2)*((5-x1-x2)^2)*((6+2*x1)^3)
                                                                                                                                                                                                //df1
18
                           df1_dx1=d3-(d4/d5)
                                     /dx1- partial derivative of f1 wrt to x1
                           d6=3*(x1-x2)*((3*x1+x2)^2)-(3*x1+x2)^3
19
                           d7 = (1-x1)*(5-x1-x2)*((6+x1*2)^2)
20
                           d8 = ((x1-x2)*(3*x1+x2)^3)/((1-x1)*((5-x1-x2)^2)
21
                                     *(6+2*x1)^2
                                                                                                                                                                                                //df1
                           df1_dx2 = (d6/d7) + d8
22
                                     /dx2- partial derivative of f1 wrt to x2
23
                          d9 = (x1 - x2) * (5 - x1 - x2)
                           df2_dx1=3*x2/d9-(x2*(3*x1+x2)*(5-2*x1))/(d9^2)
24
                                                               //df1/dx2- partial derivative of f1
                                     wrt to x2
                          d10 = (3 * x1 + 2 * x2) / d9
25
                          d11=x2*(3*x1+x2)*(2*x2-5)/(d9^2)
26
                           df2_dx2=d10-d11
27
                                     df1/dx2- partial derivative of f1 wrt to x2
                           dm=df1_dx1*df2_dx2-df1_dx2*df2_dx1
28
                           delta_x1 = (f2*df1_dx2-f1*df2_dx2)/dm
29
30
                           delta_x2=(f1*df2_dx1-f2*df1_dx1)/dm
31 x1new=x1+delta_x1
                                                                                                                                                                         //updating
                      the values of x1 & x2
32 \quad x2new=x2+delta_x2
33 r1 = abs(x1 - x1new), r2 = abs(x2new - x2)
34 end
35 disp(x2,x1,"the value of X1 and X2 respectively is")
36 \text{ m}_{C}H4=1-x1, m_{H}20=5-x1-x2, m_{C}0=x1-x2, m_{H}2=3*x1+x2,
                     m_C02=x2
                                                                           //moles of reactants and products
                     at eqm.
37 \text{ total} = m_CO2 + m_H2 + m_CO + m_H2O + m_CH4
38 disp(m_CO2,m_H2,m_CO,m_H2O,m_CH4,"the moles at eqm
                      of CH4, H2O, CO, H2, CO2 are")
39 disp(total, "total number of moles at eqm. is")
```

Scilab code Exa 3.10 adiabatic flame temperature

```
1 clc
2 disp("the soln of eg 3.10--> Adiabatic Flame
      Temperature");
3 u1=1, u2=3.5, u3=2, u4=3
                                                      //moles
      given 1-C2H6, 2-O2, 3-CO2, 4-H2O
4 a1=1.648, a2=6.085, a3=5.316, a4=7.7
5 b1=4.124e-2, b2=.3631e-2, b3=1.4285e-2, b4=.04594e-2
6 c1=-1.53e-5, c2=-.1709e-5, c3=-.8362e-5, c4=.2521e-5
7 d1=1.74e-9, d2=.3133e-9, d3=1.784e-9, d4=-.8587e-9
8 \text{ n1=1}, \text{n2=4}, \text{n3=10}, \text{n4=0}, \text{t0=298.15}, \text{t1=25}, \text{e1=1}
9 t1=t1+273.15
10 //calc. of sum of co-efficients of heat capacity of
      the rxn.
11 \quad \text{sa=n1*a1+n2*a2+n3*a3+n4*a4}
12 	ext{ sb=n1*b1+n2*b2+n3*b3+n4*b4}
13 \text{ sc}=n1*c1+n2*c2+n3*c3+n4*c4
14 \text{ sd} = n1*d1+n2*d2+n3*d3+n4*d4
15 da=u4*a4+u3*a3-u2*a2-u1*a1
16 db = u4 * b4 + u3 * b3 - u2 * b2 - u1 * b1
17 dc = u4 * c4 + u3 * c3 - u2 * c2 - u1 * c1
18 dd=u4*d4+u3*d3-u2*d2-u1*d1
19 h0=(u4*(-57.798)+u3*(-94.05)-u2*0-u1*(-20.236))*1000
                         //enthalpy of the rxn.
20 \text{ tnew} = 1000
21 while e1>1e-6 do t=tnew,
22
        function f=ft(t),
        f=sa*(t-t1)+(sb/2)*(t^2-t1^2)+(sc/3)*(t^3-t1^3)
23
           +(sd/4)*(t^4-t^4)+h0+da*(t-t0)+(db/2)*(t^2-
           t0^2+(dc/3)*(t^3-t0^3)+(dd/4)*(t^4-t0^4)
24 endfunction
25 dr=derivative(ft,t),
26 \text{ tnew=t-ft(t)/dr,}
```

```
27 e1=abs((tnew-t)/tnew)
28 end
29 disp(tnew,"the adiabatic flame temp in K is");
```

Chapter 4

INITIAL VALUE PROBLEMS

Scilab code Exa 4.1 solution of ordinary differential equation

```
1 clc
2 disp("the solution of e.g. 4.1 -->Integration of
      Ordinary Differential Equation")
\frac{3}{\sqrt{x}} in this problem \frac{dy}{dx} = x + y
4 x_0 = 0
                             //initial values given
5 y_0 = 0
7 function ydash=fs(x,y),
8
        ydash=x+y,
9 endfunction
10
11 for x_0=0:0.1:0.2,
                                                        //step
12
       h = 0.1
           increment of 0.1
       f_0=fs(x_0,y_0)
13
14
       k1=h*f_0
15
       k2=h*fs(x_0+h/2,y_0+k1/2)
16
       k3=h*fs(x_0+h/2,y_0+k2/2)
17
       k4=h*fs(x_0+h,y_0+k3)
        y_0 = y_0 + (k_1 + 2 * k_2 + 2 * k_3 + k_4) / 6
18
19 end
```

Scilab code Exa 4.2 solution of ordinary differential equation

```
1 clc
2 disp("the solution of e.g. 4.2 -->Ordinary
      Differential Eqn.-Runge Kutta method")
3 // in this problem dy/dx=-y/(1+x)
4 x_0 = 0
                            //initial values given
5 y_0 = 2
6 function ydash=fr(x,y),
       ydash=-y/(1+x),
8 endfunction
9 for x_0=0:0.01:2.5,
       h = 0.01
10
                                                        //step
            increment of 0.01
       f_0=fr(x_0,y_0)
11
12
       k1 = h * f_0
       k2=h*fr(x_0+h/2,y_0+k1/2)
13
       k3=h*fr(x_0+h/2,y_0+k2/2)
14
15
       k4=h*fr(x_0+h,y_0+k3)
16
       y_0 = y_0 + (k_1 + 2 * k_2 + 2 * k_3 + k_4) / 6
17 end
18 \quad y_0 = y_0 - (k1 + 2 * k2 + 2 * k3 + k4) / 6
                                                         //
      final value at x=2.5
19 disp(y_0), "the value of y at x=2.5 using Runge Kutta
      method is");
```

Scilab code Exa 4.3 double pipe heat exchanger

```
1 clc
2 disp("the solution of e.g. 4.3 --> Double Pipe Heat
      Exchanger");
3 \text{ rho=1000, v=1, dia=2.4*10^--2, Cp=4184}
                                                          //
      given data
4 mdot=rho*v*%pi*dia^2/4
5 t1=mdot*Cp
6 U = 200
7 \text{ Ts} = 250
                         //initial values given
8 z=0
9 // dT/dz=U*pi*dia*(Ts-T)/(mdot*Cp)
10 function Tgrad=fr(z,T),
       Tgrad=U*\%pi*dia*(Ts-T)/(mdot*Cp),
11
12 endfunction
13 T=20
14 for z=0:0.01:10,
                                                      //step
15
       h = 0.01
           increment of 0.01
       k1=h*fr(z,T)
16
17
       k2=h*fr(z+h/2,T+k1/2)
18
       k3=h*fr(z+h/2,T+k2/2)
       k4=h*fr(z+h,T+k3)
19
       T=T+(k1+2*k2+2*k3+k4)/6
20
       if z==5 then T=T-(k1+2*k2+2*k3+k4)/6,
21
            disp(T," the value of T in deg Celsius at z=5
22
               m using Runge Kutta method is");
23
       end
24 end
25 \quad T=T-(k1+2*k2+2*k3+k4)/6
                                                   //final
      value at z=10 \text{ m}
  disp(T," the value of T in deg Celsius at z=10 m
      using Runge Kutta method is");
```

Scilab code Exa 4.4 stirred tank with coil heater

```
1 clc
2 disp("the solution of e.g. 4.4 -->Stirred Tank with
      Coil Heater")
3 \text{ vol} = .5 * .5 * 2
                                            //given data
4 rho=1000
5 \text{ m=vol*rho}
6 \text{ vol_rate} = .001
7 mdot=vol_rate*rho
8 \text{ out}_A = 1
9 U = 200
10 \text{ Cp} = 4184
11 T1=20, Ts=250, T_exit=28
      //temp in Celsius
12 t1=(mdot*Cp*T1+U*out_A*Ts)/(m*Cp)
      //terms of the function
13 t2=(mdot*Cp+U*out_A)/(m*Cp)
14 / dt / dt = (mdot * Cp (T1-T) + Q_dot) / m * Cp
15 function tgrad=fv(tm,T),
        tgrad=t1-t2*T
16
17 endfunction
                                                             //
18 T=20
      initial value
19 funcprot(0)
20 \text{ for } tm=0:1:5000,
       h=1
                                                      //step
21
           increment of 1 sec
22
       k1=h*fv(tm,T)
23
       k2=h*fv(tm+h/2,T+k1/2)
       k3=h*fv(tm+h/2,T+k2/2)
24
       k4=h*fv(tm+h,T+k3)
25
        e1=abs(T-T_exit)
26
        if e1<1e-3 then disp(tm,"the time at which exit
27
```

Scilab code Exa 4.5 stirred tank with coil heater

```
1 clc
2 disp("the solution of e.g. 4.5 ->Stirred Vessel
      with Coil Heater");
3 m = 760
                                                       //
      given data
4 \text{ mdot} = 12/60
5 U_into_A=11.5/60
6 Cp = 2.3
7 T1 = 25, Ts = 150
8 t1=(mdot*Cp*T1+U_into_A*Ts)/(m*Cp)
9 t2=(mdot*Cp+U_into_A)/(m*Cp)
10 //using energy balance we know accumulation=input-
      output
11 //T is the temp. of fluid in stirred tank
12 function tgrade=fg(t,T);
        tgrade = (t1 - t2 * T),
13
14 endfunction
15 T=25
16 \text{ for } t=0:1:3000,
                                                   //step
17
       h = 1
          increment of 1 sec
18
       k1=h*fg(t,T)
       k2=h*fg(t+h/2,T+k1/2)
19
20
       k3=h*fg(t+h/2,T+k2/2)
       k4=h*fg(t+h,T+k3)
21
```

Scilab code Exa 4.6 pneumatic conveying

```
1 clc
2 disp("the soln of eg 4.6-->Pneumatic Conveying")
3 \text{ dia}=3*10^-4
                                               //given data
4 v_sprfcl=12
5 rho_p=900
6 meu=1.8*10^-5
7 P=101325
8 T=298.15
9 R=8.314
10 M = 28.84 * 10^{-3}
11 rho_air=P*M/(R*T)
12 proj_A=%pi*(dia^2)/4
13 volm=%pi*(dia^3)/6
14 t1=rho_air*proj_A/(volm*rho_p)
                               //terms of the function
15 t2=((rho_air/rho_p)-1)*9.81*2
16 y = 0
17 for z=.01:.01:10,
18
       h = .01
       vn1=sqrt(y)
19
20
       Re=rho_air*(12-vn1)*dia/meu
       Cd = 24 * (1 + .15 * Re^{.687}) / Re
21
       function dy_by_dz=fy(z,y),
22
23
       dy_by_dz = t1*Cd*(12-sqrt(y))^2+t2,
24 endfunction
```

```
25
       kk1=h*fy(z,y)
       kk2=h*fy(z+h/2,y+kk1/2)
26
27
       kk3=h*fy(z+h/2,y+kk2/2)
       kk4=h*fy(z+h,y+kk3)
28
29
       y=y+(kk1+2*kk2+2*kk3+kk4)/6
30
       end
                                    //final value of
31 \text{ v=} \text{sqrt}(y)
      velocity
32 disp(v," the value of v at the end of the pneumatic
      conveyor is");
```

Scilab code Exa 4.7 simultaneous ordinary differential equations

```
1 clc
2 disp("the soln of eg 4.7-->Simultaneous O.D.E.")
3 function dx_dt=fw(t,x,y);
             dx_dt = x + 2 * y,
4
5 endfunction
6 function dy_dt=fq(t,x,y);
             dv_{dt} = 3 * x + 2 * y
7
8 endfunction
9 \text{ y=4, x=6}
                                       //initial values
10 //solving by Runge-Kutta method
11 for t=0:.1:.2,
12
       h = .1
                                                    //step
          increment of 0.1
       k1=h*fw(t,x,y)
13
14
       11=h*fq(t,x,y)
15
       k2=h*fw(t+h/2,x+k1/2,y+11/2)
       12=h*fq(t+h/2,x+k1/2,y+11/2)
16
       k3=h*fw(t+h/2,x+k2/2,y+12/2)
17
       13=h*fq(t+h/2,x+k2/2,y+12/2)
18
       k4=h*fw(t+h,x+k3,y+13)
19
20
       14=h*fq(t+h,x+k3,y+13)
21
       x=x+(k1+2*k2+2*k3+k4)/6
```

```
22     y=y+(11+2*12+2*13+14)/6
23     end
24     x=x-(k1+2*k2+2*k3+k4)/6
25     y=y-(11+2*12+2*13+14)/6
26     disp(y,x,"the values of x and y repectively are");
27     t_an=.2
28     x_an=4*exp(4*t)+2*exp(-t)
29     y_an=6*exp(4*t)-2*exp(-t)
30     disp(y_an,x_an,"the analytical values of x and y are respectively");
```

Scilab code Exa 4.8 simultaneous ordinary differential equations

```
1 clc
2 disp("the soln of eg 4.8-->Simultaneous O.D.E.")
3 function dy_dx=fw(x,y,z);
            dy_dx=z,
4
5 endfunction
6 function dz_dx=fq(x,y,z);
            dz_dx = -y
7
8 endfunction
9 y=2, z=1
                                      //initial values
10 for x=0:.1:3,
                                                  //step
11
       h = .1
          increment of 0.1
       k1=h*fw(x,y,z)
12
       11=h*fq(x,y,z)
13
       k2=h*fw(x+h/2,y+k1/2,z+l1/2)
14
15
       12=h*fq(x+h/2,y+k1/2,z+11/2)
       k3=h*fw(x+h/2,y+k2/2,z+12/2)
16
       13=h*fq(x+h/2,y+k2/2,z+12/2)
17
       k4=h*fw(x+h,y+k3,z+13)
18
       14=h*fq(x+h,y+k3,z+13)
19
20
       y=y+(k1+2*k2+2*k3+k4)/6
21
       z=z+(11+2*12+2*13+14)/6
```

```
22     end
23     y=y-(k1+2*k2+2*k3+k4)/6
24     z=z-(11+2*12+2*13+14)/6
25     disp(z,y,"the values of y and z respectively are");
26     // for the given analytical eqns the values of A and alpha can be determined using initial values of y and z
27     alpha=atan(2)
28     A=2/sin(alpha)
29     y_an=A*sin(alpha+x)
30     z_an=A*cos(alpha+x)
31     disp(z_an,y_an,"the analytical values of y and z are ");
```

Scilab code Exa 4.9 simultaneous ordinary differential equations

```
1 clc
2 disp("the soln of eg 4.9-->Simultaneous O.D.E.")
3 function dy_dx=fw(x,y,z);
                                                 //let us
      have dy/dx=z, therefore d2y/dx2=dz/dx
4
            dy_dx=z,
5 endfunction
6 function dz_dx=fq(x,y,z);
7
            dz_dx = -y * x,
8 endfunction
9 y=2, z=1
10 for x=0:.1:3,
11
       h = .1
                                                  //step
          increment of 0.1
       k1=h*fw(x,y,z)
12
13
       11=h*fq(x,y,z)
       k2=h*fw(x+h/2,y+k1/2,z+11/2)
14
       12=h*fq(x+h/2,y+k1/2,z+11/2)
15
16
       k3=h*fw(x+h/2,y+k2/2,z+12/2)
17
       13=h*fq(x+h/2,y+k2/2,z+12/2)
```

Scilab code Exa 4.10 series of stirred tank with coil heater

```
1 clc
2 disp("the solution of eg 4.10 --> Series of Stirred
      Tanks with Coil Heaters")
4 Cp=2000, A=1, U=200, m=1000, mdot=2, Ts=250
                        //given data
5 \text{ T0=20}, \text{ T1=0}, \text{ T2=0}, \text{ T3=0}
7 //from energy balances for the tanks we have
      accumulation=inlet-outlet
8 T1_steady = (mdot*Cp*(T0)+U*A*(Ts))/(mdot*Cp+U*A)
9 disp(T1_steady,"the steady state temperature of tank
       1 is");
10 T2\_steady = (mdot*Cp*(T1\_steady)+U*A*(Ts))/(mdot*Cp+U*
11 disp(T2_steady," the steady state temperature of tank
       2 is"):
12 T3\_steady = (mdot*Cp*(T2\_steady)+U*A*(Ts))/(mdot*Cp+U*
13 disp(T3_steady," the steady state temperature of tank
       3 is");
14 \text{ final}_T3 = .99 * T3_steady
15 function dT1_by_dt=f1(t,T1,T2,T3),
16
       dT1_by_dt = (mdot*Cp*(T0-T1)+U*A*(Ts-T1))/(m*Cp),
```

```
17 endfunction
18 function dT2_by_dt=f2(t,T1,T2,T3),
       dT2_by_dt = (mdot*Cp*(T1-T2)+U*A*(Ts-T2))/(m*Cp),
19
20 endfunction
21 function dT3_by_dt=f3(t,T1,T2,T3),
22
       dT3_by_dt = (mdot*Cp*(T2-T3)+U*A*(Ts-T3))/(m*Cp),
23 endfunction
24 \quad T1=20, T2=20, T3=20
25 //solving by Newton's Method
26 \quad \text{for} \quad t=0:1:10000
                                                  //step
       h=1
27
          increment of 1
28
       k1=h*f1(t,T1,T2,T3)
       11=h*f2(t,T1,T2,T3)
29
30
       m1=h*f3(t,T1,T2,T3)
       k2=h*f1(t+h/2,T1+k1/2,T2+11/2,T3+m1/2)
31
       12=h*f2(t+h/2,T1+k1/2,T2+11/2,T3+m1/2)
32
       m2=h*f3(t+h/2,T1+k1/2,T2+11/2,T3+m1/2)
33
       k3=h*f1(t+h/2,T1+k2/2,T2+12/2,T3+m2/2)
34
35
       13=h*f2(t+h/2,T1+k2/2,T2+12/2,T3+m2/2)
       m3=h*f3(t+h/2,T1+k2/2,T2+12/2,T3+m2/2)
36
       k4=h*f1(t+h,T1+k3,T2+13,T3+m3)
37
       14=h*f2(t+h,T1+k3,T2+13,T3+m3)
38
       m4=h*f3(t+h,T1+k3,T2+13,T3+m3)
39
40
       T1=T1+(k1+2*k2+2*k3+k4)/6
41
       T2=T2+(11+2*12+2*13+14)/6
       e1=abs(T3-final_T3)
42
       if e1<1e-3 then disp(t,"the approx. time when
43
          Temperature in 3rd tank is 99% of steady
          value is"); break
44
45
       T3=T3+(m1+2*m2+2*m3+m4)/6
46 end
```

Scilab code Exa 4.11 batch and stirred tank reactor

```
1 clc
2 //batch reactors
3 disp("the solution of e.g. 4.11 --> Batch and Stirred
       Tank Reactors")
4 // rxn given A \rightarrow B
5 rate_const_k=1
6 function dCa_by_dt=fs1(t,Ca),
       dCa_by_dt = - rate_const_k * Ca,
8 endfunction
9 \text{ Ca}=1
10 for t=0.1:0.1:3,
11
                                                     //step
       h = 0.1
          increment of 0.1
12
       k1=h*fs1(t,Ca)
       k2=h*fs1(t+h/2,Ca+k1/2)
13
14
       k3=h*fs1(t+h/2,Ca+k2/2)
       k4=h*fs1(t+h,Ca+k3)
15
       Ca=Ca+(k1+2*k2+2*k3+k4)/6
16
17 end
18 disp(Ca," the value of conc. at t=3 using Runge Kutta
       method is");
                                       //analytical
19 Ca_anl = exp(-t)
      solution
20 disp(Ca_anl,"the analytical soln. is")
```

Scilab code Exa 4.12 batch and stirred tank reactor

```
7 Ca0=1, F=1, V=10
9 function dVCa_by_dt=fr(t,Ca1),
       dVCa_by_dt=F*Ca0-F*Ca1-rate_const_k*Ca1*V,
10
11 endfunction
12 Ca1=1
13 for t=0.1:0.1:10,
                                                   //step
14
       h = 0.1
          increment of 0.1
       k1=h*fr(t,Ca1)
15
       k2=h*fr(t+h/2,Ca1+k1/2)
16
17
      k3=h*fr(t+h/2,Ca1+k2/2)
18
       k4=h*fr(t+h,Ca1+k3)
       Ca1 = Ca1 + (k1 + 2 * k2 + 2 * k3 + k4)/6
19
20 end
                            //final value
21 disp(Ca1," the value of Ca at t=10 s using Runge
      Kutta method is");
22 Ca_steady=F*Ca0/(F+rate_const_k*V)
23 disp(Ca_steady,"the steady state value of conc. is")
```

Scilab code Exa 4.13 batch and stirred tank reactor

```
1 clc
2 //given rxn A--->B--->C
3 k1=1, k2=1
                               //given data
4 disp("the solution of eg 4.13 --> Batch Reactors")
5 function dA_by_dt=f1a(t,A,B,C),
                                                        //
      functions defined
6
       dA_by_dt = -A,
7 endfunction
8 function dB_by_dt=f2a(t,A,B,C),
9
       dB_by_dt = A - B,
10 endfunction
11 function dC_by_dt=f3a(t,A,B,C),
```

```
12
       dC_by_dt=B,
13 endfunction
                                        //initial values
14 \quad A=1, B=0, C=0
15 for t=0.1:.1:10,
                                                    //step
16
       h = .1
          increment of 0.1
       k1=h*f1a(t,A,B,C)
17
       11=h*f2a(t,A,B,C)
18
       m1=h*f3a(t,A,B,C)
19
       k2=h*f1a(t+h/2,A+k1/2,B+11/2,C+m1/2)
20
       12=h*f2a(t+h/2,A+k1/2,B+l1/2,C+m1/2)
21
22
       m2=h*f3a(t+h/2,A+k1/2,B+11/2,C+m1/2)
23
       k3=h*f1a(t+h/2,A+k2/2,B+12/2,C+m2/2)
       13=h*f2a(t+h/2,A+k2/2,B+12/2,C+m2/2)
24
25
       m3=h*f3a(t+h/2,A+k2/2,B+12/2,C+m2/2)
       k4=h*f1a(t+h,A+k3,B+l3,C+m3)
26
       14=h*f2a(t+h,A+k3,B+13,C+m3)
27
       m4=h*f3a(t+h,A+k3,B+13,C+m3)
28
       A = A + (k1 + 2 * k2 + 2 * k3 + k4)/6
29
30
       B=B+(11+2*12+2*13+14)/6
       C=C+(m1+2*m2+2*m3+m4)/6
31
       if t==.5 | t==1 | t==2 | t==5  then disp(C,B,A,"secs
32
          is",t,"the conc. of A,B,C after");
33
       end
34 end
35 disp(C,B,A," the conc. of A,B,C after 10 secs
      respectively is");
```

Scilab code Exa 4.14 batch and stirred tank reactor

```
5 disp("the solution of eg 4.14 --->Batch Reactors")
6 function dA_by_dt=f1a(t,A,B,C,D),
       dA_by_dt = -A*B,
8 endfunction
9 function dB_by_dt=f2a(t,A,B,C,D),
10
       dB_by_dt = -A*B-B*C,
11 endfunction
12 function dC_by_dt=f3a(t,A,B,C,D),
       dC_bv_dt = A*B-B*C,
13
14 endfunction
15 function dD_by_dt=f4a(t,A,B,C,D),
       dD_by_dt = B*C,
16
17 endfunction
18 A=1, B=1, C=0, D=0
                                                  //initial
       values
19 for t = .1 : .1 : 10,
                                                   //step
       h = .1
20
          increment of 0.1
       k1=h*f1a(t,A,B,C,D)
21
22
       11=h*f2a(t,A,B,C,D)
23
       m1=h*f3a(t,A,B,C,D)
       n1=h*f4a(t,A,B,C,D)
24
25
       k2=h*f1a(t+h/2,A+k1/2,B+11/2,C+m1/2,D+n1/2)
       12=h*f2a(t+h/2,A+k1/2,B+11/2,C+m1/2,D+n1/2)
26
       m2=h*f3a(t+h/2,A+k1/2,B+l1/2,C+m1/2,D+n1/2)
27
28
       n2=h*f4a(t+h/2,A+k1/2,B+l1/2,C+m1/2,D+n1/2)
29
       k3=h*f1a(t+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
30
       13=h*f2a(t+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
       m3=h*f3a(t+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
31
       n3=h*f4a(t+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
32
       k4=h*f1a(t+h,A+k3,B+13,C+m3,D+n3)
33
34
       14=h*f2a(t+h,A+k3,B+13,C+m3,D+n3)
35
       m4=h*f3a(t+h,A+k3,B+13,C+m3,D+n3)
36
       n4=h*f4a(t+h,A+k3,B+13,C+m3,D+n3)
       A = A + (k1 + 2 * k2 + 2 * k3 + k4)/6
37
       B=B+(11+2*12+2*13+14)/6
38
       C=C+(m1+2*m2+2*m3+m4)/6
39
       D=D+(n1+2*n2+2*n3+n4)/6
40
```

Scilab code Exa 4.15 plug flow reactor

```
1 clc
2 disp("the solution of eg 4.15 --> Plug Flow Reactor")
3 \text{ rc}_k1=1
                                   //given rate constant
                         //mean axial velocity
4 u=1
5 function dCa_by_dx=fm(x,Ca),
       dCa_by_dx = -Ca,
7 endfunction
8 \text{ Ca}=1
9 for x = .1 : .1 : 10,
                                                     //step
10
       h=0.1
          increment of 0.1
       k1=h*fm(x,Ca)
11
       k2=h*fm(x+h/2,Ca+k1/2)
12
       k3=h*fm(x+h/2,Ca+k2/2)
13
14
       k4=h*fm(x+h,Ca+k3)
       Ca=Ca+(k1+2*k2+2*k3+k4)/6
15
       if x==.5 | x==1 | x==2 | x==5 then disp(Ca, "length is"
16
          ,x,"the value of conc. at");
17
       end
18 end
19 disp(Ca," the value of Ca at x=10 using Runge Kutta
      method in plug flow reactor is");
```

Scilab code Exa 4.16 plug flow reactor

```
1 clc
2 //given rxn A--->B--->C
                                                   //given
3 rc_k1=1, rc_k2=1
      rate constants
4 u = 1
                                            //mean axial
      velocity
5 disp("the solution of eg 4.16 -->Plug Flow Reactor")
6 function dA_by_dx=f1e(x,A,B,C),
7
       dA_by_dx = -A,
8 endfunction
9 function dB_by_dx=f2e(x,A,B,C),
       dB_by_dx = A - B,
10
11 endfunction
12 function dC_by_dx=f3e(x,A,B,C),
       dC_by_dx=B,
13
14 endfunction
15 \quad A=1, B=0, C=0
16 for x = .1 : .1 : 10,
       h = .1
                                                    //step
17
          increment of 0.1
       k1=h*f1e(x,A,B,C)
18
       11=h*f2e(x,A,B,C)
19
20
       m1=h*f3e(x,A,B,C)
       k2=h*f1e(x+h/2,A+k1/2,B+l1/2,C+m1/2)
21
       12=h*f2e(x+h/2,A+k1/2,B+l1/2,C+m1/2)
22
23
       m2=h*f3e(x+h/2,A+k1/2,B+11/2,C+m1/2)
24
       k3=h*f1e(x+h/2,A+k2/2,B+12/2,C+m2/2)
25
       13=h*f2e(x+h/2,A+k2/2,B+12/2,C+m2/2)
       m3=h*f3e(x+h/2,A+k2/2,B+12/2,C+m2/2)
26
27
       k4=h*f1e(x+h,A+k3,B+13,C+m3)
       14=h*f2e(x+h,A+k3,B+13,C+m3)
28
29
       m4=h*f3e(x+h,A+k3,B+13,C+m3)
30
       A = A + (k1 + 2 * k2 + 2 * k3 + k4) / 6
31
       B=B+(11+2*12+2*13+14)/6
       C=C+(m1+2*m2+2*m3+m4)/6
32
       if x==.5 | x==1 | x==2 | x==5 then disp(C,B,A," mtr is
33
          ",x," the conc. of A,B,C at a distance of");
34
       end
```

```
35 end
36 disp(C,B,A,"the conc. of A,B,C at a distance of 10 mtr is");
```

Scilab code Exa 4.17 plug flow reactor

```
1 clc
\frac{2}{\sqrt{given}} rxn A+B-k1-->C
                B+C---k2--->D
                                                   //rate
4 rc_k1=1,rc_k2=1
      constants
5 disp("the solution of eg 4.17 --> Plug Flow Reactor")
6 function dA_by_dx=f1a(x,A,B,C,D),
7
       dA_by_dx = -A*B,
8 endfunction
9 function dB_by_dx=f2a(x,A,B,C,D),
       dB_by_dx = -A*B-B*C,
10
11 endfunction
12 function dC_by_dx=f3a(x,A,B,C,D),
       dC_by_dx = A*B-B*C,
13
14 endfunction
15 function dD_by_dx=f4a(x,A,B,C,D),
16
       dD_by_dx = B*C,
17 endfunction
18 A=1, B=1, C=0, D=0
19 for x = .1 : .1 : 10,
20
       h = .1
                                                    //step
          increment of 0.1
21
       k1=h*f1a(x,A,B,C,D)
       11=h*f2a(x,A,B,C,D)
22
23
       m1=h*f3a(x,A,B,C,D)
24
       n1=h*f4a(x,A,B,C,D)
       k2=h*f1a(x+h/2,A+k1/2,B+11/2,C+m1/2,D+n1/2)
25
26
       12=h*f2a(x+h/2,A+k1/2,B+11/2,C+m1/2,D+n1/2)
27
       m2=h*f3a(x+h/2,A+k1/2,B+l1/2,C+m1/2,D+n1/2)
```

```
28
       n2=h*f4a(x+h/2,A+k1/2,B+l1/2,C+m1/2,D+n1/2)
       k3=h*f1a(x+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
29
       13=h*f2a(x+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
30
       m3=h*f3a(x+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
31
32
       n3=h*f4a(x+h/2,A+k2/2,B+12/2,C+m2/2,D+n2/2)
33
       k4=h*f1a(x+h,A+k3,B+13,C+m3,D+n3)
       14=h*f2a(x+h,A+k3,B+13,C+m3,D+n3)
34
       m4=h*f3a(x+h,A+k3,B+13,C+m3,D+n3)
35
       n4=h*f4a(x+h,A+k3,B+13,C+m3,D+n3)
36
37
       A = A + (k1 + 2 * k2 + 2 * k3 + k4) / 6
       B=B+(11+2*12+2*13+14)/6
38
       C=C+(m1+2*m2+2*m3+m4)/6
39
40
       D=D+(n1+2*n2+2*n3+n4)/6
       if x==.5 | x==1 | x==2 | x==5  then disp(D,C,B,A," secs
41
           is",x,"the conc. of A,B,C,D after");
42
       end
43 end
       disp(D,C,B,A," the conc. of A,B,C,D after 10 secs
44
           respectively is");
```

Scilab code Exa 4.18 non isothermal plug flow reactor

```
10 / dX_by_dV = k*(1-X)/F
11 //from energX balance
12 / mdot*Cp*dT_by_dz+ra*A*H_RXN-q=0
13 / q = U * \% pi * dia * (Ts - T)
14 //-mdot*Cp*dT_by_dV+4*U/dia*(Ts-T)-ra*H_rxn=0
15 F=mdot/rho
16 \ t1 = A * k1/F
17
18 \text{ s1=mdot*Cp/A}
19 	 s2=4*U/dia
20 \quad s3=H_rxn*t1
21
22 function dX_by_dz=fg1(z,X,T),
             dX_by_dz = t1*(1-X)*exp(b*(1-T1/T))
23
24 endfunction
25 function dT_by_dz=fd1(z,X,T),
             ra=na0/A*(t1*(1-X)*exp(b*(1-T1/T)))
26
27
             dT_by_dz = (ra*H_rxn-s2*(Ts-T))/-s1
28
29 endfunction
30
31 \quad X=0, T=294.15
32 \text{ for } z=0:.1:350,
       h = .1
                                                     //szep
33
           incremenz of 0.1
34
       k1=h*fg1(z,X,T)
35
       11=h*fd1(z,X,T)
       k2=h*fg1(z+h/2,X+k1/2,T+l1/2)
36
37
       12=h*fd1(z+h/2,X+k1/2,T+11/2)
38
       k3=h*fg1(z+h/2,X+k2/2,T+12/2)
39
       13=h*fd1(z+h/2,X+k2/2,T+12/2)
40
       k4=h*fg1(z+h,X+k3,T+13)
       14=h*fd1(z+h,X+k3,T+13)
41
42
       X = X + (k1 + 2 * k2 + 2 * k3 + k4)/6
       T=T+(11+2*12+2*13+14)/6
43
       //condition for height calc. for 90% conversion
44
       if X>.9 &X<.9005 then disp(z,"the height of the
45
           tower required for 90% conversion in mtrs is"
```

```
); break
46 end
47 end
```

Chapter 5

BOUNDARY VALUE PROBLEMS

Scilab code Exa 5.1 discretization in 1 D space

```
1 clc
2 //finite difference method
3 disp("the solution of eg 5.1--> Discretization in 1-D
       space");
4 //given d2y_by_dx_2-2=0 hence it is dirichlet's
      problem
                                 //initial boundary
6 x_1=0, y_1=0
      conditions
7 x_3=1, y_3=0
9 \text{ delta_x=.5}
                                //since we have to find
      v_2 at x = .5 so x_2 = .5
10 //in the central difference method substituting i=2
11 //(y_3-2*y_2+y_1)/(delta_x)^2=2
12 // \text{since y}_1 \& y_3 = 0 \text{ as per B.C.}
13 y_2 = (y_3 + y_1 - 2*delta_x^2)/2
14 disp(y_2,"the value of y at x=.5 from finite
```

```
difference method is");
15 x=.5
16 y_exact=x^2-x
17 disp(y_exact,"the value of y from exact soln at x=.5
    is");
```

Scilab code Exa 5.2 discretization in 1 D space

```
1 clc
2 disp("the solution of eg 5.2 --> Discretization in 1-
      D space");
3 //boundary conditions are: x=0 at y=0; dy/dx=1 at x
4 disp("to solve this problem we will take delta x=.5
      since we have to find the value at x=.5");
5 \text{ delta_x=.5}
6 y_1=0
7 //using central difference equ
8 	 dy_by_dx=1
                                 // at x=1, i=3
9 //y_4 = dy/dx * 2 * delta_x + y_2
                                              sincefrom B.C.
       at node 3
10
11 / y_2 = delta_x^2 + y_3 - delta_x
                                              on
      substituting the value of y<sub>-</sub>4
12 y_3 = -(2*delta_x^2 + 2*(delta_x^2 - delta_x) - y_1) //on
      substituting the value of y<sub>-</sub>2
13 y_2 = delta_x^2 + y_3 - delta_x
14 disp(y_2,"the value of y at x=.5 is");
```

Scilab code Exa 5.3 discretization in 1 D space

1 clc

```
2 disp("the solution of eg 5.3 --> Discretization in 1-
     D space");
3 // given the source term f(x)=4x^2-2x-4
4 //given eqn d2y/dx2-2y=f(x)
5 y_1 = 0
6 y_4 = -1
7 \text{ delta_x=1/3}
                          //since given 3 parts and
     length=1
8 for i=0:3,j=0:delta_x:1;
9 end
10 //given to divide the line in 3 parts
11 //at node 2
12 / y_3 - 2 * y_2
13 function d=fx3(x),
14 d = (4 * x^2 - 2 * x - 4)
15 endfunction
16 f2=fx3(j(2))
17 f3=fx3(j(3))
18 y_3=((f2)*delta_x^2+(2+2*delta_x^2)*((f3)*delta_x^2-
      y_4)-y_1)/(1-(2+2*delta_x^2)^2)
19 y_2 = (f3+2*y_3)*delta_x^2+2*y_3-y_4
20 disp(y_3,y_2,"is respectively",j(3),j(2),"the value
      of y at x=");
```

Scilab code Exa 5.4 discretization in 1 D space

```
9 //given to divide the line in 3 parts
10 function d=fx3(x),
11 d = (4 * x^2 - 2 * x - 4)
12 endfunction
13 f2=fx3(j(2))
14 f3=fx3(j(3))
15 f4=fx3(j(4))
16 disp("the exact analytical soln are");
17 for i=1:3, y(i)=-2*j(i+1)^2+j(i+1), disp(y(i));
18 end
19 // using B.C. -2 at node 4 we get
20 //(y_5-y_3)/(2*delta_x)=-3
21 //eqn at node 2
22 //-20*y_2+9*y_3=f2
23 //at node 3
24 / 9 * y_2 - 20 * y_3 + 9 * y_4 = f3
25 //at node 4
26 / 18 * y_3 - 20 * y_4 = 16
27 disp(f4,f3,f2," the value of f(x) at node 2 3 and 4
      are");
28 //now solving the equations using TDMA method
29
30 \ a(2) = 9, a(3) = 18
                                //sub diagonal assignment
31
32 for j=1:3, b(j)=-20;
                                      //main diagonal
      assignment
33 end
34 \text{ for } k=1:2, c(k)=9;
                                     //super diagonal
      assignment
35 end
36 d(1) = f2
                                  //given values
      assignment
37 d(2) = f3
38 d(3) = 16
39
40 i = 1;
41 n=3;
42 beta1(i)=b(i);
                                     //initial b is equal
```

Scilab code Exa 5.5 discretization in 1 D space

```
1 clc
2 disp("the soln of eqn 5.5-->");
3 \text{ delta_x=.1}
4 y_11=1
                           //dy/dx at x=0
5 dy_by_dx_1=0
6 // given eqn d2y/dx2=y
7 disp("the analytical soln are");
8 for i=1:10, y_an(i)=cosh((i-1)/10)/cosh(1), disp(
     y_an(i));
9 end
10 //using central difference method we have
11 //y(i-1) - (2+delat_x^2)y(i) + y(i+1)=0
12 //therefore the eqns can be solved using TDMA method
13 for i=2:10, a(i)=1
                                 //sub diagonal
     assignment
14 end
15 for j=1:10, b(j)=-2.01;
                                     //main diagonal
     assignment
```

```
16 \text{ end}
17 c(1) = 2
18 for k=2:9, c(k)=1;
                                   //super diagonal
      assignment
19 end
20 \text{ for } 1=1:9, d(1)=0;
21
                                  //given values
       end
          assignment
22 d(10) = -1
23 i = 1;
24 n = 10;
25 beta1(i)=b(i);
                                    //initial b is equal
      to beta since a1=0
26 gamma1(i)=d(i)/beta1(i);
                                   //\sin ce c7=0
27 m = i + 1;
28 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
29 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
30 end
31 \times (n) = gamma1(n);
                                    //\sin ce c7=0
32 n1=n-i;
33 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
      j);
34 end
35 disp("the values of y from y1 to y10 by TDMA method
      are");
36 for i=1:10, disp(x(i));
37 end
```

Scilab code Exa 5.6 1 D steady state heat conduction

```
//since 9
5 \text{ delta_x} = (T_10 - T_1)/9
      divisions are to be made
6 //using central difference method we get
7 // for node 2--> 2*T_2-T_3=100
8 \text{ for } i=2:8, a(i)=-1
                                    //sub diagonal
      assignment
9 end
10 for j=1:8, b(j)=2;
                          //main diagonal
      assignment
11 end
12 for k=1:7, c(k)=-1;
                                   //super diagonal
      assignment
13 end
14 d(1) = 100, d(8) = 200
15 for 1=2:7, d(1)=0;
16 \text{ end}
                             //given values assignment
17 i=1;
18 n=8;
19 beta1(i)=b(i);
                                    //initial b is equal
      to beta since a1=0
20 gamma1(i)=d(i)/beta1(i);
                                   //\sin ce c7=0
21 m = i + 1;
22 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
23 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
24 end
                                    //\sin ce c7=0
25 \times (n) = gamma1(n);
26 \quad n1=n-i;
27 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
      j);
28 end
29 disp ("the values of T from T2 to T9 by TDMA method
      are");
30 for i=1:8, disp(x(i));
31 end
```

Scilab code Exa 5.7 1 D steady state heat conduction

```
1 clc
2 disp("the soln of eqn 5.7-->1-D Steady Heat
      Conduction");
3 \text{ dia}=.02
4 1=.05
5 T_0 = 320
6 \text{ delta_x=1/4}
7 k = 50
8 h = 100
9 T_surr=20
10 //B.C \rightarrow d(theta)/dx + h(theta)/k = 0 at x = 0.05
11 / let m = sqrt(hP/kA)
12 P = \%pi * dia
13 A = \%pi*dia^2/4
14 m = sqrt(h*P/(k*A));
15 //using central difference method we get
16 //-theta(i-1)+(2+(m*delta_x^2)*theta(i)+theta(i+1))
      =0
17 \text{ theta}_0=T_0-T_surr
18 //using B.C. at node 4 we get \rightarrow theta(5)=theta(3)-2
      h*theta(4)*delta_x/k
19 //now the eqns can be solved using TDMA method
20 \text{ for } i=2:3, a(i)=-1
                                       //sub diagonal
      assignment
21 end
22 \quad a(4) = -2
23 for j=1:3, b(j)=2.0625;
                                            //main diagonal
      assignment
24 end
25 b(4) = 2.1125
26 \text{ for } k=1:3, c(k)=-1;
                                        //super diagonal
      assignment
27 \text{ end}
28 \text{ for } 1=2:4, d(1)=0;
29
                                     //given values
        end
           assignment
```

```
30 d(1) = 300
31 i = 1;
32 n = 4;
33 beta1(i)=b(i);
                                      //initial b is equal
      to beta since a1=0
34 gamma1(i)=d(i)/beta1(i);
                                      //\sin ce c7=0
35 \text{ m} = \text{i} + 1;
36 \text{ for } j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
37 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
                                      //\sin ce c7=0
39 \times (n) = gamma1(n);
40 \text{ n1=n-i};
41 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
      j);
42 end
43 disp("the values of T from T1 to T4 in Celsius by
      TDMA method are");
44 for i=1:4, disp(x(i)-T_surr);
45 end
```

Scilab code Exa 5.8 chemical reaction and diffusion in pore

```
method
11 for i=2:99, a(i)=1
                                  //sub diagonal
     assignment
12 end
13 a(100) = 2
                              //since C99=C100 using B.C
14 for j=1:100, b(j)=-2.0001,
                                          //main diagonal
       assignment
15 end
16 for k=1:99, c(k)=1;
                                   //super diagonal
      assignment
17 end
18 d(1) = -1
19 for l=2:100, d(l)=0;
                            //given values assignment
20 end
21 i = 1;
22 n = 100;
23 beta1(i)=b(i);
                                  //initial b is equal
     to beta since a1=0
24 gamma1(i)=d(i)/beta1(i);
                                  //\sin ce c7=0
25 \text{ m=i+1};
26 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
27 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
28 end
29 \times (n) = gamma1(n);
                                   //\sin ce c7=0
30 n1=n-i;
31 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
     j);
32 end
33 disp(x(50)), "the values of conc. at x=.5mm or at the
     50th node is");
```

Chapter 6

CONVECTION DIFFUSION PROBLEMS

Scilab code Exa 6.1 upwind scheme

```
1 //given convective diffusive eqn \rightarrow -u*(dc/dx)+D*(
     d2C/dx2)=0
2 C_ini=0
                         //at x=0
                         //at x=1
3 C_end=1
4 clc
5 disp("the soln of eg 6.1");
7 //using central difference method for both diffusion
       and convective term
  //-u*(C(i+1)-C(i-1))/(2*delta_x) + D*(C(i+1)+C(i-1))
      -2*C(i))/delta_x^2 = 0
9 \text{ delta_x=1/50}
10 //on solving the given eqns and by using the given
      boundary eqns we have
11 \text{ Pe} = 50
                                         //given
12 Pe_local=50*delta_x
                                         //u/D=50 as l=1
13 alpha=Pe_local-2
                                         //co-eff of C(i
      +1)
                                         //co-eff of C(i
14 Beta=Pe_local+2
```

```
-1)
15 //multipling with -2*delta_x^2/D we get
16 //-(Pe_local+2)*C(i-1) + 4*C(i) + (Pe_local-2)*C(i)
      +1)=0
17 //solving eqns using TDMA method
18 for i=2:49, a(i)=-Beta
                                         //sub diagonal
      assignment
19 \, \text{end}
20 for j=1:49, b(j)=4,
                                    //main diagonal
      assignment
21 end
                                          //super diagonal
22 for k=1:48, c(k)=alpha;
      assignment
23 end
24 d(1) = Beta*C_ini, d(49) = -alpha*C_end
25 for 1=2:48, d(1)=0;
26 end
                             //given values assignment
27 i = 1;
28 n = 49;
29 beta1(i)=b(i);
                                    //initial b is equal
      to beta since a1=0
                                    //\sin ce c7=0
30 gamma1(i)=d(i)/beta1(i);
31 m = i + 1;
32 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
33 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
34 end
                                    //\sin ce c7=0
35 \times (n) = gamma1(n);
36 \text{ n1=n-i};
37 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
      j);
38 end
39 disp("the values of conc. using CDS method for x=.84
       to 1 are")
40 for i=42:49, disp(x(i));
42 //part (ii) using CDS and UDS method
43 // \text{multipling with } - \text{delta_x^2/D we get}
44 //-(Pe_local+1)*C(i-1) + (Pe_local+2)*C(i)-C(i+1)=0
```

```
45 BEta=Pe_local+2
46 Gamma=Pe_local+1
47 for i=2:49, a(i)=-Gamma
                                        //sub diagonal
      assignment
48 end
49 for j=1:49, b(j)=BEta,
                                       //main diagonal
      assignment
50 end
51 for k=1:48, c(k)=-1;
                                      //super diagonal
      assignment
52 end
53 d(1) = Gamma * C_ini, d(49) = C_end
54 for 1=2:48, d(1)=0;
55 end
                              //given values assignment
56 i = 1;
57 n = 49;
58 beta1(i)=b(i);
                                    //initial b is equal
      to beta since a1=0
59 gamma1(i)=d(i)/beta1(i);
                                    //\sin ce c7=0
60 \text{ m} = \text{i} + 1;
61 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
62 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
63 end
64 \times (n) = gamma1(n);
                                     //\sin ce c7=0
65 \text{ n1=n-i};
66 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
      j);
67 end
68 disp("the values of conc. using CDS/UDS method for x
      =.84 to 1 are")
69 for i=42:49, disp(x(i));
70 end
71 disp("the analytical soln is");
72 for i=42:49;
        C_{an}(i) = C_{ini} + ((exp(Pe*.02*i)-1)*(C_{end}-C_{ini})
           /(exp(Pe)-1));
       disp(C_an(i));
74
75
       end
```

Scilab code Exa 6.2 upwind scheme

```
1 //given convective diffusive eqn \rightarrow -u*(dc/dx)+D*(
      d2C/dx2)=0
                         //at x=0
//at x=1
2 C_ini=0
3 C_end=1
4 clc
5 disp("the soln of eg 6.2-->");
7 //using central difference method for both diffusion
       and convective term
  //-u*(C(i+1)-C(i-1))/(2*delta_x) + D*(C(i+1)+C(i-1))
      -2*C(i))/delta_x^2 = 0
9 \text{ delta_x=1/50}
  //on solving the given eqns and by using the given
      boundary eqns we have
11 \text{ Pe} = 500
                                           //given
                                          //u/D=50 as l=1
12 Pe_local=500*delta_x
13 alpha=Pe_local-2
                                          //co-eff of C(i
      +1)
                                         //co-eff of C(i
14 Beta=Pe_local+2
      -1)
15 // multipling with -2*delta_x^2/D we get
16 //-(Pe_local+2)*C(i-1) + 4*C(i) + (Pe_local-2)*C(i)
      +1)=0
17 //solving eqns using TDMA method
18 for i=2:49, a(i)=-Beta
                                        //sub diagonal
      assignment
19 end
20 for j=1:49, b(j)=4,
                                    //main diagonal
      assignment
21 end
22 \text{ for } k=1:48, c(k)=alpha;
                                         //super diagonal
      assignment
```

```
23 end
24 d(1) = Beta*C_ini, d(49) = -alpha*C_end
25 for 1=2:48, d(1)=0;
                              //given values assignment
26 \, \text{end}
27 i = 1;
28 n = 49;
29 beta1(i)=b(i);
                                     //initial b is equal
      to beta since a1=0
                                    //\sin ce c7=0
30 gamma1(i)=d(i)/beta1(i);
31 m = i + 1;
32 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
33 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
34 end
                                    //\sin ce c7=0
35 \times (n) = gamma1(n);
36 \text{ n1=n-i};
37 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(j)
      j);
38 end
39 disp("the values of conc. using CDS method for x=.84
       to 1 are")
40 for i=42:49, disp(x(i));
41 end
42 //part (ii) using CDS and UDS method
43 // \text{multipling with } - \text{delta_x^2/D we get}
44 //-(Pe_local+1)*C(i-1) + (Pe_local+2)*C(i)-C(i+1)=0
45 BEta=Pe_local+2
46 Gamma=Pe_local+1
47 \text{ for } i=2:49, a(i)=-Gamma
                                          //sub diagonal
      assignment
48 end
49 for j=1:49, b(j)=BEta,
                                       //main diagonal
      assignment
50 end
51 for k=1:48, c(k)=-1;
                                     //super diagonal
      assignment
52 end
53 d(1) = Gamma * C_ini, d(49) = C_end
54 for 1=2:48, d(1)=0;
```

```
//given values assignment
55 end
56 i = 1;
57 n = 49;
58 beta1(i)=b(i);
                                     //initial b is equal
      to beta since a1=0
59 gamma1(i)=d(i)/beta1(i);
                                     //\sin ce c7=0
60 \text{ m} = \text{i} + 1;
61 for j=m:n, beta1(j)=b(j)-a(j)*c(j-1)/beta1(j-1);
62 gamma1(j)=(d(j)-a(j)*gamma1(j-1))/beta1(j);
63 end
                                     //\sin ce c7=0
64 \times (n) = gamma1(n);
65 \text{ n1=n-i};
66 for k=1:n1, j=n-k; x(j)=gamma1(j)-c(j)*x(j+1)/beta1(
      j);
67 end
68 disp("the values of conc. using CDS/UDS method for x
      =.84 to 1 are")
69 for i=42:49, disp(x(i));
70 end
71 disp("the analytical soln is");
72 for i=42:49;
         C_{an}(i) = C_{ini} + ((exp(Pe*.02*i)-1)*(C_{end}-C_{ini})
73
            /(exp(Pe)-1));
        disp(C_an(i));
74
75
        end
```

TUBULAR REACTOR WITH AXIAL DISPERSION

Scilab code Exa 7.1 boundary value problem in chemical reaction engineering

```
1 clc
2 disp("soln of eg 7.1-->First Order Reaction-50 parts
3 e1=1, e2=1
      //assumed values
4 u=1,D=10^-4,k=1,C_a_in=1,delta_x=10/50
                                //given data
5 \text{ cf_ca1_n1} = -2*D/\text{delta_x^2} - 3*u/\text{delta_x-k-2}*u^2/D
                       //co-efficient of C-A1 at node 1
6 cf_ca2_n1=2*D/delta_x^2+u/delta_x
7 cf_da1_n1=-(2*u^2/D+2*u/delta_x)*C_a_in
                                //right hand side co-
      efficient
8 cf_ca1_n2=D/delta_x^2+u/delta_x
9 	 cf_ca2_n2 = -2*D/delta_x^2-u/delta_x-k
10 cf_ca3_n2=D/delta_x^2
11 cf_da1_n2=0
```

```
12 cf_ca2_n3=cf_ca1_n2
13 cf_ca3_n3=cf_ca2_n2
14 \text{ cf}_{ca4_n3=cf}_{ca3_n2}
15 cf_da1_n3=0
16 \text{ cf_ca50_n51=2*D/delta_x^2+u/delta_x}
                                   //co-efficient of C-A50
       at node 51
17 \text{ cf_ca51_n51} = -2*D/delta_x^2-u/delta_x-k
18 cf_da51_n51=0
19 for i=2:50, a(i)=cf_ca1_n2,
20 end
21 a(51) = cf_ca2_n1, c(1) = cf_ca2_n1
22 for i=2:50,c(i)=cf_ca3_n2,
23 end
24 d(1)=cf_da1_n1
25 for i=2:51,d(i)=cf_da1_n2
26 \text{ end}
27 for i=1:51, x(i)=0,
28 end
29 b(1)=cf_ca1_n1,
30 for i=2:51,b(i)=cf_ca2_n2,end
31 while e1>1e-6 & e2>1e-6 do for i=1:51,x1(i)=x(i),end
32 i=1, n=51, Beta(i)=b(i),
       Gamma(i)=d(i)/Beta(i)
33
34
       i1 = i + 1,
35
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
            Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
36
37
       end
       x(n) = Gamma(n)
38
39
       n1=n-i,
40
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
          (j)
41
       end
42 e1=abs(x(42)-x1(42)), e2=abs(x(18)-x1(18))
43 end
44 for i=1:51, disp(x(i))
45 end
```

Scilab code Exa 7.2 boundary value problem in chemical reaction engineering second order

```
1 clc
2 disp("soln of eg 7.2-->Second Order Reaction-20
      parts")
3 e1=1, e2=1
4 u=1, D=10^-4, k=1, C_a_in=1, delta_x=10/20
5 cff_ca2_n1=2*D/delta_x^2+u/delta_x
                              //co-efficient of C-A2 at
      node 1
6 cff_da1_n1 = -(2*u^2/D+2*u/delta_x)*C_a_in
                       //right hand side co-efficient
7 cff_ca1_n2=D/delta_x^2+u/delta_x
8 cff_ca3_n2=D/delta_x^2
                                            //co-efficient
       of C-A3 at node 2
9 cff_da1_n2=0
10 cff_ca2_n3=cf_ca1_n2
11 cff_ca4_n3=cf_ca3_n2
12 cff_da1_n3=0
13 \text{ cff_ca20_n21=2*D/delta_x^2+u/delta_x}
                               //co-efficient of C-A20 at
       node 21
14 cff_da21_n21=0
15 for i=2:20, a(i)=cff_ca1_n2,
16 \text{ end}
17 a(21) = cff_ca2_n1, c(1) = cff_ca2_n1
18 for i=2:20,c(i)=cff_ca3_n2,
19 end
20 d(1) = cff_da1_n1
21 for i=2:21,d(i)=cff_da1_n2
22 end
23 for i=1:21, x(i)=0,
```

```
24 end
25 while e1>1e-6 & e2>1e-6 do for i=1:21,x1(i)=x(i),end
      cff_ca1_n1 = -2*D/delta_x^2 - 3*u/delta_x - x1(1) - 2*u
26
         ^2/D
                                //main diagonal elements
         dependence on conc.
      b(1) = cff_ca1_n1,
27
      for i=2:21,b(i)=-2*D/delta_x^2-u/delta_x-x(i),end
28
29
30 //solving by TDMA method
      i=1, n=21, Beta(i)=b(i),
31
32
       Gamma(i)=d(i)/Beta(i)
33
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
34
           Gamma(j)=(d(j)-a(j)*Gamma(j-1))/Beta(j),
35
36
       end
       x(n) = Gamma(n)
37
38
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
39
          (j)
40
       end
41 e1=abs(x(1)-x1(1)), e2=abs(x(21)-x1(21))
43 for i=1:21, disp(x(i))
44 end
```

CHEMICAL REACTION AND DIFFUSION IN SPHERICAL CATALYST PELLET

Scilab code Exa 8.1 first order reaction

```
1 clc
2 disp("the soln of eg 8.1-->");
3 for i=1:100, x(i)=0
4 end
5 iter=0, e1=1, f=1
6 while e1>1e-6 & f>1e-6 do iter=iter+1, for i=1:100,
      x1(i)=x(i),
       end, for i=2:100, a(i)=1-(1/(i-1))
7
8
       end, b(1) = -6.01, for i = 2:100, b(i) = -2.01
       end, c(1)=6, for i=2:99, c(i)=1+(1/(i-1))
9
       end, for i=1:99, d(i)=0, end, d(100)=-100/99,
10
       i=1, n=100, Beta(i)=b(i),
11
       Gamma(i)=d(i)/Beta(i)
12
13
       i1 = i + 1,
14
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
           Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
15
16
       end
```

```
17
        x(n) = Gamma(n)
        n1=n-i,
18
        for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
19
           (j)
20
        end
21
        e1 = abs(x(1) - x1(1)),
22
        f = abs(x(100) - x1(100)),
23 end
24 disp(iter," the solution by TDMA of node 77 to 99 by
      1st order rxn. is");
25 \text{ for } i=78:100,
        disp(x(i));
26
27 \text{ end}
```

Scilab code Exa 8.2 second order reaction

```
1 clc
2 disp("the soln of eg 8.2-->");
3 \text{ for } i=1:100, x(i)=0
4 end
5 iter=0, e1=1, f=1
6 k=.1,D=10^-9,r=.01,delta_r=r/10,t1=k*delta_r^2/D
7 while e1>1e-6 & f>1e-6 do iter=iter+1, for i=1:100,
      x1(i)=x(i),
       end, for i=2:100, a(i)=1-(1/(i-1))
8
       end, b(1) = -6 - .t1 * x1(1), for i = 2:100, b(i) = -2 - t1 *
9
          x1(i)
10
       end, c(1)=6, for i=2:99, c(i)=1+(1/(i-1))
11
       end, for i=1:99, d(i)=0, end, d(100)=-100/99,
       i=1, n=100, Beta(i)=b(i),
12
       Gamma(i)=d(i)/Beta(i)
13
14
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
15
16
            Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
17
       end
```

```
x(n) = Gamma(n)
18
19
       n1=n-i,
        for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
20
           (j)
21
        end
22
        e1 = abs(x(1) - x1(1)),
23
        f = abs(x(100) - x1(100)),
24 end
25 disp ("the solution by TDMA of node 77 to 99 by 2nd
      order rxn. is");
26 \text{ for } i=77:100,
        disp(x(i));
27
28 end
```

Scilab code Exa 8.3 non isothermal condition

```
1 clc
2 disp("the soln of eg 8.3-->");
3 \text{ for } i=1:100, x(i)=0
                                                 //initial
       values
4 end
5 e2=1, f1=1, iter=0
                                                 //assumed
       values
6 k=.1*10^-2, D=10^-9,r=.01,delta_r=r/100,t1=k*delta_r
                  //given data
7 //now solving the eqns for all the nodes and then
      simplifying we get the following relations
8 while e2>1e-6 & f1>1e-6 do iter=iter+1, for i=1:100,
      x1(i)=x(i),
9
       end, for i=2:100, a(i)=1-(1/(i-1))
10
       end, b(1) = -6 - t1 * exp((1-x1(1))/(2-x1(1))), for i
          =2:100, b(i)=-2-t1*exp((1-x(i))/(2-x(i)))
       end, c(1)=6, for i=2:99, c(i)=1+(1/(i-1))
11
12
       end, for i=1:99, d(i)=0, end, d(100)=-100/99,
13
       i=1, n=100, Beta(i)=b(i),
```

```
14
        Gamma(i)=d(i)/Beta(i)
15
        i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
16
            Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
17
18
        end
19
       x(n) = Gamma(n)
20
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
21
           (j)
22
       end
        e2=abs(x(1)-x1(1)),
23
       f1=abs(x(100)-x1(100)),
24
25 end
26 disp ("the solution by TDMA of node 77 to 100 by 1st
      order rxn. is");
27 \text{ for } i=76:100,
       disp(x(i));
28
29 end
```

Scilab code Exa 8.4 non isothermal condition

```
1 clc
2 disp("the soln of eg 8.4-->");
3 \text{ for } i=1:100, x(i)=0
4 end
5 iter=0, e1=1, f1=1
6 while e1>1e-6 & f1>1e-6 do iter=iter+1, for i=1:100,
      x1(i)=x(i),
       end, for i=2:100, a(i)=1-(1/(i-1))
7
       end, b(1) = -6 - .01 * exp((10 - 10 * x1(1))/(11 - 10 * x1(1))
          ), for i=2:100, b(i)=-2-.01*exp((10-10*x1(i))
          /(11-10*x1(i))
       end, c(1)=6, for i=2:99, c(i)=1+(1/(i-1))
9
       end, for i=1:99, d(i)=0, end, d(100)=-100/99,
10
11
       i=1, n=100, Beta(i)=b(i),
```

```
12
       Gamma(i)=d(i)/Beta(i)
13
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
14
            Gamma(j) = (d(j) - a(j) * Gamma(j-1)) / Beta(j),
15
16
       end
       x(n) = Gamma(n)
17
18
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
19
           (j)
20
       end
       e1=abs(x(1)-x1(1)),
21
       f1=abs(x(100)-x1(100)),
22
23 end
24 disp("the solution by TDMA of node 77 to 99 by 1st
      order rxn. is");
25 \text{ for } i=76:100,
26
       disp(x(i));
27 end
```

ONE DIMENSIONAL TRANSIENT HEAT CONDUCTION

Scilab code Exa 9.1 transient conduction in rectangular slab

```
1 clc
2 disp("the soln of eg 9.1-->Transient heat conduction
       in a Rectangular slab")
3 disp("the values of Temp measured from centre at the
       gap of .2 cm are")
4 alpha=10^-5, delta_t=.1, delta_x=10^-3
                                                       //
      given data
5 m=alpha*delta_t/(delta_x^2)
6 for i=2:4, a(i)=m
                                                      //
     sub-diagonal
7 end
8 b(1)=(-2*m-1)/2
9 for i=2:4, b(i)=-2*m-1
     //diagonal
10 \text{ end}
                                                      //
11 for i=1:3, c(i)=m
     super-diagonal
```

```
12 end
                                                      //
13 for i=1:4, x(i)=20
      initial temperature
14 end
15 for t=0.1:.1:3.1, for i=1:4, y(i)=x(i), end
                //TDMA method
       d(1) = -.5*y(1),
16
       d(2) = -y(2)
17
       d(3) = -y(3)
18
       d(4) = -y(4) - 300
19
20
       i=1, n=4
21
       Beta(i)=b(i),
22
       Gamma(i)=d(i)/Beta(i)
23
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
24
           Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
25
26
       end
27
       x(n) = Gamma(n)
28
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
29
          (j)
30
       end
31 for i=1:4, disp(x(i));
                                        //solution of
      temperature
32 end
33 disp("----")
34 end
35 disp("-----");
```

Scilab code Exa 9.2 transient conduction in rectangular slab

```
3 delta_t=1, delta_x=.05, alpha=10^-5
4 t1=alpha*delta_t/delta_x^2
5 for i=2:9, a(i)=-t1
6 end
7 for i=1:9,b(i)=1+2*t1
8 end
9 \text{ for } i=1:8, c(i)=-t1
10 \, \text{end}
11 t=1, tf=3000
12 for i=1:9, x(i)=300
13 end
14 \text{ e1} = 425,
15 disp ("time when centre temp is 425 K in secs. is")
16 for t=1:1:tf,for i=1:9, y(i)=x(i),end
       d(1) = y(1) + 1.7,
17
       d(9) = y(9) + 2.4,
18
       for i=2:8,d(i)=y(i)
19
20
       end
       i=1, n=9
21
22
       Beta(i)=b(i),
23
       Gamma(i)=d(i)/Beta(i)
24
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
25
            Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
26
27
       end
28
       x(n) = Gamma(n)
29
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
30
           (j)
31
       end
       if abs(x(5)-e1)>0 \& abs(x(5)-e1)<.1 then disp(t)
32
           ; break;
33
       end
34 end
35 disp("the values of temp. at req. time is");
36 for i=1:9, disp(x(i)); end
```

Scilab code Exa 9.3 transient conduction in cylinder

```
1 clc
2 disp("the soln of eg 9.3-->Transient Conduction in
      cylinder");
3 \text{ delta\_t=.1}, \text{ delta\_r=.001}, \text{ alpha=10^-5}
      //given data
4 t1=alpha*delta_t/delta_r^2
5 a(2) = .5*t1, a(3) = .75*t1, a(4) = .833*t1
      //sub-diagonal
6 b(1) = -4*t1-1
7 for i=2:4,b(i)=-2*t1-1
      //main diagonal
8 end
9 c(1)=4*t1, c(2)=1.5*t1, c(3)=1.25*t1
      //super-diagonal
10 for i=1:4, x(i)=20
11 end
12 disp("T1,T2,T2 & T4 at time interval of .1 sec is")
13 for t=.1:.1:2.1, for i=1:4, y(i)=x(i), end
                              //TDMA Method
       d(4) = -y(4) - 7*t1*300/6,
14
15
       for i=1:3, d(i)=-y(i)
16
       end
17
       i=1, n=4
18
       Beta(i)=b(i),
19
       Gamma(i)=d(i)/Beta(i)
20
       i1 = i + 1,
21
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
            Gamma(j)=(d(j)-a(j)*Gamma(j-1))/Beta(j),
22
23
       end
       x(n) = Gamma(n)
24
25
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
26
```

```
(j)
27 end
28 disp(x(4),x(3),x(2),x(1));
29 disp("-----");
30 end
```

Scilab code Exa 9.4 transient conduction in sphere

```
1 clc
2 disp("the soln of eg 9.4-->Transient conduction in
      Sphere");
3 \text{ delta_t=.1}, \text{ delta_r=.001}, \text{ alpha=10^-5}
4 t1=alpha*delta_t/delta_r^2
5 a(2) = 0, a(3) = .5, a(4) = .667
6 b(1) = -7*t1
7 for i=2:4, b(i)=-3
8 end
9 c(1)=6, c(2)=2, c(3)=1.5
10 for i=1:4, x(i)=20
11 end
12 disp("T1, T2, T2 & T4 at time interval of .1 sec is")
13 for t=.1:.1:1.4, for i=1:4, y(i)=x(i), end
       d(4) = -y(4) - 400,
14
15
       for i=1:3, d(i)=-y(i)
16
       end
       i=1, n=4
17
       Beta(i)=b(i),
18
19
       Gamma(i)=d(i)/Beta(i)
20
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
21
            Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
22
23
       end
       x(n) = Gamma(n)
24
25
       n1=n-i,
26
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
```

```
(j)
27 end
28 disp(x(4),x(3),x(2),x(1));
29 disp("-----");
30 end
```

Scilab code Exa 9.5 transient diffusion in sphere

```
1 clc
2 disp("the soln of eg 9.5-->");
3 R=.326, D=3*10^-7
4 delta_t=1, delta_r=.0326, conc_ini=10/(1.33*%pi*R^3)
5 t1=D*delta_t/delta_r^2
6 disp(conc_ini,"the initial conc. of drug is");
7 for i=2:10, a(i)=-(1-1/(i-1))
8 end
9 b(1) = 591.4
10 for i=2:10, b(i)=3544.5
11 end
12 c(1)=-1, for i=2:9, c(i)=-(1+1/(i-1))
13 end
14 for i=1:10, x(i)=conc_ini
15 end
16 disp ("Conc. at centre at t=3hr, 12 hr, 24 hr, 48 hr
      is");
17 for t=1:delta_t:172800, for i=1:10, y(i)=x(i), end
18
       d(1) = y(1) *590.4,
19
       for i=2:10, d(i)=3542.5*y(i)
20
       end
       i=1, n=10
21
22
       Beta(i)=b(i),
23
       Gamma(i)=d(i)/Beta(i)
24
       i1=i+1,
25
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
26
           Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
```

```
27
       end
       x(n) = Gamma(n)
28
29
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
30
          (j)
31
       end
       if t==10800| t==43200| t==86400|t==172800 then
32
          disp(x(6));
33
       end
34 \text{ end}
```

TWO DIMENSIONAL STEADY AND TRANSIENT HEAT CONDUCTION

Scilab code Exa 10.1 discretization in 2 D space gauss seidel method

```
1 clc
2 disp("the soln of eg 10.1-->2-D steady heat
      conduction-Gauss Seidel method ");
3 for i=1:9, tnew(i)=101, e(i)=1
      //assumed values
4 \, \text{end}
5 t = 1e - 6
6 //since all the nodes are interior nodes so
      discretized eqn used is eqn 10.10
7 while e(1)>t&e(2)>t&e(3)>t&e(4)>t&e(5)>t&e(6)>t&e(6)>t
      (7) > t \& e(8) > t \& e(9) > t do
       for i=1:9, told(i)=tnew(i),end
       tnew(1) = (told(2) + 40 + told(4))/4
                                   //on solving eqns for
           various nodes we get,
10
       tnew(2) = (tnew(1) + told(3) + told(5) + 20)/4
       tnew(3) = (tnew(2) + told(6) + 420)/4
11
```

```
tnew(4) = (told(5) + tnew(1) + told(7) + 20)/4
12
13
        tnew(5) = (tnew(2) + told(8) + told(6) + tnew(4))/4
        tnew(6) = (tnew(3) + tnew(5) + told(9) + 400) / 4
14
        tnew(7) = (tnew(4) + told(8) + 40)/4
15
16
        tnew(8) = (tnew(5) + tnew(7) + told(9) + 20)/4
17
        tnew(9) = (tnew(6) + 420 + tnew(8))/4
        for i=1:9,e(i)=abs(tnew(i)-told(i))
18
19
        end
20 end
21 disp("the values of T from 1st element to last is");
22 for i=1:9, disp(tnew(i));
23 end
```

Scilab code Exa 10.2 discretization in 2 D space gauss seidel method

```
1 clc
2 disp("the soln of eg 10.2-->");
3 for i=1:5, tnew(i)=101, e(i)=1
4 end
5 t = 1e - 6
6 //since there is no source term so we get the
      following eqns.
  while e(1) > t\&e(2) > t\&e(3) > t\&e(4) > t\&e(5) > t do
8
       for i=1:5, told(i)=tnew(i),end
       tnew(1) = (told(2) *2+300)/4
9
       tnew(2) = (tnew(1) + told(3) + 300)/4
10
       tnew(3) = (tnew(2) + told(4) + 200)/4
11
12
       tnew(4) = (told(5) + tnew(3) + 300)/4
       tnew(5) = (2*tnew(4)+300)/4
13
       for i=1:5, e(i)=abs(tnew(1)-told(i))
14
15
       end
16 \, \text{end}
17 disp("the values of T from 1st element to last is");
18 for i=1:5, disp(tnew(i));
19 end
```

Scilab code Exa 10.3 discretization in 2 D space

```
1 clc
2 disp ("the soln of eg 10.3-->Red-Black Gauss-Seidel
      Method");
3 for j=1:5, tn(j,1)=400, end
                                                         //
      defining conditions
4 for j=2:4, tn(1,j)=20, tn(5,j)=20, tn(j,5)=20, end
5 \text{ for } i=1:9, e(i)=1
6 end
7 for i=2:4, j=2:4, tn(i,j)=60
8 end
9 t1 = 1e - 6
10 while e(1) > t1 & e(2) > t1 & e(3) > t1 & e(4) > t1 & e(5) > t1 & e(6) >
      t1\& e(7)>t1\& e(8)>t1 \& e(9)>t1 do for i=2:4,j
      =2:4,t(i,j)=tn(i,j),end
11 //using red-black gauss-seidel method
12 for i=2:4, j=2:4, tn(i,j)=(tn(i+1,j)+tn(i-1,j)+tn(i,j)
      +1)+tn(i,j-1))/4, end
13 //now getting the absolute difference of the 9
      variables
14 e(1) = abs(t(2,2) - tn(2,2)), e(2) = abs(t(2,3) - tn(2,3)), e(2)
      (3) = abs(t(2,4) - tn(2,4)), e(4) = abs(t(3,2) - tn(3,2)),
      e(5) = abs(t(3,3) - tn(3,3)), e(6) = abs(t(3,4) - tn(3,4))
      e^{(7)} = abs(t(4,2) - tn(4,2)), e^{(8)} = abs(t(4,3) - tn(4,3))
      ), e(9) = abs(t(4,4) - tn(4,4)),
15 end
16 //now defining positions of the various nodes
      according to red black combination
17 R1=t(2,4), R2=t(4,4), R3=t(3,3), R4=t(2,2), R5=t(2,4), B1
      =t(4,3),B2=t(3,2),B3=t(3,4),B4=t(2,3)
18 disp(R5,R4,R3,R2,R1,"the value of RED points
      respectively is");
19 disp(B4,B3,B2,B1," the value of BLUE points
```

Scilab code Exa 10.8 discretization in 2 D space

```
1 clc
2 disp("the soln of eg 10.8-->Gauss Seidel Method");
3 \text{ for } i=1:9, tnew(i)=101, e(i)=1
      assumed values
4 end
5 t = 1e - 6
6 while e(1)>t&e(2)>t&e(3)>t&e(4)>t&e(5)>t&e(6)>t&e(6)
       (7) > t \& e(8) > t \& e(9) > t do
        for i=1:9, told(i)=tnew(i),end
7
8
        //using eqn 10.10 for the interior nodes and
            convective boundary conditions for corner
            nodes
9
        tnew(1) = (told(2) + 50 + .5 * told(4) + 100/3) * 3/7
        tnew(2) = (tnew(1) + told(3) + told(5) + 100)/4
10
        tnew(3) = (tnew(2) + told(6) + 600)/4
11
12
        tnew (4) = (\text{told}(5) + .5*\text{tnew}(1) + .5*\text{told}(7) + 100/3)
            *3/7
13
        tnew(5) = (tnew(2) + told(8) + told(6) + tnew(4))/4
        tnew (6) = (tnew(3) + tnew(5) + told(9) + 500)/4
14
15
        tnew(7) = (.5*tnew(4) + .5*told(8) + 100/3)*3/4
        tnew (8) = (\text{tnew}(5) + .5*\text{tnew}(7) + .5*\text{told}(9) + 100/3)
16
            *3/7
        tnew (9) = (\text{tnew}(6) + 100/3 + .5 * \text{tnew}(8) + 250) * 3/7
17
18
        for i=1:9, e(i)=abs(tnew(i)-told(i))
19
        end
20 end
21 disp("the values of T from 1st element to last is");
22 for i=1:9, disp(tnew(i));
23 end
```

Scilab code Exa 10.9 discretization in 2 D space

```
1 clc
2 disp("the soln of eg 10.9-->Steady state heat
      conduction in L-shaped body");
3 \text{ for } i=1:9, tnew(i)=101, e(i)=1
                                                  //assumed
      values
4 end
5 t = 1e - 6
6 while e(1)>t&e(2)>t&e(3)>t&e(4)>t&e(5)>t&e(6)>t&e(6)>t
      (7) > t \& e(8) > t \& e(9) > t do
7
       for i=1:9, told(i)=tnew(i),end
       //using the basic discretization eqn. for all
           the nodes since the boundary conditions vary
           for each point
        tnew(1) = (told(2) + 1.25 + told(4))/2.05
9
       tnew(2) = (.5*tnew(1) + .5*told(3) + told(5) + 1.25)
10
           /2.05
11
        tnew(3)=(.5*tnew(2)+.5*told(6)+1.25)/1.05
12
        tnew(4) = (told(5) + .5*tnew(1) + 45)/2
       tnew(5) = (tnew(2) + told(8) + 90 + tnew(4))/4
13
       tnew (6) = (.5*tnew(3)+tnew(5)+.5*told(7)+91.25)
14
           /3.05
       tnew (7) = (.5*tnew(6) + .5*told(8) + 91.25)/2.05
15
16
       tnew (8) = (91.25 + .5 * tnew (7) + .5 * told (9))/2.05
17
        tnew (9) = (47.125 + .5 * tnew (8)) / 1.025
18
       for i=1:9, e(i)=abs(tnew(i)-told(i))
19
        end
20 end
21 disp("the values of T from 1st element to last is");
22 for i=1:9, disp(told(i));
23 end
```

Scilab code Exa 10.10 ADI method

```
1 clc
2 disp ("the soln of eg 10.10--> Alternating Direction
      Implicit Method");
3 \text{ nmax} = 25
                                                       //
4 a(2)=1, a(3)=1,
      defining variables
5 b(1) = -4, b(2) = -4, b(3) = -4
6 c(1)=1, c(2)=1
7 t(1,2)=20, t(1,3)=20, t(1,4)=20, t(2,1)=20, t(3,1)=20, t
      (4,1)=20, t(5,2)=20, t(5,3)=20, t(5,4)=20, t(2,5)
      =400, t(3,5)=400, t(4,5)=400
  tstar(1,2)=20, tstar(1,3)=20, tstar(1,4)=20, tstar(2,1)
      =20, tstar(3,1)=20, tstar(4,1)=20, tstar(5,2)=20,
      tstar(5,3)=20, tstar(5,4)=20, tstar(2,5)=400, tstar(5,4)=20
      (3,5)=400, tstar(4,5)=400
9 for i=2:4, for j=2:4 t(i,j)=20
10
       end
11 end
12 //solving by TDMA Method
13 for nn=1:nmax, for jj=2:4, d(1)=-t(1,jj)-t(2,jj+1)-
      tstar(2, jj-1),
            d(2) = -t(3, jj+1) - tstar(3, jj-1),
14
15
            d(3) = -t(5, jj) - t(4, jj+1) - tstar(4, jj-1)
16
            i=1, n=3
17
       Beta(i)=b(i),
       Gamma(i)=d(i)/Beta(i)
18
19
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
20
            Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
21
22
23
       x(n) = Gamma(n)
24
       n1=n-i,
```

```
for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
25
           (j)
       end
26
       tstar(2,jj)=x(1)
27
28
       tstar(3,jj)=x(2)
       tstar(4,jj)=x(3)
29
30 end
31 for ii=2:4,d(1)=-t(ii,1)-tstar(ii+1,2)-tstar(ii-1,2)
       d(2) = -tstar(ii+1,3) - tstar(ii-1,3)
32
       d(3) = -t(ii, 5) - tstar(ii+1, 4) - tstar(ii-1, 4)
33
       i=1, n=3
34
35
       Beta(i)=b(i),
       Gamma(i)=d(i)/Beta(i)
36
37
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
38
            Gamma(j)=(d(j)-a(j)*Gamma(j-1))/Beta(j),
39
40
       end
       x(n) = Gamma(n)
41
42
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
43
           (j)
44
       end
       t(ii, 2) = x(1)
45
46 \text{ t(ii,3)} = x(2)
47 t(ii,4)=x(3)
48 end
49 end
50 disp("the soln by ADI method is");
51 \text{ disp}(t(2,4),t(2,3),t(2,2));
52 disp("----");
53 \quad disp(t(3,4),t(3,3),t(3,2));
54 disp("----");
55 \text{ disp}(t(4,4),t(4,3),t(4,2));
```

Scilab code Exa 10.11 ADI method for transient heat conduction

```
1 clc
2 disp("the soln of eg 10.11-->");
3 for k=2:10, a(k)=-1, b(k)=2.4, c(k)=-1
4 end
5 alpha=1, delta_t=.05, delta_x=.1
6 m=alpha*delta_t/delta_x^2
7 b(1) = 2.4
8 c(1) = -2
9 for k=1:11, t(11,k)=400, tstar(11,k)=400, t(k,11)
      =400, tstar(k, 11) =400
10 \, \text{end}
11 for i=1:10, for j=1:10, t(i,j)=0, tstar(i,j)=0
12
       end
13 end
14 for tm = .05 : .05 : .5, for jj = 1 : 10, if jj = 1 then for ii
      =1:10,d(ii)=2*t(ii,2)-1.6*t(ii,1),end,d(10)=d(10)
      +400, else for ii=1:10, d(ii)=t(ii,jj+1)+t(ii,jj
      -1) -1.6*t(ii,jj), end, d(10) = d(10) + 400, end,
       i=1, n=10
15
       Beta(i)=b(i),
16
       Gamma(i)=d(i)/Beta(i)
17
18
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
19
20
            Gamma(j)=(d(j)-a(j)*Gamma(j-1))/Beta(j),
21
       end
22
       x(n) = Gamma(n)
       n1=n-i,
23
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
24
       end, for count=1:10, tstar(count,jj)=x(count),
25
          end
26
       end
27
       for ii=1:10,
            if ii == 1 then for jj = 1:10, d(jj) = 2*tstar(ii)
28
               +1,1)-1.6*tstar(ii,1),end, d(10)=d(10)
               +400, else for jj=1:10, d(jj)=tstar(ii-1, jj
```

```
)+tstar(ii+1,jj)-1.6*tstar(ii,jj), end, d
              (10) = d(10) + 400, end
       i=1, n=10
29
       Beta(i)=b(i),
30
31
       Gamma(i)=d(i)/Beta(i)
32
       i1 = i + 1,
       for j=i1:n, Beta(j)=b(j)-a(j)*c(j-1)/Beta(j-1),
33
           Gamma(j) = (d(j)-a(j)*Gamma(j-1))/Beta(j),
34
35
       end
       x(n) = Gamma(n)
36
37
       n1=n-i,
       for k=1:n1, j=n-k, x(j)=Gamma(j)-c(j)*x(j+1)/Beta
38
       end,
39
       for count=1:10, t(ii,count)=x(count), end
40
41
42 end
43 disp("the soln by ADI is");
44 for i=1:10, j=1:10, disp(t(i,j));
45 end
46 disp("the table is actually interchanged row &
      column.. horizontally are the elements of the
      column");
```