

Scilab Textbook Companion for
Chemical Engineering Thermodynamics
by S. Sundaram¹

Created by
Jyoti Kumari
B.TECH
Chemical Engineering
NIT TIRUCHIRAPPALLI
College Teacher
Dr. Prakash Kotecha
Cross-Checked by

August 10, 2013

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: Chemical Engineering Thermodynamics

Author: S. Sundaram

Publisher: R. N. Ahuja Book Company, New Delhi

Edition: 1

Year: 1998

ISBN: 81-7619-001-2

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

List of Scilab Codes	5
1 Introduction	10
2 P V T Relations	16
3 First Law of Thermodynamics	31
4 Second Law of Thermodynamics	44
5 Thermodynamic Potentials and Maxwell Relation	54
6 Thermodynamic Relations	56
7 Ideal Gases	57
8 Third Law of Thermodynamics	66
9 Fluid Flow in Pipes and Nozzles	68
10 Compressor	74
11 Liquefaction of Gases	79
12 Refrigeration	83
13 Thermodynamics in Phase Equilibria	88
14 Thermodynamics of Chemical Reactions	110

List of Scilab Codes

Exa 1.1	To determine the force exerted	10
Exa 1.2	Theoretical problem	11
Exa 1.3	Theoretical problem	11
Exa 1.4	To determine the mass of water required	12
Exa 1.5	To Calculate the work obtained	12
Exa 1.6	To Calculate the work done	14
Exa 2.1	To determine the temperature required	16
Exa 2.2	Theoretical problem	17
Exa 2.3	Theoretical problem	17
Exa 2.4	Theoretical problem	18
Exa 2.5	To calculate the volume of Methane	18
Exa 2.6	To calculate the final pressure acheived	20
Exa 2.7	To compute the work required	21
Exa 2.8	To determine the vapour pressure of Chlorine	23
Exa 2.9	To calculate the pressure exerted by the gas mixture	25
Exa 2.10	To calculate the amount of Ammonia leaving the reactor and the velocity of gaseous product leaving the reactor	28
Exa 3.1	To calculate the change in internal energy	31
Exa 3.2	To calculate the change in internal energy	32
Exa 3.3	To calculate the work done by the expanding gas and increase in internal energy	32
Exa 3.4	To calculate the time taken for the gas to attain 10 atm	33
Exa 3.5	Theoretical problem	34
Exa 3.6	To calculate the flow work per kg of air	35
Exa 3.7	To calculate the horse power output of the turbine	35
Exa 3.8	To find out the enthalpy of water of tank2 and find out the temperature of water in the second tank	36
Exa 3.9	To calculate the mass of steam required	38

Exa 3.10	To calculate the pump work required	38
Exa 3.11	To calculate the quality of exit steam	39
Exa 3.12	To calculate the internal energy of the steam in the chamber	40
Exa 3.13	To calculate the final weight and the final temperature of the air in the tank	41
Exa 3.14	Theoretical problem	42
Exa 4.1	To Calculate work output heat rejected entropy change of system and the surrounding and total change in entropy and the efficiency of the heat engine	44
Exa 4.2	To calculate the total change in entropy and hence determine the reversibility of the process	45
Exa 4.3	To find out entropy change of block air and total entropy change	46
Exa 4.4	To calculate the total change in entropy	48
Exa 4.5	To calculate the entropy change	49
Exa 4.6	Theoretical problem	49
Exa 4.7	To calculate the horse power of the compressor	50
Exa 4.8	To calculate the effectiveness of the process	51
Exa 4.9	To Calculate the maximum work obtained and the entropy change	52
Exa 4.10	Theoretical problem	53
Exa 5.1	To Calculate the efficiency of the separation process	54
Exa 6.0	Theoretical problem	56
Exa 7.1	Theoretical problem	57
Exa 7.2	Theoretical problem	57
Exa 7.3	To Calculate the final temperature of the ideal gas and work done in an open and closed system and internal energy change for the process	58
Exa 7.4	Theoretical problem	60
Exa 7.5	To Compute change in enthalpy entropy heat work and for the processes given above and to indicate the quantities that are state functions and to verify that the work required in an isothermal process is less than that in an adiabatic process	60
Exa 8.1	To calculate the absolute entropy of copper at 300 K	66
Exa 9.1	To find out the pressure at the final point	68
Exa 9.2	To find out the mass rate of alcohol	69

Exa 9.3	To plot velocity and specific volume and mass velocity against the ratio of P2 and P1 and to calculate the critical pressure and critical mass velocity and mass rate of flow	70
Exa 9.4	To calculate the area at exit of nozzle and hence decide the type of the nozzle	72
Exa 10.1	To calculate the horsepower required	74
Exa 10.2	To calculate the volumetric efficiency and the maximum possible pressure that can be attained in a single stage	75
Exa 10.3	To calculate the capacity and the actual horse power of the compressor	76
Exa 10.4	To Calculate the theoretical horse power required	77
Exa 10.5	To find out the pressure between stages	78
Exa 11.1	To Calculate the dryness fraction of exit stream and the ratio of upstream to downstream diameters	79
Exa 11.2	To Calculate the temperature of the throttled gas	80
Exa 11.3	To Calculate the fraction of air liquified at steady state and temperature of air before throttling	81
Exa 12.1	To Calculate the theoretical horse power required	83
Exa 12.2	To Calculate the compressor load	84
Exa 12.3	To Calculate the COP mass of refrigerant required and compressor horse power required and the COP and compressor horse power for a reversed Carnot cycle	85
Exa 12.4	To calculate the pressure in the tank and the amount of make up water required	86
Exa 13.1	To Calculate the fugacity of N2 at 373K and 100 atm	88
Exa 13.2	To Calculate the fugacity of liquid water	89
Exa 13.3	To Calculate the bubble point pressure of the solution	90
Exa 13.4	To Calculate the equilibrium data and compare with the experimental values	91
Exa 13.5	Theoretical problem	92
Exa 13.6	To Calculate the volume of 10 percent dichloromethane solution	93
Exa 13.7	To Calculate the vapour pressure of the solution and bubble point at 686 mm Hg and the vapour composition at equilibrium	94
Exa 13.8	To Calculate the heating load required for the process	96
Exa 13.9	Theoretical problem	97

Exa 13.10	Theoretical problem	97
Exa 13.11	Theoretical problem	98
Exa 13.12	To Calculate the partial pressure of toluene in the solution and check with the experimental value	98
Exa 13.13	To Check whether the activity coefficient of the solution can be represented by the Margules equation	99
Exa 13.14	To Calculate the composition of the vapour evolved	101
Exa 13.15	To plot a graph between temperature and vapour phase composition	102
Exa 13.16	To Calculate the heat of vapourization of toluene by using ideal gas law and second virial coefficient but neglecting v_l and including v_l	103
Exa 13.17	To Calculate the heat of vapourisation of water by Vishwanath and Kuloor method and by Riedel method and compare with the experimental value	105
Exa 13.18	To Calculate the latent heat of saturated ethane at 0 deg cel	106
Exa 13.19	To calculate the latent heat of the solution and compare it with the one which calculated from the given vapour pressure equation	108
Exa 14.1	To Calculate the standard heats of reaction at 25 deg celsius	110
Exa 14.2	To Calculate the sensible heat required	111
Exa 14.3	To Calculate the heat must be removed if the product temperature should not exceed 260 deg cel	111
Exa 14.4	To Calculate the theoretical flame temperature when both air and CO ₂ enter at 95 deg celsius	114
Exa 14.5	To Calculate the standard free energy for the reaction	116
Exa 14.6	To show the variation of the standard heats of reaction with temperature and the equilibrium constant with temperature graphically in the given temperature range	117
Exa 14.7	To Calculate the conversion of SO ₂ to SO ₃ at 1atm and at various temperature	119
Exa 14.8	Theoretical problem	124
Exa 14.9	To find out the equilibrium has been attained or not If not then calculate the equilibrium composition and also find out whether the equilibrium composition will change or not if pressure were increased to 3 atm	125

Exa 14.10	To Calculate the final temperature for various conversions and the maximum conversion that can be attained in a single reactor operating adiabatically	127
Exa 14.11	To Calculate the conversion of benzene at 25 degree celsius and 1 atm	129
Exa 14.12	To Calculate the maximum CH ₄ concentration under the condition of 2 atm and the quantity of methane obtained if pressure is 1 atm	130
Exa 14.13	To Calculate the partial pressure of CO ₂ required for decomposition and thus determine whether Ag ₂ CO ₃ will decomposes or not at the given pressure and temperature	131
Exa 14.14	Theoretical problem	133
Exa 14.15	To Calculate the equilibrium composition of the mixture	134
Exa 15.1	To Calculate the emf of the cell and the cell efficiency and heat to be removed to maintain isothermal conditions	136

Chapter 1

Introduction

Scilab code Exa 1.1 To determine the force exerted

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 1
3 //Introduction
4
5 //Example 1.1
6 clear all;
7 clc;
8
9 //Given
10 m = 100;//m is the mass of the object in kg
11 a = 10;//a is the acceleration due to gravity in m/
    s^2
12
13 //To determine the force exerted
14 F = m*a;//F is the force exerted by the object in kg
15 mprintf('Force exerted by the object= %f N',F);
16 F = (1/9.8065)*m*a;//F is the force exerted by the
    object in kgf
17 mprintf('\n Force exerted by the object= %f N',F);
18 //end
```

Scilab code Exa 1.2 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter
3 //Introduction
4
5 //Example 1.2
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end
```

Scilab code Exa 1.3 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter
3 //Introduction
4
5 //Example 1.3
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end
```

Scilab code Exa 1.4 To determine the mass of water required

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 1
3 //Introduction
4
5 //Example 1.4
6 clear all;
7 clc;
8
9 //Given
10 h = 100; //h is the height of the water fall in m
11 n = .855; //n is the efficiency of the turbine
12 g = 9.8; //g is the acceleration due to gravity in m
    /(s^2)
13 E = 100*10*3600; //E is the potential enery of water
    available to the bulb for 10 hours in watt or J/s
14
15 //To determine the mass of water required
16 m = (E/(g*h*n)); //m is the mass of water required
    for lighting the bulb for 10 hours in Kg
17 mprintf('Mass of water required for lighting the
    bulb for 10 hours in Kg= %f Kg',m);
18 mprintf('\n Mass of water required for lighting the
    bulb for 10 hours in tonnes= %f Kg',m/907.2);
19 //end
```

Scilab code Exa 1.5 To Calculate the work obtained

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 1
3 //Introduction
4
5 //Example 1.5
6 clear all;
```

```

7  clc;
8
9  //Given
10 n = 1; //n is the Kg mole of an ideal gas
11 P = 700*(10^4); //P is the pressure of the system in
    N/(m^2)
12 W = 45; //W is the weight of the mass in Kg
13 M = 20; //M is the weight of the piston and piston
    rod together in Kg
14 T = 300; //T is the constant temperature of the bath
    in K
15 h = .4; //h is the height difference of the piston
    after expansion in m
16
17 //To calculate the work obtained
18 a = (10^-4); //a is the cross sectional area of the
    cylinder in m^2
19 V = h*a; //V is the volume changed as gas expands in
    m^3
20
21 //(i). If gas alone is the system
22 //1Kgf = 9.8065Nm
23 P1 = ((W+M)*9.8065)/(10^-4); //P1 is the resisting
    pressure when the gas confined in the cylinder
    taken as a system
24 W1 = P1*V; //W1 is the work done if the gas confined
    in the cylinder us taken as system
25 mprintf('Work done by the system if the gas confined
    in the cylinder is taken as a system is %f Nm',
    W1);
26
27 //(ii). If gas + piston + piston rod is a system
28 P2 = ((W*9.8065)/(10^-4)); //P2 is the resisting
    pressure when the gas plus piston plus piston rod
    is taken as a system
29 W2 = P2*V; //W2 is the Work done by the system if the
    gas plus piston plus piston rod is taken as a
    system

```

```

30 mprintf('\\n Work done by the system if the gas plus
    piston plus piston rod is taken as system is %f
    Nm',W2);
31
32 //(iii). If gas + piston + piston rod +weight is
    system
33 P3 = 0;//P3 is the resisting pressure when the gas
    plus piston plus piston rod plus weight is taken
    as a system
34 W3 = P3*V;//W3 is the work done by the system if the
    gas plus piston plus piston rod plus weight is
    taken as a system
35 mprintf('\\n Work done by the system if the gas plus
    piston plus piston rod plus weight is taken as a
    system is %f',W3);
36 //end

```

Scilab code Exa 1.6 To Calculate the work done

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 1
3 //Introduction
4
5 //Example 1.6
6 clear all;
7 clc;
8
9 //Given
10 n = 1;//n is the Kg mole of ideal gas.
11 P1 = 700*(10^4);//P1 is the initial pressure of the
    system in N/(m^2)
12 P2 = 638*(10^4);//P2 is the final pressure of the
    system in N/(m^2)
13 T = 300;//T is temperature of the system in K
14 R = 8314.4;//R is gas constant in Nm/Kgmole deg K

```

```
15
16 //To calculate the work done
17 W = n*R*T*log(P1/P2); //W is the work done by the
    system in Nm
18 mprintf('Work done by the system is %4.2e Nm',W);
19 //end
```

Chapter 2

P V T Relations

Scilab code Exa 2.1 To determine the temperature required

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.1
6 clear all;
7 clc;
8
9 //Given
10 m = 140; //m is the mass of N2 in Kg
11 P = 4.052*(10^5); //P is the pressure of the system
    in Pa
12 V = 30; //V is the volume of the system in m^3
13 R = 8314.4; // R is the gas constant
14
15 //To determine temperature required
16 T = P*V/((m/28)*R); //T is the temperature of the
    system in K
17 mprintf('Temperature of the system is %f K',T);
18 //end
```

Scilab code Exa 2.2 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.2
6 clear all;
7 clc;
8
9 //Given
10 //This example is a theoretical problem and does not
    involve any numerical computation
11 //end
```

Scilab code Exa 2.3 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.3
6 clear all;
7 clc;
8
9 //Given
10 //This example is a theoretical problem and does not
    involve any numerical computation
11 //end
```

Scilab code Exa 2.4 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.4
6 clear all;
7 clc;
8
9 //Given
10 //This example is a theoretical problem and does not
    involve any numerical computation
11 //end
```

Scilab code Exa 2.5 To calculate the volume of Methane

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.5
6 clear all;
7 clc;
8
9 //Given
10 n = 1; //n is Kg moles of methane
11 T = 423; //T is the temperatue of the system in
    kelvin
12 P = 100; //P is the pressure of the system in atm
13 Tc = 191; //Tc is the critical temperature of the
    system in K
14 Pc = 45.8; //Pc is the critical pressure of the
    system in atm
15 R = 0.08206; //R is the gas constant in (m3 atm/Kg
```

```

    mole K)
16
17 //To calculate the volume of methane
18 //(i)Using ideal gas equation
19 V1 = (n*R*T)/P;//V1 is the volume of the gas in m^3
20 fprintf('(i)Volume of the gas using ideal gas
    equation is %f cubic meter',V1);
21
22 //(ii)Using Vander Waals' equation
23 a = (27*(R^2)*(Tc^2))/(64*Pc);//Vander Waais
    constant
24 b = (R*Tc)/(8*Pc);//Vander Waais constant
25 v = poly(0, 'v');
26 q = -((a*b)/P)+(a/P)*v-(((R*T)+(b*P))/P)*v^2+(v^3);
    //According to Vander Waals equation
27 r = roots(q);
28 fprintf('\n (ii)Volume of the gas using Vander Waals
    equation is %f cubic meter',r(1));
29
30 //(iii)Using generalized Z chart
31 Tr = T/Tc;//Tr is the reduced temperatue
32 Pr = P/Pc;//Pr is the reduced pressure
33 //From the figure A.2.2,
34 Z = 0.97;//Z is the compressibility factor
35 V = (Z*R*T)/P;
36 fprintf('\n (iii)Volume of the gas using Z chart is
    %f cubic meter',V);
37
38 //(iv)Using molar polarisation method
39 //From Table 2.2
40 Pmc = 6.82;//Pmc is the molar polarisation for
    methane
41 //From figure A.2.4
42 Z0 = .965;
43 Z1 = 14.8*(10^-4);
44 Z = Z0+(Z1*Pmc);
45 V = (Z*R*T)/P;
46 fprintf('\n (iv)Volume of the gas using molar

```

```

    polarisation method is %f cubic meter',V);
47
48 //(v)From experiment
49 //Given
50 Z = 0.9848;
51 V = (0.9848*n*R*T)/P;
52 mprintf('\n (v)Volume of the gas calculated by
    experimental Z value is %f cubic meter',V);
53 //end

```

Scilab code Exa 2.6 To calculate the final pressure achieved

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.6
6 clear all;
7 clc;
8
9 //Given
10 P1 = 266;
11 T1 = 473.16; //Initial temperature in Kelvin
12 T2 = 273.16; //Final temperature in Kelvin
13 V1 = 80; V2 = 80; //Initial & final volume in litres
14 N1 = (14.28/28); N2 = (14.28/28); //Initial and final
    Kg moles are equal
15 Tc = 126; //Critical temperature of N2 in K
16 Pc = 33.5; //Critical pressure of N2 in atm
17
18 //To calculate the final pressure achieved
19 //(i)Using ideal gas law
20 p2 = (P1*V1*N2*T2)/(V2*N1*T1);
21 mprintf('(i)Final pressure of N2 using ideal gas
    law is %f atm',p2);

```

```

22
23 //(ii)Using generalized Z chart
24 Tr1 = T1/Tc;//reduced initial temp in k
25 Pr1 = P1/Pc;//reduced initial press in K
26 //From the Z-chart compressibility factor
    coressponding to the above Tr1 &Pr1 is
27 Z1 = 1.07;
28 P2 = [125,135,150];
29 Z2 = [0.95, 0.96, 0.98];
30 F = [0,0,0];
31 for i = 1:3
32     F(i) = (P2(i)/(Z2(i)*T2))-(P1/(Z1*T1));
33 end
34 clf;
35 plot(P2,F);
36 xtitle("P2 vs F", "P2", "F");
37 P3 = interp1n([F;P2],0);
38 mprintf('\n (ii)Final pressure of N2 from Z chart is
    %f atm',P3);
39
40 //(iii)Using Pseudo reduced density chart
41 R = 0.082;//gas constant
42 v = V1/N1;//Volume per moles of nitrogen in m^3/Kg
    mole
43 Dr = (R*Tc)/(Pc*v);
44 Tr2 = T2/Tc;//final reduced temp in K
45 //From figure A.2.1, reduced pressure coressponding
    to this Dr and Tr2 is
46 Pr2 = 4.1//final reduced pressure in atm
47 p2_ = Pr2*Pc;
48 mprintf('\n (iii)Final pressure achieved using Dr
    chart is %f atm',p2_);
49 //end

```

Scilab code Exa 2.7 To compute the work required

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.7
6 clear all;
7 clc;
8
9 //Given
10 n = 1; //n is the Kg mole of methane gas
11 T = 298; //T is the constant temperature in K
12 P1 = 1; //P1 is the initial pressure of the system
13 P2 = 100; //P2 is the final pressure of the system
14 R = 8314.4; //R is the gas constant in Nm/Kgmole deg
    K
15
16 //To compute the work required
17 //(i) Using ideal gas law
18 W = R*T*log(P1/P2);
19 mprintf('(i) Work done by the system if the gas obeys
    ideal gas law is %4.2e Nm', W);
20
21 //(ii) Using Vander Waals' equation
22 //Given
23 //For methane
24 a = 2.32*(10^5); //Vander Wals' constant a in N/m^2
25 b = 0.0428; //Vanderwaals' constant b in m^3
26 //V1 and V2 are evaluated by trial and error using
    Vanderwaals' equation as P1 and P2 are known
27 V1 = 11.1; //initial volume of the gas in m^3
28 V2 = 0.089; //final volume of the gas in m^3
29 W = (R*T*log((V2-b)/(V1-b)))+(a*((1/V2)-(1/V1)))
30 mprintf('\n (ii) Work done by the system if the gas
    obeys Vander Waals equation is %4.2e Nm', W);
31 //end

```

Scilab code Exa 2.8 To determine the vapour pressure of Chlorine

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.8
6 clear all;
7 clc;
8
9 //Given
10 V = 27*(10^-3); //Volume of the container in m^3
11 n = (15/70.91); //n is the Kg moles of chlorine
12 T = 293; //T is the temperature in K
13 R = 0.08206;
14 P = 10^(4.39-(1045/293)); //P is the vapour pressure
    of chlorine
15 Pc = 76.1; //Critical pressure of Chlorine
16 Tc = 417; //Critical temperature of Chlorine
17 Pr = P/Pc; //Reduced pressure of Chlorine
18 Tr = T/Tc; //Critical temperature of Chlorine
19 M = 70.91; //Molecular weight of the Chlorine
20
21 //To determine the vapour pressure of chlorine ,
    amount of liquid Cl2 and temperature required
22 //(i) Specific volume of liquid Chlorine
23 //From figure A.2.2
24 Zg = 0.93;
25 //From figure A.2.6
26 Zl = 0.013;
27 vl = ((Zl*R*T)/P);
28 mprintf('(i) Specific volume of liquid Chlorine from
    compressibility chart is %f cubic meter /Kgmole',
    vl);
```



```

29
30 //From Francis relation , taking the constants from
    Table 2.3
31 D = (1.606-(216*(10^-5)*20)-(28/(200-20)))*10^3; //
    Density of liq Cl2 in Kg/m^3
32 V1 = M/D;
33 mprintf('\n Specific volume of liquid Chlorine
    from Francis relation is %f cubic meter /Kgmole',
    V1);
34
35 //(ii)Amount of liquid Cl2 present in the cylinder
36 vg = ((Zg*R*T)/P);
37 V1 = V-vg; //V1 is the volume of liquid Chlorine
38 Vct = 0.027; //volume of the container
39 Vg = (0.212-(Vct/v1))/((1/vg)-(1/v1)); //By material
    balance
40 W = ((V-Vg)*70.9)/v1;
41 mprintf('\n\n (ii)Weight of Chlorine at 20deg cel is
    %f Kg',W);
42
43 //(iii)Calculation of temperature required to
    evaporate all the liquid chlorine
44 //log P' = 4.39 - 1045/T (given)
45 //Assume the various temperature
46 Ng = 0.212; //total Kg moles of gas
47 Ta = [413 415 417];
48 N = [0,0,0];
49 for i = 1:3
50     Tr(i) = Ta(i)/Tc; //reduced temperature in K
51     P(i) = 10^(4.39-(1045/Ta(i)));
52     Pr(i) = P(i)/Pc; //reduced pressure in K
53 //From the compressibility factor chart,Z values
    coressponding to the above Tr &Pr are given as
54 Z = [0.4 0.328 0.208];
55 N(i) = (P(i)*Vct)/(Z(i)*R*Ta(i));
56 end
57
58 clf;

```

```

59 plot(N,Ta);
60 xtitle("Ta vs N", "N", "Ta");
61 T1 = interp1n([N;Ta],0.212); //in K
62 mprintf('\n (iii)The temperature required to
    evaporate all the liquid chlorine is %f deg
    celsius ',T1-273);
63 //end

```

Scilab code Exa 2.9 To calculate the pressure exerted by the gas mixture

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.9
6 clear all;
7 clc;
8
9 //Given
10 N1 = 0.7; //Kg mole of CH4
11 N2 = 0.3; //Kg mole of N2
12 R = 0.08206; //Gas constant
13 T = 323; //Temperature in Kelvin
14 V = 0.04; //Volume in m^3
15 a1 = 2.280; b1 = 0.0428; //Vanderwaals constants for
    CH4
16 a2 = 1.345; b2 = 0.0386; //Vanderwaals constants for
    N2
17 Tc1 = 191; Pc1 = 45.8; //Critical temperature in K
    and pressure of CH4 in atm
18 Tc2 = 126; Pc2 = 33.5; //Critical temperature in K and
    pressure of N2 in atm
19
20 //To find Approx Value
21 function [A]=approx(V,n)

```

```

22     A=round(V*10^n)/10^n; //V-Value  n-To what place
23     funcprot(0)
24 endfunction
25
26 //To calculate the pressure exerted by the gas
    mixture
27 //(i)Using ideal gas law
28 P = (N1+N2)*((R*T)/V);
29 mprintf('(i) Pressure exerted by the gas mixture
    using ideal gas law is %d atm',P);
30
31 //(ii)Using Vander waal equation
32 P1 = ((N1*R*T)/(V-(N1*b1)))-((a1*(N1^2))/(V^2)); //
    Partial pressure of CH4
33 P2 = ((N2*R*T)/(V-(N2*b2)))-((a2*(N2^2))/(V^2)); //
    Partial pressure of N2
34 Pt = P1+P2;
35 mprintf('\n(ii) Pressure exerted by the gas mixture
    using Vander waal equation is %f atm', Pt);
36
37 //(iii)Using Zchart and Dalton's law
38 Tra = T/Tc1; //reduced temperature of CH4
39 Trb = T/Tc2; //reduced temperature of N2
40 //Assume the pressure
41 P = [660 732 793 815 831];
42 for i = 1:5
43     Pa(i) = N1*P(i); // partial pressure of CH4 for
        the ith total pressure
44     Pb(i) = N2*P(i); // partial pressure of N2 for
        the ith total pressure
45     Pra(i) = Pa(i)/Pc1; //reduced pressure of CH4 for
        the ith total pressure
46     Prb(i) = Pb(i)/Pc2; //reduced pressure of N2 for
        the ith total pressure
47 end
48
49 //For the above Pr and Tr values compressibility
    factors from the figure A.2.3 are given as

```

```

50 Za = [1.154 1.280 1.331 1.370 1.390]; //Z values of
    CH4
51 Zb = [1 1 1 1 1]; //Z values of N2
52 V3 = 0.0421;
53 for i = 1:5
54     Pa(i) = Za(i)*N1*((R*T)/V); //partial pressure of
        CH4 coressponding to the ith total presure
55     Pb(i) = Zb(i)*N2*((R*T)/V); //partial pressure of
        N2 coressponding to the ith total pressure
56     Pt(i) = Pa(i)+Pb(i); //total pressure of the gas
        mixture
57     if Pt(i)-P(i) < 15
58         mprintf('\n(iii) pressure exerted by the gas
            mixture using Z chart and Dalton Law is %d
            atm ',Pt(i));
59     else
60     end
61 end
62
63 //(iv) Using Amagat's law and Z chart
64 P = [1000 1200 1500 1700];
65 for i=1:4
66     Pra(i) = P(i)/Pc1;
67     Prb(i) = P(i)/Pc2;
68 end
69 //For the above Pr and Tr values compressibility
    factors from the figure A.2.3 are given as
70 Za = [1.87 2.14 2.52 2.77];
71 Zb = [1.80 2.10 2.37 2.54];
72 for i = 1:4
73     Va(i) = approx((N1*Za(i))*((R*T)/P(i)),4);
74     Vb(i) = approx((N2*Zb(i))*((R*T)/P(i)),4);
75     V1(i) = approx((Va(i)+Vb(i)),4);
76     if V1(i)-V <= 0.003
77         mprintf('\n(iv) Pressure exerted by the gas
            mixture using Amagat law and Zchart is %d
            atm ',P(i));
78     else

```

```
79 end
80 end
81 //end
```

Scilab code Exa 2.10 To calculate the amount of Ammonia leaving the reactor and the velocity of gaseous product leaving the reactor

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 2
3 //P-V-T Relations
4
5 //Example 2.10
6 clear all;
7 clc;
8
9 //Given
10 yN2 = 1/4; //mole fraction of N2 in the mixture
11 yH2 = 3/4; //mole fraction of H2 in the mixture
12 V = 5.7; //V is the rate at which mixture enters in m
    ^3 in 1 hour
13 P = 600; //P is in atm
14 T = 298; //T is in K
15 TcN2 = 126; //critical temp of N2 in K
16 TcH2 = 33.3; //critical temp of H2 in K
17 TcNh3 = 406.0; //critical temp of NH3 in K
18 PcN2 = 33.5; //critical pressure of N2 in atm
19 PcH2 = 12.8; //critical pressure of H2 in atm
20 PcNH3 = 111.0; //critical pressure of NH3 in atm
21 R = 0.082; //gas constant
22
23 //To calculate the amount of ammonia leaving the
    reactor and the velocity of gaseous product
    leaving the reactor
```

```

24 //(i) Calculation of amount of NH3 leaving the
    reactor
25 Tcm = (TcN2*yN2)+(TcH2*yH2); // critical temperature
    of the mixture
26 Pcm = (PcN2*yN2)+(PcH2*yH2); // critical pressure of
    the mixture
27 Trm = T/Tcm;
28 Prm = P/Pcm;
29 //From figure A.2.3
30 Zm = 1.57; //compressibility factor of the mixture
31 N = (P*V)/(Zm*R*T); //Kg mole of the mixture
32 N1 = 0.25*N; //Kg mole of N2 in feed
33 //N2+3H2 - 2NH3
34 W = 2*0.15*N1*17;
35 mprintf('(i) Ammonia formed per hour is %f Kg',W);
36
37 //(ii) Calculation of velocity
38 N1 = 0.25*N-(0.25*N*0.15); //Kg mole of N2 after
    reactor
39 N2 = 0.75*N-(0.75*N*0.15); //Kg mole of H2 after
    reactor
40 N3 = 0.25*N*2*0.15; //Kg mole of NH3 after reactor
41 Nt = N1+N2+N3; //total Kg moles after reactor
42 y1NH3 = N3/Nt; //mole fraction of NH3 after reactor
43 y1N2 = N1/Nt; //mole fraction of N2 after reactor
44 y1H2 = N2/Nt; //mole fraction of H2 after reactor
45 T1cm = (TcN2*y1N2)+(TcH2*y1H2);
46 P1cm = (PcN2*y1N2)+(PcH2*y1H2);
47 T1 = 448; //in K
48 P1 = 550; //in atm
49 T1rm = T1/T1cm;
50 P1rm = P1/P1cm;
51 //From Figure A.2.2
52 Zm1 = 1.38;
53 V1 = (Zm1*Nt*R*T1)/P1;
54 d = 5*(10^-2); //diameter of pipe
55 v = V1/((%pi/4)*(d^2)*3600);
56 mprintf('\n (ii) Velocity in pipe is %f m/sec',v);

```

57 //end

Chapter 3

First Law of Thermodynamics

Scilab code Exa 3.1 To calculate the change in internal energy

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.1
6 clear all;
7 clc;
8
9 //Given
10 W = -((2*745.6*(10^-3)/4.18)*3600); //work added to
    the system in Kcal/hr
11 m = 10; //Amount of fluid in tank in Kg
12 Q = -378; //Heat losses from the system in Kcal/hr
13
14 //To calculate the change in internal energy
15 delE=(Q-W)/m; // Change in internal energy in Kcal/hr
    kg
16 mprintf('Change in Internal energy is %f Kcal/hr Kg'
    ,delE);
17 //end
```

Scilab code Exa 3.2 To calculate the change in internal energy

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.2
6 clear all;
7 clc;
8
9 //Given
10 n = 1; //kg moles of a gas
11 Cv = 5; //specific heat in Kcal/Kgmole
12 delT = 15; //increase in temperature in deg celsius
13
14 //To calculate the change in internal energy
15 Q = n*Cv*delT; //heat given to the system in Kcal
16 W = 0; //work done
17 delE = Q-W; //Change in internal energy
18 mprintf('Change in internal energy is %f Kcal',delE)
19 //end
```

Scilab code Exa 3.3 To calculate the work done by the expanding gas and increase in internal energy

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.3
6 clear all;
```

```

7  clc;
8
9  //Given
10 P = 1; //constant pressure throughout the process in
    atm
11 T1 = 273; //Initial temperature in K
12 T2 = 373; //Final temperature in K
13 V1 = 0; //Volume of liquid water or initial volume
14 V0 = 22.4; //volume of vapour at standard condition
    in cubic meter
15 Q = 9.7 //Heat of vapourisation in Kcal
16
17 //To calculate the work done by the expanding gas
    and increase in internal energy
18 //(i) Calculation of work done
19 V2 = 22.4*(T2/T1)*(P)*(10^-3); //Volume of final
    vapour in cubic meter
20 w = P*(V2-V1); //Work done in atm cubic meter
21 W = w*(1.03*10^4)/427; //Work done in Kcal
22 mprintf('(i)Work done by the expanding gas is %f
    Kcal',W);
23
24 //(ii) Calculation of change in internal energy
25 delE = Q-W;
26 mprintf('\n\n (ii)Increase in internal energy is %f
    Kcal',delE);
27 //end

```

Scilab code Exa 3.4 To calculate the time taken for the gas to attain 10 atm

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4

```

```

5 //Example 3.4
6 clear all;
7 clc;
8
9 //Given
10 W = 0; //work done during the process
11 P1 = 1; //Initial pressure in atm
12 P2 = 10; //Final pressure in atm
13 V2 = V1; //Initial & final volume are equal
14 Cv = 0.23 //specific heat at constant volume in Kcal/
    Kg deg K
15 //((delQ/delT)=Q
16 Q = 1.3; //Rate of heat addition in Kcal/min
17 m = 2.5 //Weight of an ideal gas in Kg
18 T1 = 298 //Initial temperature in Kelvin
19
20 //To calculate the time taken for the gas to attain
    10 atm
21 //Q = m*Cv*(delT/delt)=1.3
22 T2 = (P2*T1)/(P1); //Final temperature in Kelvin
23 t = ((m*Cv)/1.3)*(T2-T1); //time taken in minutes
24 mprintf('The time taken to attain a pressure of 10
    atm is %f hrs ',t/60);
25 //end

```

Scilab code Exa 3.5 Theoretical problem

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.5
6 clear all;
7 clc;
8

```

```
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end
```

Scilab code Exa 3.6 To calculate the flow work per kg of air

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.6
6 clear all;
7 clc;
8
9 //Given
10 R = 1.98; //gas constant in kcal/Kgmole deg K
11 T = 293; //Temperature in K
12 M = 29; //Molecular weight of air
13
14 //To calculate the flow work per kg of air
15 //W=(P*V)=(R*T)
16 W = R*T; //Flow work in Kcal/Kg mole
17 W1 = W/M;
18 mprintf('Flow work is %f Kcal/Kg',W1);
19 //end
```

Scilab code Exa 3.7 To calculate the horse power output of the turbine

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
```

```

5 //Example 3.7
6 clear all;
7 clc;
8
9 //Given
10 m = 5000; //Amount of steam recived per hour in Kg
11 H1 = 666; //Specific enthalpy when steam entered in
    the turbine in Kcal/Kg
12 H2 = 540; //Specific enthalpy when steam left the
    turbine in Kcal/Kg
13 u1 = 3000/60; //velocity at which steam entered in m/
    sec
14 u2 = 600/60; //velocity at which steam left in m/sec
15 Z1 = 5; //height at which steam entered in m
16 Z2 = 1; //height at which steam left in m
17 Q = -4000; //heat lost in Kcal
18 g = 9.81;
19
20 //To calculate the horsepower output of the turbine
21 delH = H2-H1; //change in enthalpy in Kcal
22 delKE = ((u2^2)-(u1^2)/(2*g))/(9.8065*427); //change
    in kinetic energy in Kcal; 1kgf = 9.8065 N
23 delPE = ((Z2-Z1)*g)/(9.8065*427); //change in
    potential energy in Kcal
24 W = -(m*(delH+delKE+delPE))+Q; //work delivered in
    Kcal/hr
25 W1 = W*(427/(3600*75)); //work delivered by turbine
    in hp
26 mprintf('Work delivered by turbine is %f hp',W1);
27 //end

```

Scilab code Exa 3.8 To find out the enthalpy of water of tank2 and find out the temperature of water in the second tank

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.8
6 clear all;
7 clc;
8
9 //Given
10 m = 183; //rate of water flow in Kg/min
11 H1 = 95; //enthalpy of storage tank 1 in Kcal/Kg
12 h = 15; //height difference between two storage tanks
    in m
13 Q = -10100; //extraced heat from storage tank 1 in a
    heat exchanger in Kcal/min
14 W = -2; //work delivered by motor in hp
15
16 // To find out the enthalpy of water tank2 and the
    temperature of water in the second tank
17 delPE = h/427; //change in potential energy in Kcal/
    Kg
18 delKE = 0; //change in kinetic energy
19 W1 = W*(75/427); //work delivered by motor in Kcal/
    sec
20 W2 = W1*60; //work delivered by motor in Kcal/min
21 H2 = ((Q+W2)/m)-delKE-delPE+H1; //enthalpy of storage
    tank 2 in Kcal/Kg
22 mprintf('The enthalpy of storage tank 2 is %f Kcal/
    Kg',H2);
23
24 //The enthalpy H2=39.66 corresponds to the
    temperature T according to steam table
25 T=40; //Temperature is in deg celsius
26 mprintf('\n The temperature of water in the second
    tank is %d deg celsius ',T);
27 //end

```

Scilab code Exa 3.9 To calculate the mass of steam required

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.9
6 clear all;
7 clc;
8
9 //To calculate the mass of steam required
10 //Given
11 m2 = 100; //mass of water to be heated
12 //From diagram ,
13 //m3 = m1+m2; .. (a)
14 //Hs = H1; ..(b) since throttling is a constant
    enthalpy process
15 //m3*H3-(m1*H1+m2*H2)=0; ..(c) since delH=0
16
17 //From steam tables ,
18 Hs = 681.7 //enthalpy of steam at 200 deg cel bleded
    at the rate of 5Kgf/(cm^2) in Kcal/Kg
19 H2 = 5.03; //enthalpy of liquid water at 5 deg cel
20 H3 = 64.98; //enthalpy of liquid water at 65 deg cel
21 //from equn (a),(b)&(c);(page no 80)
22 m1 = ((H3-H2)/(Hs-H3))*m2; //mass of steam required
    in Kg (page no 80)
23 mprintf('The mass of steam required to heat 100 Kg
    of water is %f Kg',m1);
24 //end
```

Scilab code Exa 3.10 To calculate the pump work required

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.10
6 clear all;
7 clc;
8
9 //Given
10 V = 0.3; //Volume of the tank in m^3
11 P1 = 1; //Initial pressure of the tank in atm
12 P2 = 0; //Final pressure of the tank in atm
13 T = 298; //Temperature of the tank in K
14 t = 10; //evacuation time in min
15
16 //delN=(V/(R*T)*delP)..(a) change in moles as V and
    T are constant
17 //delW=delN*R*T*lnP..(b)pump work required
18 //From (a)&(b),delW=V*delP*lnP
19
20 //To calculate the pump work required
21 //On doing integration of dW we will get
22
23 W = V*(P1-P2); //pump work done in J/sec
24 W1=(W*(1.033*10^4))/(75*600);
25 mprintf('The pump work required is %f hp',W1);
26 //end

```

Scilab code Exa 3.11 To calculate the quality of exit steam

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.11

```



```

6 clear all;
7 clc;
8
9 //Given
10 H1 = 680.6; //Enthalpy of entering steam at 6Kgf/cm^2
    &200 deg cel in Kcal/Kg
11 u1 = 60; //velocity at which steam entered the nozzle
    in m/sec
12 u2 = 600; //velocity at which steam left the nozzle
    in m/sec
13 g = 9.8;
14 Hg = 642.8; H1q = 110.2; //Enthalpy of saturated
    vapour & saturated liquid at 1.46 Kgf/cm^2
    respectively
15
16 //To calculate the quality of exit steam
17 H2 = H1+((u1^2)-(u2^2))/(2*g*427); //enthalpy of
    leaving steam in Kcal/Kg
18 x = (H2-H1q)/(Hg-H1q);
19 mprintf('The quality of exit steam is %f percent',x
    *100);
20 //end

```

Scilab code Exa 3.12 To calculate the internal energy of the steam in the chamber

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.12
6 clear all;
7 clc;
8
9 //Given

```

```

10 W = 0; //pump work
11 Mi = 0; //chamber is initially evacuated
12 M2 = 0; //no exist stream
13 H1 = 684.2; //enthalpy of steam at 200 deg cel & 3
    Kgf/cm^2
14
15 //To calculate the internal energy of the steam in
    the chamber
16 //Q=150*m1;.. (a) heat lost from the chamber in Kcal
    /Kg
17 //m1=mf;..(b) mass of steam added from large pipe is
    equal to steam in chamber
18 //H1*M1-Q=Mf*Ef; using (a)&(b)
19 Ef = H1-150;
20 mprintf('The internal energy of steam in chamber is
    %f Kcal ',Ef);
21 //end

```

Scilab code Exa 3.13 To calculate the final weight and the final temperature of the air in the tank

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3
3 //First Law of Thermodynamics
4
5 //Example 3.13
6 clear all;
7 clc;
8
9 //Given
10 //Q=W=delPE=delKE=0;
11 //M2=0; no exit stream
12 Ti = 288; //initial temperature in K
13 H = 7*Ti; //enthalpy of air in Kcal/Kgmole
14 Ei = 5*Ti; // initial internal energy of air in Kcal/

```

```

    Kgmole
15 //Ef=5*Tf;Final internal energy of air in Kcal/
    Kgmole
16 Pi = 0.3; //initial pressure in atm
17 V = 0.57; //volume of the tank in m^3
18 R = 848; //gas constant in mKgf/Kg mole K
19 Pf = 1; //final prssure in atm
20
21 //To calculate the final weight and the final
    temperature of the air in the tank
22 Mi = (Pi*V*1.03*10^4)/(R*Ti); //initial quantity of
    air in tank in Kg mole
23 //Tf=(Pf*V*1.033*10^4)/(Mf*R)..(a) final temperature
    ,Mf=final quantity of air in tank in Kg mole
24 //M1=Mf-Mi..(b) M1 is mass of steam added in Kg mole
25 //H*M1=(Ef*Mf)-(Ei*Mi)
26 //H*M1=((5*Pf*V*1.033*10^4)/(Tf*R))*Tf-(Ei*Mi)...(c)
27 A = [1 -1;0 -H];
28 B = [Mi;((Ei*Mi)-((5*Pf*V*1.03*10^4)/R))];
29 x = A\B;
30 Mf = x(1);
31 mprintf('The final weight of air in the tank is%f Kg
    ',Mf);
32
33 Tf = (Pf*V*1.03*10^4)/(Mf*R);
34 mprintf('\\n The final temperature of air in the tank
    is %f K',Tf);
35 //end

```

Scilab code Exa 3.14 Theoretical problem

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 3

```

```
3 //First Law of Thermodynamics
4
5 //Example 3.14
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end
```

Chapter 4

Second Law of Thermodynamics

Scilab code Exa 4.1 To Calculate work output heat rejected entropy change of system and the surrounding and total change in entropy and the efficiency of the heat engine

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.1
6 clear all;
7 clc;
8
9 //Given
10 Q1 = 250; //Heat absorbed in Kcal
11 T1 = (260+273); //Temperature at which engine absorbs
    heat
12 T0 = (40+273); //Temperature at which engine discards
    heat
13 //To Calculate work output, heat rejected, entropy
    change of system, surrounding & total change in
    entropy and the efficiency of the heat engine
```

```

14
15 //(i) Calculation of work output
16 W = (Q1*((T1-T0)/T1)); //Work done using equations
    4.7 & 4.9 given on page no 98
17 mprintf('(i)The work output of the heat engine is %f
    Kcal ',W);
18
19 //(ii) Calculation of heat rejected
20 Q2 = (Q1*T0)/T1;
21 mprintf('\n (ii)The heat rejected is %f Kcal ',Q2);
22
23 //(iii) Calculation of entropy
24 del_S1 = -(Q1/T1); //Change in the entropy of source
    in Kcal/Kg K
25 del_S2 = Q2/T0; //Change in the entropy of sink in
    Kcal/Kg K
26 del_St = del_S1+del_S2; //Total change in entropy in
    Kcal/Kg K
27 mprintf('\n (iii)Total change in entropy is %d
    confirming that the process is reversible ',del_St
    );
28
29 //(iv) Calculation of efficiency
30 n = (W/Q1)*100;
31 mprintf('\n (iv)The efficiency of the heat engine is
    %f percent ',n);
32 //end

```

Scilab code Exa 4.2 To calculate the total change in entropy and hence determine the reversibility of the process

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4

```

```

5 //Example 4.2
6 clear all;
7 clc;
8
9 //Given
10 T1 = 373; //Temperature of the saturated steam in K
11 T2 = 298; //Temperature of the saturated water in K
12 //To calculate the total change in entropy and hence
    determine the reversibility of the process
13
14 //del_H = del_Q+(V*del_P)
15 //del_H =del_Q; since it is a constant pressure
    process
16
17 //From steam table ,
18 //enthalpy of saturated steam at 373K is
19 H1 = 6348.5; // in Kcal/Kg
20 //enthalpy of saturated liquid water at 373K is
21 H2 = 99.15; //in Kcal/Kg
22 Q = H2-H1; //heat rejected in Kcal/Kg
23 del_S1 = Q/T1; //change in entropy of the system in
    Kcal/Kg K
24 del_S2 = Q/T2; //change in entropy of the surrounding
    in Kcal/Kg K
25 del_St = del_S1+del_S2; //total change in the entropy
    in Kcal/Kg K
26 if(del_St == 0)
27     mprintf('Process is reversible ');
28 else
29     mprintf('Process is irreversible ');
30 end
31 //end

```

Scilab code Exa 4.3 To find out entropy change of block air and total entropy change

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.3
6 clear all;
7 clc;
8
9 //Given
10 Cp = 0.09; //specific heat of metal block in Kcal/Kg
    K
11 m = 10; //mass of metal block in Kg
12 T1 = 323; //initial temperature of the block in K
13 T2 = 298; //final temperature of the block in K
14 //constant pressure process
15 //To find out entropy change of block, air and total
    entropy change
16
17 //(i)To calculate the entropy change of block
18 del_S1 = m*Cp*log(T2/T1);
19 fprintf('(i)Entropy change of block is %f Kcal/Kg K'
    ,del_S1);
20
21 //(ii)To calculate the entropy change of air
22 Q = m*Cp*(T1-T2); //heat absorbed by air = heat
    rejected by block in Kcal
23 del_S2 = (Q/T2);
24 fprintf('\n (ii)Entropy change of air is %f Kcal/Kg
    K',del_S2);
25
26 //(iii)To calculate the total entropy change
27 del_St = del_S1+del_S2;
28 fprintf('\n (iii)Total entropy change is %f Kcal/Kg
    K',del_St);
29 if(del_St == 0)
30     fprintf('\n Process is reversible');
31 else
32     fprintf('\n Process is irreversible');

```



```
33 end
34 //end
```

Scilab code Exa 4.4 To calculate the total change in entropy

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.4
6 clear all;
7 clc;
8
9 //Given
10 m1 = 10; //mass of metal block in Kg
11 m2 = 50; //mass of water in Kg
12 Cp1 = 0.09; //Specific heat of metal block in Kcal/Kg
    K
13 Cp2 = 1; //Specific heat of water in Kcal/Kg K
14 T1 = 50; //Initial temperature of block in deg
    celsius
15 T2 = 25; //Final temperature of block in deg celsius
16
17 //To calculate the total change in entropy
18 //Heat lost by block = Heat gained by water
19 Tf = ((m1*Cp1*T1)+(m2*Cp2*T2))/((m1*Cp1)+(m2*Cp2));
    //final temperature of water in deg celsius
20 Tf1 = Tf+273.16; //final temperature in K
21 del_S1 = m1*Cp1*log(Tf1/(T1+273)); //change in
    entropy of the block in Kcal/K
22 del_S2 = m2*Cp2*log(Tf1/(T2+273)); //change in
    entropy of the block in Kcal/K
23 del_St = del_S1+del_S2;
24 mprintf('The total change entropy is %f Kcal/K',
    del_St);
```

25 //end

Scilab code Exa 4.5 To calculate the entropy change

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.5
6 clear all;
7 clc;
8
9 //Given
10 //Air at 20 deg celsius
11 //P1 = 250;initial pressure in atm
12 //P2 = 10;final pressure after throttling in atm
13
14 //To calculate the entropy change
15 //According to the given conditions from figure4.5(
    page no 103)
16 S1 = -0.38;//initial entropy in Kcal/Kg K
17 S2 = -0.15;//final entroy in Kcal/Kg K
18 del_S = S2-S1;
19 mprintf('Change in entropy for the throttling
    process is %f Kcal/Kg K',del_S);
20 //From figure 4.6(page no 104), the final
    temperature is -10 deg celsius
21 //end
```

Scilab code Exa 4.6 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 4
```

```

3 //Second Law of Thermodynamics
4
5 //Example 4.6
6 clear all;
7 clc;
8
9 //Given
10 //The given problem does not involve any numerical
    computation
11 //end

```

Scilab code Exa 4.7 To calculate the horse power of the compressor

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.7
6 clear all;
7 clc;
8
9 //Given
10 //Basis: 1 hour
11 m = 10; //mass of air in Kg
12 T = 293; //Constant temperature throughout the
    process in K
13 //P1 = 1; //Initial pressure in atm
14 //P2 = 30; //Final pressure in atm
15 //According to the given data and using the graph
    or figure A.2.7 given in page no 105
16 S1 = 0.02; //Initial entropy in Kcal/Kg
17 S2 = -0.23; //Final entropy in Kcal/Kg
18 H1 = 5; //Initial enthalpy in Kcal/Kg
19 H2 = 3; //Final enthalpy in Kcal/Kg
20

```

```

21 W = -((H2-H1)+T*(S2-S1))*m*(427/(3600*75));
22 mprintf('The horse power of the compressor is %f hp',
           ,W);
23 //end

```

Scilab code Exa 4.8 To calculate the effectiveness of the process

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.1
6 clear all;
7 clc;
8
9 //Given
10 //Basis: 1 Kg of steam
11 //P1 = 30;Initial pressure in Kgf/cm^2
12 //P2 = 3;Final pressure in Kgf/cm^2
13 //T = 300;//Operating temperature
14 //From figure A.2.8,
15 H1 = 715;//Initial enthalpy of steam in Kcal/Kg
16 H2 = 625;//Final enthalpy of steam in Kcal/Kg
17 S1 = 1.56;//Initial entropy of steam in Kcal/Kg K
18 S2 = 1.61;//Final entropy of steam in Kcal/Kg K
19 Q = -1;//heat loss in Kcal/Kg
20 To = 298;//The lowest surrounding temperature in K
21
22 //To calculate the effectiveness of the process
23 W = -(H2-H1)+Q);//Actual work output by the turbine
           in Kcal
24 //The maximum or available work can be calculated
           from equation 4.14
25 del_B = -((H2-H1)-(To*(S2-S1)));// Maximum work that
           can be obtained in Kcal

```

```

26 E = (W/del_B)*100;
27 mprintf('The effectiveness of the process is %f
    percent ',E);
28 //end

```

Scilab code Exa 4.9 To Calculate the maximum work obtained and the entropy change

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.9
6 clear all;
7 clc;
8
9 //Given
10 m = 1; //mass of liquid water in Kg
11 T1 = 1350; //initial temperature in deg celsius
12 T2 = 400; //final temperature in deg celsius
13 Cp = 1; //Specific heat of water in Kcal/Kg K
14 Cpg = 0.2; //Specific heat of combustion gases in
    Kcal/Kg K
15 Hv = 468.35; //Heat of vapourisation at 14 Kgf/cm^2
    and 194.16 deg celsius in Kcak/Kg
16 To = 298; //Surronding temperature
17 Tb = 194.16+273; //Boiling point of liquid water
18
19 //To Calculate the maximum work obtained and the
    entropy change
20 //(i) Calculation of maximum work
21 //Q = del_H = m*Cp*(T2-T1); gas can be assumed to
    cool at constant pressure
22 //From equation 4.14 (page no 110)
23 del_B = -((m*Cpg*(T2-T1))-(To*m*Cp*log((T2+273)/(T1

```

```

+273))));
24 mprintf('(i)The maximum work that can be obtained is
    %f Kcal/Kg of gas ',del_B);
25
26 //(ii)To Calculate the change in entropy
27 del_S =(m*Cp*log(Tb/To))+((m*Hv)/Tb);
28 mprintf('\\n(ii)The entropy change per Kg of water is
    %f ',del_S);
29 //end

```

Scilab code Exa 4.10 Theoretical problem

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 4
3 //Second Law of Thermodynamics
4
5 //Example 4.10
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end

```

Chapter 5

Thermodynamic Potentials and Maxwell Relation

Scilab code Exa 5.1 To Calculate the efficiency of the separation process

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 5
3 //Thermodynamic Potentials and Maxwell's Relation
4
5 //Example 5.1
6 clear all;
7 clc;
8
9 //Given
10 T = 293; //Constant temperature in K
11 w_NH3 = 20/100; //weight of NH3 in an aqueous
    solution in Kg
12 w_H2O = 80/100; //weight of H2O in an aqueous
    solution in Kg
13 V_f = 40; //feed rate in Kg/min
14 M_NH3 = 17; //Molecular weight of NH3
15 M_H2O = 18; //Molecular weight of H2O
16 R = 1.98; //gas constant in Kcal/Kg mole K
17 V_s = 62; //Rate of heating steam in Kg/min
```

```

18 P1_H2O = 11.6; //Vapour pressure of water in feed in
    mm Hg
19 P2_H2O = 17.5; //Vapour pressure of pure water in mm
    Hg
20 P1_NH3 = 227; //Vapour pressure of NH3 in feed in mm
    Hg
21 P2_NH3 = 6350; //Vapor pressure of pure NH3 in mm Hg
22 //From steam tables:
23 Hs = 666.4; //Enthalpy of steam at 160 deg celsius &
    2Kgf/cm^2 in Kcal /Kg
24 Ss = 1.75; //Entropy of steam at 160 deg celsius & 2
    Kgf/cm^2V in Kcal/Kg K
25 Hl = 20.03; //Enthalpy of liquid water at 20 deg
    celsius in Kcal/Kg
26 Sl = 0.0612; //Entropy of liquid water at 20 deg
    celsius in Kcal/Kg K
27
28 //To Calculate the efficiency of the separation
    process
29 //Material Balance:
30 n_NH3 = (V*w_NH3)/M_NH3; //Kg moles of NH3 in feed(
    tops)
31 n_H2O = (V*w_H2O)/M_H2O; //Kg moles of H2O in feed(
    bottoms)
32 //del_F = del_F_NH3 +del_F_H2O;
33 del_F = (R*T*n_NH3*log(P2_NH3/P1_NH3))+(R*T*n_H2O*
    log(P2_H2O/P1_H2O)); //Theoretical minimum work
    done in Kcal
34 //The available energy of the steam can be
    calculated from equation 4.14(page no 110)
35 del_B = -V_s*((Hl-Hs)-T*(Sl-Ss)); //Available energy
    of the steam in Kcal
36 E = (del_F/del_B)*100;
37 mprintf('The efficiency of the separation process is
    %f percent ',E);
38 //end

```

Chapter 6

Thermodynamic Relations

Scilab code Exa 6.0 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 6
3 //Thermodynamic Relations
4
5 clear all;
6 clc;
7
8 //Given
9 //The chapter does not contain any example which
   involve numerical computation
10 //end
```

Chapter 7

Ideal Gases

Scilab code Exa 7.1 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 7
3 //Ideal Gases
4
5 //Example 7.1
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end
```

Scilab code Exa 7.2 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 7
3 //Ideal Gases
```

```

4
5 //Example 7.2
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end

```

Scilab code Exa 7.3 To Calculate the final temperature of the ideal gas and work done in an open and closed system and internal energy change for the process

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 7
3 //Ideal Gases
4
5 //Example 7.3
6 clear all;
7 clc;
8
9 //Given
10 P1 = 15; //initial pressure in Kgf/cm^2
11 P2 = 1; //final pressure in Kgf/cm^2
12 V1 = 0.012; //initial volume in m^3
13 V2 = 0.06; //final volume in m^3
14 T1 = 420; //initial temperature in K
15 M = 28; //molecular weight of the gas
16 Cp = 0.25; //specific heat at constant pressure in
    Kcal/Kg K
17 R = 1.98; //gas constant in Kcal/Kg mole K
18 R2 = 848; //gas constant in mKgf/Kgmole K
19 //Cv = a+0.0005*T1; Specific heat at constant volume
20

```

```

21 //To Calculate the final temperature of the ideal
    gas, work done in an open and closed system,
    internal energy change for the process
22 //(a) Calculation of final temperature
23 //Using ideal gas law:(P*V)/(R*T)
24 T2 = (P2*V2*T1)/(P1*V1);
25 mprintf('(a)The final temperature is %d K',T2);
26
27 //(b) Calculation of work in an open and closed
    system
28 //From equation 7.22(page no 147): P1*(V1^n)=P2*(V2^
    n)
29 n = (log(P2/P1))/(log(V1/V2));
30 //From equation 7.25(page no 149)
31 W = ((P1*V1)-(P2*V2))/(n-1)*10^4; //work in mKgf
32 W1 = W/427; //Work in Kcal
33 mprintf('\n (b)The work in a closed system is %f
    Kcal',W1);
34 Ws = n*W1; //from equation 7.28(page no 149)
35 mprintf('\n    The work in an open system is %f Kcal
    ',Ws);
36
37 //(c) Calculation of internal energy change
38 R1 = R/M; //gas constant in Kcal/Kg
39 Cv = Cp-R1; //specific heat at constant volume in
    Kcal/Kg K
40 a = Cv-(0.0005*T1);
41 m = (P1*10^4*V1*M)/(R2*T1); //mass of gas in Kg
42 function y = f(T)
43     y = m*(a+(0.0005*T));
44 endfunction
45 del_E = intg(T1,T2,f); //internal energy change in
    Kcal/Kg
46 del_E1 = M*del_E; //internal energy change in Kcal/
    Kgmole
47 mprintf('\n (c)The internal energy change for the
    process is %f Kcal/Kgmole',del_E1);

```

Scilab code Exa 7.4 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 7
3 //Ideal Gases
4
5 //Example 7.4
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
    does not involve any numerical computation
11 //end
```

Scilab code Exa 7.5 To Compute change in enthalpy entropy heat work and for the processes given above and to indicate the quantities that are state functions and to verify that the work required in an isothermal process is less than that in an adiabatic process

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 7
3 //Ideal Gases
4
5 //Example 7.5
6 clear all;
7 clc;
8
9 //Given
10 P1 = 1; //Initial pressure of air in atm
11 T1 = 15+273; //Initial temperature in K
12 P2 = 5; //Final pressure of air in atm
```

```

13 T2 = 15+273; //Final temperature in K
14 Cv = 5; //specific heat of air at constant volume in
    Kcal/Kgmole K
15 Cp = 7; //specific heat of air at constant pressure
    in Kcal/Kgmole K
16 R = 0.082; //gas constant in atm-m3/Kgmole K
17 R1 = 2; //gas constant in Kcal/Kgmole K
18 //From the P-V diagram given in page no 155:
19 //Line 12 represents Isothermal process
20 //Line b2,c2 & 1a represent Isometric process
21 //Line a2 & 1c represent Isobaric process
22 //Line 1b represent Adiabatic process
23
24 //To find Approx Value
25 function [A]=approx(V,n)
26     A=round(V*10n)/10n; //V-Value n-To what place
27     funcprot(0)
28 endfunction
29
30 //To Compute del_H , del_E , Q, W, del_S for the
    processes given above.
31 //To indicate the quantities that are state
    functions
32 //To verify that the work required in an isothermal
    process is less than that in an adiabatic process
33
34 //Basis:1 Kgmole of air
35 V1 = (R*T1)/P1; //Initial volume in cubic meter
36 V2 = (R*T2)/P2; //Final volume in cubic meter
37
38 //(i) Isothermal path 12
39 //Equations 7.7 to 7.9 will be used (page no 145)
40 del_E_12 = Cv*(T2-T1);
41 del_H_12 = Cp*(T2-T1);
42 W_12 = R1*T1*log(P1/P2);
43 Q_12 = W_12;
44 del_S_12 = approx((R1*log(P1/P2)),4);
45 mprintf('\n(i) For isothermal process or path 12

```

```

    change in internal energy is %f',del_E_12);
46 mprintf('\n For isothermal process or path 12
    change in enthalpy is %f',del_H_12);
47 mprintf('\n For isothermal process or path 12 heat
    released is %f Kcal',Q_12);
48 mprintf('\n For isothermal process or path 12 work
    is %f Kcal',W_12);
49 mprintf('\n For isothermal process or path 12
    change in entropy is %f Kcal/Kgmole K',del_S_12);
50
51 //(ii)Path 1a2 = 1a(isometric)+a2(isobaric)
52 //Equation 7.1 to 7.6 will be used (page no 144 &
    145)
53 Pa = P2;
54 Ta = (Pa/P1)*T1;//in K
55 Q_1a = Cv*(Ta-T1);
56 del_E_1a = Q_1a;
57 del_H_1a = Cp*(Ta-T1);
58 W_1a = 0;// Constant volume process
59 del_E_a2 = Cv*(T2-Ta);
60 del_H_a2 = Cp*(T2-Ta);
61 Q_a2 = del_H_a2;
62 W_a2 = P2*(V2-V1)*((10^4*1.03)/427);
63 del_H_1a2 = del_H_1a+del_H_a2;
64 del_E_1a2 = del_E_1a+del_E_a2;
65 Q_1a2 = Q_1a+Q_a2;
66 W_1a2 = W_1a+W_a2;
67 del_S_1a = Cv*log(Ta/T1);
68 del_S_a2 = Cp*log(T2/Ta);
69 del_S_1a2 = approx((del_S_1a+del_S_a2),4);
70 mprintf('\n\n(ii)For path 1a2 change in internal
    energy is %f',del_E_1a2);
71 mprintf('\n For path 1a2 change in enthalpy is %f'
    ,del_H_1a2);
72 mprintf('\n For path 1a2 heat released is %f Kcal'
    ,Q_1a2);
73 mprintf('\n For path 1a2 work is %f Kcal',W_1a2);
74 mprintf('\n For path 1a2 change in entropy is %f

```

```

    Kcal/Kgmole K',del_S_1a2);
75
76 //(iii)Path 1b2 = 1b(adiabatic)+b2(isometric)
77 //From equation 7.11 (page no 146)
78 y = Cp/Cv;
79 Tb = T1*((V1/V2))^(y-1);
80 //From equation 7.1 to 7.3,7.10 & 7.21,(page no
    144,146,147)
81 Q_1b = 0;//adiabatic process
82 del_E_1b = Cv*(Tb-T1);
83 del_H_1b = Cp*(Tb-T1);
84 W_1b = -del_E_1b;
85 Q_b2 = Cv*(T1-Tb);
86 del_H_b2 = Cp*(T1-Tb);
87 W_b2 = 0;//constant volume prcess
88 del_E_b2 = Cv*(T2-Tb);
89 del_H_1b2 = del_H_1b+del_H_b2;
90 del_E_1b2 = del_E_1b+del_E_b2;
91 W_1b2 = W_1b+W_b2;
92 Q_1b2 = Q_1b+Q_b2;
93 del_S_1b2 = approx((Cv*log(T1/Tb)),4);
94 mprintf('\n\n(iii)For path 1b2 change in internal
    energy is %f',del_E_1b2);
95 mprintf('\n    For path 1b2 change in enthalpy is %f'
    ,del_H_1b2);
96 mprintf('\n    For path 1b2 heat released is %f Kcal'
    ,Q_1b2);
97 mprintf('\n    For path 1b2 work is %f Kcal',W_1b2);
98 mprintf('\n    For path 1b2 change in entropy is %f
    Kcal/Kgmole K',del_S_1b2);
99
100 //(iv)Path 1c2 = 1c(isobaric)+c2(isometric);
101 Pc = P1;
102 Vc = V2;
103 Tc = (Pc/P2)*T2;
104 del_E_1c = Cv*(Tc-T1);
105 Q_1c = Cp*(Tc-T1);
106 del_H_1c = Q_1c;

```



```

107 W_1c = P1*(Vc-V1)*((10^4*1.03)/427);
108 del_E_c2 = Cv*(T2-Tc);
109 Q_c2 = del_E_c2;
110 del_H_c2 = Cp*(T2-Tc);
111 W_c2 = 0; //constant volume process
112 del_E_1c2 = del_E_1c+del_E_c2;
113 del_H_1c2 = del_H_1c+del_H_c2;
114 Q_1c2 = Q_1c+Q_c2;
115 W_1c2 = W_1c+W_c2;
116 del_S_1c = Cp*log(Tc/T1);
117 del_S_c2 = Cv*log(T2/Tc);
118 del_S_1c2 = approx((del_S_1c+del_S_c2),4);
119 fprintf('\n\n(iv)For path 1c2 change in internal
        energy is %f',del_E_1c2);
120 fprintf('\n    For path 1c2 change in enthalpy is %f'
        ,del_H_1c2);
121 fprintf('\n    For path 1c2 heat released is %f Kcal'
        ,Q_1c2);
122 fprintf('\n    For path 1c2 work is %f Kcal',W_1c2);
123 fprintf('\n    For path 1c2 change in entropy is %f
        Kcal/Kgmole K',del_S_1c2);
124
125 //Determination of state & path functions
126 if((del_E_12 == del_E_1a2)&(del_E_12 == del_E_1b2)&(
        del_E_12 == del_E_1c2))
127     fprintf('\n\n del_E is a state function');
128 else
129     fprintf('\n\n del_E is a path function');
130 end
131 if((del_H_12 == del_H_1a2)&(del_H_12 == del_H_1b2)&(
        del_H_12 == del_H_1c2))
132     fprintf('\n\n del_H is a state function');
133 else
134     fprintf('\n\n del_H is a path function');
135 end
136 if(del_S_12 == del_S_1a2)&(del_S_12 == del_S_1b2)&(
        del_S_12 == del_S_1c2)
137     fprintf('\n\n del_S is a state function');

```

```

138 else
139     mprintf('\n\n del_S is a path function');
140 end
141 if((Q_12 == Q_1a2)&(Q_12 == Q_1b2)&(Q_12 == Q_1c2))
142     mprintf('\n\n Q is a state function');
143 else
144     mprintf('\n\n Q is a path function');
145 end
146 if((W_12 == W_1a2)&(W_12 == W_1b2)&(W_12 == W_1c2))
147     mprintf('\n\n W is a state function');
148 else
149     mprintf('\n\n W is a path function');
150 end
151
152 //Comparison of work required by isothermal &
    adiabatic process
153 if(-(W_12)<-(W_1b2))
154     mprintf('\n\n Work required by isothermal
        process is less than the work required by an
        adiabatic process');
155 else
156     mprintf('\n\n Statement is incorrect');
157 end
158 //end

```

Chapter 8

Third Law of Thermodynamics

Scilab code Exa 8.1 To calculate the absolute entropy of copper at 300 K

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 8
3 //Third Law of Thermodynamics
4
5 //Example 8.1
6 clear all;
7 clc;
8
9 //Given
10 C_ps = 0.1; //Molal heat capacity of copper at 20 K
11 Ti = 0; //Initial temperature in K
12 Tf = 20; //melting point in K
13 Tb = 300; //boiling point in K
14
15 //To calculate the absolute entropy of copper at 300
    K
16 //From equation 8.4(page no 164)
17 a = C_ps/(Tf^3); // a is the charateristic constant
18 C_p = [0.1 0.80 1.94 3.0 3.9 5.0];
19 //T1 = log(T);
20 T1 = [1.301 1.6021 1.7782 1.9031 2.000 2.1761];
```

```
21 plot(T1,C_p);
22 xtitle("C_p vs T1","T1","Cp");
23 // Area under the curve is given as
24 A = 7.82;
25 //From equation 8.5(page no 164)
26 S = (a*((Tf^3)/3))+A;
27 mprintf('The absolute entropy of copper is %f Kcal/
    Kgmole ',S);
28 //end
```

Chapter 9

Fluid Flow in Pipes and Nozzles

Scilab code Exa 9.1 To find out the pressure at the final point

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 9
3 //Fluid Flow in Pipes and Nozzles
4 //Example 9.1
5 clear all;
6 clc;
7
8 //Given
9 R = 848; //gas constant in m Kgf/Kgmole K
10 M = 29; //molecular weight of air
11 g = 9.81;
12 T1 = 90+273; //initial temperature in K
13 y = 1.4; //gamma = Cp/Cv
14 W = 800/3600; //Mass rate of air in Kg/sec
15 P1 = 3.5; //initial pressure in atm
16 d = 2.5; //diameter of the pipe in cm
17
18 //To find out the pressure at the final point
19 v1 = (R*T1)/(M*P1*1.033*10^4); //specific volume in
```

```

        cubic meter/Kg
20 u1 = (W*v1)/(%pi*(d^2*(10^-4))/4); // initial velocity
    in m/sec
21 // Assume final temperature as
22 T2 = [300 310];
23 // Assume specific heat capacity in J/KgK
    corresponding to the above temperature as
24 Cp = [2987.56 2983.56];
25 for i = 1:2
26     us(i) = (g*y*R*T2(i)/M)^(1/2); // sonic velocity
        attained in m/sec
27     u2(i) = ((u1^2) - ((2*g*Cp(i)/M)*(T2(i)-T1)))
        ^ (1/2); // From equation 9.18 & 9.19 (page no
        170)
28 end
29 if us(i)-u2(i) <= 1
30     u2 = u2(i);
31     T2 = T2(i);
32 else
33 end
34 v2 = u2*(%pi/4)*(d^2/10^4)*(1/W);
35 P2 = (P1*v1*T2)/(T1*v2);
36 mprintf('The pressure at the final point is %f atm',
    P2);
37 //end

```

Scilab code Exa 9.2 To find out the mass rate of alcohol

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 9
3 //Fluid Flow in Pipes and Nozzles
4 //Example 9.2
5 clear all;
6 clc;
7

```

```

8 //Given
9 A1 = 0.002; //inlet area in sq meter
10 A2 = 0.0005; //throat area in sq meter
11 P1 = 1.3*10^4; //inlet pressure in Kgf/sq m
12 P2 = 0.7*10^4; //throat pressure in Kgf/sq m
13 g = 9.81;
14 v = 12*10^-4; //specific volume in cubic m /Kg
15
16 //To find out the mass rate of alcohol
17 u2 = ((v*2*g*(P1-P2))/(1-((A2/A1)^2)))^(1/2); //
    throat velocity in m/sec
18 W = (u2*A2)/v;
19 mprintf('The mass rate of alcohol is %f Kg/sec ',W);

```

Scilab code Exa 9.3 To plot velocity and specific volume and mass velocity against the ratio of P2 and P1 and to calculate the critical pressure and critical mass velocity and mass rate of flow

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 9
3 //Fluid Flow in Pipes and Nozzles
4 //Example 9.3
5 clear all;
6 clc;
7
8 //Given
9 P1 = 50; //initial pressure in Kgf/sq m
10 T1 = 45+273; //initial temperature in K
11 g = 9.81;
12 y = 1.35; //gamma
13 R = 848; //gas constant in m Kgf/Kgmole K
14 M = 29; //molecular weight of air
15 d = 1; //pipe diameter in cm
16
17 //(i)To plot velocity ,specific volume ,mass velocity

```

```

    against P2/P1
18 //((ii)To calculate the critical pressure ,critical
    mass velocity and mass rate of flow
19 //(i)Plotting of graph
20 V1 = (R*T1)/(M*P1*1.033*10^4); //initial volume of
    the gas in cubic m/Kg
21 //P3 = P2/P1 (say)
22 //Assume P3 values as
23 P3 = [1.0 0.8 0.6 0.4 0.2 0.1 0];
24 G = [0 0 0 0 0 0 0];
25 for i = 1:7
26     u2(i) = (((2*g*y*R*T1)/((y-1)*M))*(1-(P3(i)^(y
        -1)/y))))^(1/2); //final velocity in m/sec
27 end
28 for i = 1:6
29     v2(i) = V1/(P3(i)^(1/y)); //final specific
        volume in cubic meter/Kg
30 end
31 for i = 1:6
32     G(i) = u2(i)/v2(i); //Mass velocity in Kg/sq m
        sec
33 end
34
35 clf;
36 xset('window',4);
37 plot(P3,u2,"o-");
38 xtitle("Velocity vs P2/P1","P2/P1","Velocity");
39 xset('window',5);
40 plot(P3,G,"+-");
41 xtitle("Mass velocity vs P2/P1","P2/P1","Mass
        velocity");
42 xset('window',6);
43 P_3 = [1.0 0.8 0.6 0.4 0.2 0.1];
44 plot(P_3,v2,"*-");
45 xtitle("Sp. volume vs P2/P1","P2/P1","Specific
        volume");
46
47 //((ii)Calculation of critical pressure ,critical mass

```



```

    velocity and mass rate of flow
48 //From equation 9.37(page no 181)
49 P2 = P1*(2/(y+1))^(y/(y-1));
50 mprintf('The critical pressure is %f atm',P2);
51 //From equation a (page no 183)
52 u2 = (((2*g*y*R*T1)/((y-1)*M))*(1-((P2/P1)^((y-1)/y)
    )))^(1/2);
53 mprintf('\n The critical velocity is %f m/sec ',u2);
54 //From equation b (page no 183)
55 v2 = ((R*T1)/(M*P1*1.033*10^4))/((P2/P1)^(1/y));
56 mprintf('\n The critical specific volume is %f cubic
    meter/Kg',v2);
57 //From relation c (page no 183)
58 G = u2/v2;
59 mprintf('\n The critical mass velocity is %f Kg/sq
    meter sec ',G);
60 W = G*(%pi/4)*(d/(100))^2;
61 mprintf('\n Mass rate of flow through nozzle is %f
    Kg/sec ',W);
62 //end

```

Scilab code Exa 9.4 To calculate the area at exit of nozzle and hence decide the type of the nozzle

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 9
3 //Fluid Flow in Pipes and Nozzles
4 //Example 9.4
5 clear all;
6 clc;
7
8 //Given
9 A1 = 0.1; //Inlet area in sq meter
10 u1 = 60; //inlet velocity in m/sec
11 v1 = 0.185; //inlet specific volume in cubic meter/Kg

```

```

12 H1 = 715; //inlet enthalpy in Kcal/Kg
13 H2 = 660; //exit enthalpy in Kcal/Kg
14 v2 = 0.495; //exit specific volume in cubic meter/Kg
15 g = 9.81
16
17 //To calculate the area at exit of nozzle and hence
    decide the type of the nozzle
18 //From the first law
19 u2 = ((u1^2) - (2*g*(H2-H1)*427))^(1/2);
20 W = (u1*A1)/v1; //Mass rate of gas in Kg/sec
21 A2 = (W*v2)/u2; //Area at exit of nozzle
22 if(A2 < A1)
23     mprintf('The nozzle is convergent');
24 else
25     mprintf('The nozzle is divergent');
26 end
27 //end

```

Chapter 10

Compressor

Scilab code Exa 10.1 To calculate the horsepower required

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 10
3 //Compressor
4 //Example 10.1
5 clear all;
6 clc;
7
8 //Given
9 V1 = 2.7; //flow rate of CO2 in cubic meter/min
10 T1 = 273-51; //temperature in K
11 P1 = 1; //initial pressure in Kgf/sq cm
12 P2 = 10; //final pressure in Kgf/sq cm
13 y = 1.3; //gamma
14 v1 = 0.41; //specific volume in cubic meter/Kg
15 H1 = 158.7; // initial enthalpy in Kcal/Kg
16 H2 = 188.7; //final enthalpy in Kcal/Kg
17
18 //process is isentropic
19 //To calculate the horsepower required
20
21 //(i) Assuming ideal gas behaviour
```

```

22 //From equation 10.3 (page no 189)
23 W = (y/(y-1))*(P1*1.03*10^4*V1)*(1-(P2/P1)^((y-1)/y)
    );//work in m Kgf/min
24 W1 = W/4500;
25 mprintf('(i)The horsepower required is %f hp',W1);
26
27 //(ii)Using the given data for CO2
28 //From equation 10.2 (page no 189)
29 W = -(H2 - H1);//work in Kcal/Kg
30 M = V1/v1;//Mass rate of gas in Kg/min
31 W1 = W*M*(427/4500);
32 mprintf('\n (ii)Compressor work is %f hp',W1);
33 //end

```

Scilab code Exa 10.2 To calculate the volumetric efficiency and the maximum possible pressure that can be attained in a single stage

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 10
3 //Compressor
4 //Example 10.2
5 clear all;
6 clc;
7
8 //Given
9 P1 = 1;//Initial pressure in atm
10 P2 = 29;//Final pressure in atm
11 C = 0.05;//Clearance
12 y = 1.4;//gamma of air
13
14 //To calculate the volumetric efficiency and the
    maximum possible pressure that can be attained in
    a single stage
15 //(i)Calulation of volumetric efficiency
16 //From equation 10.11 (page no 194)

```

```

17 V_E = 1+C-C*(P2/P1)^(1/y);
18 fprintf('(i) Volumetric efficiency is %f percent',V_E
    *100);
19
20 //(ii) Calculation of maximum pressure
21 V_E = 0; //Minimum efficiency
22 P2 = P1*((1+C-V_E)/C)^y);
23 fprintf('\n (ii)The maximum possible pressure
    attained is %f atm',P2);
24 //end

```

Scilab code Exa 10.3 To calculate the capacity and the actual horse power of the compressor

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 10
3 //Compressor
4
5 //Example 10.3
6 clear all;
7 clc;
8
9 //Given
10 V_d = 5.15; //displacement volume in cubic meter/min
11 P1 = 1; //initial pressure in Kgf/sq cm
12 P2 = 8.5; //final pressure in Kgf/sq cm
13 C = 0.06; //Clearance
14 M_E = 0.8; //Mechanical efficiency
15 y = 1.31; //gamma
16
17 //To calculate the capacity and the actual horse
    power of the compressor
18 v1 = V_d*(1+C-(C*((P2/P1)^(1/y))));

```

```

19 mprintf('The capacity of the copressor is %f cubic
    meter/min',v1);
20 //From equation 10.6 (page no 192)
21 W = (y/(y-1))*(P1*1*10^4*v1)*(1-(P2/P1)^((y-1)/y));
    //work in Kgf/min
22 W1 = W/4500;//work in hp
23 W2 = W1/M_E;
24 mprintf('\n The actual horse power of the compressor
    is %f hp',W2);
25 //end

```

Scilab code Exa 10.4 To Calculate the theoretical horse power required

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 10
3 //Compressor
4
5 //Example 10.4
6 clear all;
7 clc;
8
9 //Given
10 P1 = 1;//Initial pressure in Kgf/sq cm
11 Pn = 13;//Final pressure in Kgf/sq cm
12 V1 =27;//flow rate of gas in cubic meter/min
13 y = 1.6;//gamma of the gas
14 n = [1 2 3 4 7 10];//number of stages
15 mprintf('No of stages           Horse power in hp'
    );
16 //To Calculate the theoretical horse power required
17 for i = 1:6
18     W(i) = n(i)*(y/(y-1))*((P1*10^4)/4500)*V1*(1-(Pn
        /P1)^((y-1)/(n(i)*y)));
19     mprintf('\n  %d',n(i));
20     mprintf('           %f',-W(i))

```

```
21 end
22 //end
```

Scilab code Exa 10.5 To find out the pressure between stages

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 10
3 //Compressor
4
5 //Example 10.5
6 clear all;
7 clc;
8
9 //Given
10 P1 = 1; //Initial pressure in Kgf/sq cm
11 P4 = 200; //Final pressure in Kgf/sq cm
12 n = 4; //no of stages
13
14 //To find out the pressure between stages
15 r = (P4/P1)^(1/n); //Compression ratio
16 P2 = r*P1;
17 mprintf('The pressure after 1st stage is %f Kgf/sq
    cm ',P2);
18 P3 = r*P2;
19 mprintf('\n The pressure after 2nd stage is %f Kgf/
    sq cm ',P3);
20 P4 = r*P3;
21 mprintf('\n The pressure after 3rd stage is %f Kgf/
    sq cm ',P4);
22 //end
```

Chapter 11

Liquefaction of Gases

Scilab code Exa 11.1 To Calculate the dryness fraction of exit stream and the ratio of upstream to downstream diameters

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 11
3 //Liquefaction of Gases
4
5 //Example 11.1
6 clear all;
7 clc;
8
9 //Given
10 P1 = 8.74; //Initial pressure in Kgf/sq cm
11 P2 = 2.41; //Final pressure in Kgf/sq cm
12 H1 = 327.13; //Enthalpy of inlet stream in Kcal/Kg
13 H2 = H1; //Enthalpy of exit stream in Kcal/Kg ,since
    throttling is isenthalpic
14 Hl = 26.8; //Enthalpy of liquid at the final
    condition in Kcal/Kg
15 Hg = 340.3; //Enthalpy of gas at the final condition
    in Kcal/Kg
16 vl = 152*10^-5; //Specific volume of liquid at the
    final condition in cubic meter/Kg
```



```

17 vg = 0.509; // Specific volume of gas at the final
    condition in cubic meter/Kg
18 v1 = 0.1494; // Initial specific volume in cubic meter
    /Kg
19
20 //To Calculate the dryness fraction of exit stream
    and the ratio of upstream to downstream diameters
21 // (i) Calculation of the dryness fraction of exit
    stream
22 // From equation 3.13(a) (page no 82)
23 x = (H2 - H1)/(Hg - H1);
24 mprintf('(i) The dryness fraction of the exit stream
    is %f', x);
25
26 // (ii) Calculation of the ratio of upstream to
    downstream pipe diameters
27 // From equation 3.13(b) (page no 82)
28 v2 = (v1*(1-x)) + (x*vg); // Total specific volume at
    the final condition in cubic meter/Kg
29 // u1 = u2; since KE changes are negligible
30 // From continuity equation: A2/A1 = D2^2/D1^2 = v2/
    v1 ; let required ratio, r = D2/D1;
31 r = (v2/v1)^(1/2);
32 mprintf('\n (ii) The ratio of upstream to downstream
    diameters is %f', r);
33 //end

```

Scilab code Exa 11.2 To Calculate the temperature of the throttled gas

```

1 // Chemical Engineering Thermodynamics
2 // Chapter 11
3 // Liquefaction of Gases
4
5 // Example 11.2
6 clear all;

```

```

7  clc;
8
9  //Given
10 P1 = 1000*1.033*10^4; //Initial pressure in Kgf/sq m
11 P2 = 1*1.033*10^4; //Final pressure in Kgf/sq m
12 T1 = 300; //Inital temperature in K
13 Cp = 7; //Specific heat of the gas in Kcal/Kgmole K
14 //Gas obeys the relation:  $v = (R*T)/P+(b*(T^2))$ 
15 b = 5.4392*10^-8; //in cubic meter/Kgmole K^2
16
17 //To Calculate the temperature of the throttled gas
18 //From equation (a) (page no 212); which we got after
    integration
19 T2 = 1/((1/T1)-((b/Cp)*((P2-P1)/427)));
20 mprintf('The throttled gas is cooled to %f K',T2);

```

Scilab code Exa 11.3 To Calculate the fraction of air liquified at steady state and temperature of air before throttling

```

1  //Chemical Engineering Thermodynamics
2  //Chapter 11
3  //Liquefaction of Gases
4
5  //Example 11.3
6  clear all;
7  clc;
8
9  //Given
10 //From the figure 11.8 (page no 216) & from figure A
    .2.7
11 H3 = 0;
12 H7 = -47; //in Kcal/Kg
13 H6 = -93; //in Kcal/Kg
14 H8 = 7; //in Kcal/Kg
15

```

```

16 //To Calculate the fraction of air liquified at
    steady state and temperature of air before
    throttling
17 //(i) Calculation of fraction of air liquified
18 //From equation 11.3 (page no 215)
19 x = (H8-H3)/(H8-H6);
20 fprintf('The fraction of air liquified is %f',x);
21
22 //(ii) Calculation of temperature
23 H4 = H3+(H7*(1-x))-(H8*(1-x)); //enthalpy of the gas
    before throttling
24 //From figure A.2.7 temperature corresponds to
    pressure 160 atm and the enthalpy H4 is
25 T = -112;
26 fprintf('\n The temperature of air before throttling
    is %d deg celsius ',T);
27 //end

```

Chapter 12

Refrigeration

Scilab code Exa 12.1 To Calculate the theoretical horse power required

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 12
3 //Refrigeration
4
5 //Example 12.1
6 clear all;
7 clc;
8
9 //Given
10 m = 500; //mass of ice produced per hour in Kg
11 T1 = 15; //Initial temperature of water
12 T2 = -5; //Final temperature of ice
13 Ci = 0.5; //Specific heat of ice in Kcal/Kg deg
    celsius
14 Cw = 1; //Specific heat of water in Kcal/Kg deg
    celsius
15 L_f = 79.71; //Latent heat of fusion in Kcal/Kg
16 Tf = 0; //Freezing point of ice in deg celsius
17
18 //To Calculate the theoretical horse power required
19 Q2 = m*(Cw*(T1-Tf)+L_f+Ci*(Tf-T2)); //Heat to be
```

```

    extracted per hour in Kcal
20 //From equation 12.1 (page no 220)
21 C.O.P = (T2+273)/((T1+273)-(T2+273));
22 W = Q2/C.O.P;//Work in Kcal/hr
23 W1 = W*(427/(60*4500));
24 mprintf('The therotical horse power required is %f
    hp',W1);
25 //end

```

Scilab code Exa 12.2 To Calculate the compressor load

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 12
3 //Refrigeration
4
5 //Example 12.2
6 clear all;
7 clc;
8
9 //Given
10 Ta = 298;//Initial temperature in K
11 Tb = 203;//Final temperature in k
12 T1 = 298;//Water temperature in K
13 n = 1;//Kgmole of CO2
14 //Cp = 5.89+0.0112T ; Specific heat of CO2 in Kcal/
    Kgmole K
15
16 //To Calculate the compressor load
17 //From equation 12.2a and b (page no 221)
18 function y = f(T)
19     y = ((T1-T)/T)*n*(5.89+0.0112*T);
20 endfunction
21 W = intg(Ta,Tb,f);
22 mprintf('The compressor load is %f Kcal/Kgmole',W);
23 //end

```

Scilab code Exa 12.3 To Calculate the COP mass of refrigerant required and compressor horse power required and the COP and compressor horse power for a reversed Carnot cycle

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 12
3 //Refrigeration
4
5 //Example 12.3
6 clear all;
7 clc;
8
9 //Given
10 //Consider the figure 12.4 (page no 226)
11 m = 5; //tonnes of refrigeration
12 T1 = 273-10; //temperature of the saturated vapour in
    K
13 T2 = 273+35; //temperature of the super heated vapour
    in K
14 T3 = 273+25; //temperature of the saturated liquid in
    K
15 T4 = 273+25; //temperature of the wet vapour in K
16 H1 = 341.8; //enthalpy of the saturated vapour in
    Kcal/Kg
17 H2 = 409.0; //enthalpy of the super heated vapour in
    Kcal/Kg
18 H3 = 350.0; //enthalpy of the saturated liquid in
    Kcal/Kg
19 H4 = 71.3; //enthalpy of the wet vapour in Kcal/Kg
20
21 //To Calculate the C.O.P, mass of refrigerant
    required , compressor horse power required and the
```

```

        C.O.P & compressor horse power for a reversed
        Carnot cycle
22 // (i) Calculation of the C.O.P of the compression
        cycle
23 // From equation 12.6 (page no 226)
24 C.O.P = (H1-H4)/(H2-H1);
25 fprintf('(i)C.O.P of the compression cycle is %f',C.
        O.P);
26
27 // (ii) Calculation of mass of refrigerant required
28 // From equation 12.7 (page no 226)
29 M = (m*50.4)/(H1-H4);
30 fprintf('\n (ii)The mass of refrigerant required is
        %f Kg/mt',M);
31
32 // (iii) Calculation of the compressor horse power
33 // From equation 12.5 (page no 226)
34 C_hp = (H2-H1)*M*(427/4500);
35 fprintf('\n (iii)The compressor horse power is %f hp
        ',C_hp);
36
37 // (iv) Calculation for reversed Carnot cycle
38 // From equation 12.1 (page no 220)
39 C.O.P = T1/(T3-T1);
40 fprintf('\n\n (iv)C.O.P for the reversed Carnot
        cycle is %f',C.O.P);
41 Q2 = m*50.4*(427/4500); // in hp
42 C_hp = Q2/C.O.P;
43 fprintf('\n      Compressor horse power for the
        reversed Carnot cycle is %f hp',C_hp);
44 //end

```

Scilab code Exa 12.4 To calculate the pressure in the tank and the amount of make up water required

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 12
3 //Refrigeration
4
5 //Example 12.4
6 clear all;
7 clc;
8
9 //Given
10 //Water at 20 deg cel is chilled to 10 deg cel by
    flash evaporation
11 Pv = 0.012;//Vapour pressure of water at 10 deg
    celsius in Kgf/sq.cm
12 H1 = 20.03;//Enthalpy of liquid water at 20 deg cel
    in Kcal/Kg
13 H2 = 10.4;//Enthalpy of liquid water at 10 deg cel
    in Kcal/Kg
14 Hv = 601.6;//Enthalpy of saturated vapour at 10 deg
    cel in Kcal/kg
15
16 //To calculate the pressure in the tank and the
    amount of make up water required
17 P = Pv;//pressure in the tank = vapour pressure of
    water
18 mprintf('The pressure in the tank is %f Kgf/sq.cm',P
    );
19 //From equation 12.8 (page no 234)
20 x = (H1-H2)/(Hv-H2);
21 mprintf('\n The amount of make up water required is
    %f Kg',x);
22 //end

```

Chapter 13

Thermodynamics in Phase Equilibria

Scilab code Exa 13.1 To Calculate the fugacity of N2 at 373K and 100 atm

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.1
6 clear all;
7 clc;
8
9 //Given
10 //N2 obeys the relation :  $Z = 1 + (2.11 \times 10^{-4} * P)$ 
11 Tc = 126; // Critical temperature in K
12 Pc = 33.5; // Critical pressure in atm
13 T = 373; //in K
14 P = 100; //in atm
15
16 //To Calculate the fugacity of N2 at 373K and 100
    atm
17 //(i) Using the Z relation given above
```

```

18 //From equation 13.12 (page no 239)
19 phi = %e^(2.11*10^-4*(P-0)); //fugacity coefficient
20 f = phi*P;
21 mprintf('(i)The fugacity of N2 using the given Z
    relation is %f atm',f);
22
23 //(ii)Using the fugacity chart given in figure A.2.9
24 Pr = P/Pc; //Reduced pressure in atm
25 Tr = T/Tc; //Reduced temperature in K
26 //From figure A.2.9,
27 phi = 1.04
28 f = phi*P;
29 mprintf('\n (ii)The fugacity of N2 using the
    fugacity chart is %f atm',f);
30 //end

```

Scilab code Exa 13.2 To Calculate the fugacity of liquid water

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.2
6 clear all;
7 clc;
8
9 //Given
10 P1 = 50*1.03*10^4; //Initial pressure in Kgf/sq m
11 T = 373; //Temperature in K
12 P2 = 1.03*10^4; //Final pressure in Kgf/sq m
13 V = 0.001*18; //Volume in cubic meter
14 R = 848; //gas constant in m Kgf/Kgmole K
15
16 //To Calculate the fugacity of liquid water
17 //From equation 13.13(page no 240)

```

```

18 del_u = (V/(R*T))*(P2-P1); //del_u = ln(f2/f1);
    Change in chemical potential
19 f1 = P2; //in Kgf/sq m
20 f2 = f1*(%e^del_u);
21 mprintf('The fugacity of the liquid water at 50 atm
    is %4.2e Kgf/sq m',f2);
22 //end

```

Scilab code Exa 13.3 To Calculate the bubble point pressure of the solution

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.3
6 clear all;
7 clc;
8
9 //Given
10 x1 = 0.1; //mole fraction of methane
11 x2 = 0.9; //mole fraction of propane
12 P = [28.1 31.6 35.1]; //Pressure in Kgf/sq cm are
13 K1 = [5.8 5.10 4.36]; //Vapourisation constants of
    methane at the corresponding pressures
14 K2 = [0.61 0.58 0.56]; //Vapourisation constants of
    propane at the correspondig pressures
15
16 //To Calculate the bubble point pressure of the
    solution
17 //From equation 13.27 (page no 245)
18 for i = 1:3
19     y1(i) = K1(i)*x1; //mole fraction of methane in
        the vapour phase
20     y2(i) = K2(i)*x2; //mole fraction of propane in

```

```

        the vapour phase
21     y(i) = y1(i)+y2(i); //sum of the mole fraction in
        the vapour phase
22 end
23 plot(P,y);
24 xtitle("y vs pressure","P","y");
25 P1 = interp1n([y';P],1); // in Kgf/sq cm
26 mprintf('The bubble point pressure of the solution
        is %f Kgf/sq cm',P1);
27 //end

```

Scilab code Exa 13.4 To Calculate the equilibrium data and compare with the experimental values

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.4
6 clear all;
7 clc;
8
9 //Given
10 T = [80.6 79.0 77.3 61.4]; //Various temperature in
        deg cel
11 x1 = [0.0 15.0 29.0 100.0]; //mole fraction of CHCl3
        in liquid phase
12 y1 = [0.0 20.0 40.0 100.0]; //mole fraction of CHCl3
        in vapour phase
13 P1 = [1370 1310 1230 700]; //Vapour pressure of CHCl3
        in mm Hg
14 P = 760; //Total pressure in mm Hg
15
16 //To Calculate the equilibrium data i.e y/x and
        compare with the experimental values

```

```

17 //From equation 13.27 (page no 245);K = y1/x1 = Pi/P
18 mprintf('Temperature      Experimental      Calculated');
19
20 for i = 1:4
21     mprintf('\n %f',T(i));
22     if x1(i) == 0
23         mprintf('      Not defined');
24     else
25     K_ex(i) = y1(i)/x1(i);
26 mprintf('      %f',K_ex(i));
27 end
28 K_c(i) = P1(i)/P;
29 mprintf('      %f',K_c(i));
30 end
31
32 if K_ex(i) == K_c(i)
33     then mprintf('\n\n The liquid solution is
34         perfect');
35 else
36     mprintf('\n\n The liquid solution is imperfect');
37     ;
38 end
39 //end

```

Scilab code Exa 13.5 Theoretical problem

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.5
6 clear all;
7 clc;
8
9 //Given

```

```
10 //The given example is a theoretical problem and
    does not contain any numerical computation
11 //end
```

Scilab code Exa 13.6 To Calculate the volume of 10 percent dichloromethane solution

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.6
6 clear all;
7 clc;
8
9 //Given
10 x1 = 0.1; //Mole fraction of dichloromethane (CCl2H2)
11 x2 = 0.9; //Mole fraction of methyl acetate (C3H6O2)
12 M1 = 85; //Molecular weight of CCl2H2
13 M2 = 74; //Molecular weight of C3H6O2
14 D1 = 1.3163; //Density of CCl2H2 in gm/cc
15 D2 = 0.9279; //Density of C3H6O2 in gm/cc
16
17 //To Calculate the volume of 10% dichloromethane
    solution
18 V1 = M1/D1; //Specific volume of pure CCl2H2 in cc/
    gmole
19 V2 = M2/D2; //Specific volume of C3H6O2 in cc/gmole
20 //From equation 13.62(page no 256)& 13.78 (page no
    257)
21 V_e = x1*x2*(1.2672-0.771*x1); //excess volume in cc/
    gmole
22 V = V1*x1+V2*x2+V_e;
23 mprintf('The volume of 10 percent dichloromethane is
    %f cc/gmole',V);
```

24 //end

Scilab code Exa 13.7 To Calculate the vapour pressure of the solution and bubble point at 686 mm Hg and the vapour composition at equilibrium

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.7
6 clear all;
7 clc;
8
9 //Given
10 x_T = 0.957; //mole fraction of Toluene
11 x_D = 0.043; //mole fraction of 1,2-dichloroethane
12 t = [90; 100; 110]; //temperature in deg cel
13 R = 1.98; //gas constant in Kcal/Kgmole K
14
15 //To Calculate the vapour pressure of the solution ,
    bubble point at 686 mm Hg and the vapour
    composition at equilibrium ,
16 //compare the experimental value of 91.2% toluene in
    vapour with the calculated value & calculate the
    free energy of mixing
17 //(1) Calculation of vapour pressure
18 mprintf(' (1)Temp(deg cel)      P_T(mmHg)          P_D(
    mmHg)          P_s(mmHg) ');
19 for i = 1:3
20     P_T(i) = 10^(6.95464-(1344.8/(219.482+t(i))))); //
        Given as equation(a)(page no 260)
21     P_D(i) = 10^(7.03993-(1274.079/(223+t(i))))); //
        Given as equation(b)(page no 260)
22     P_s(i) = x_T*P_T(i)+x_D*P_D(i); //pressure of the
        solution in mm Hg
```

```

23     mprintf( '\n    %f', t(i));
24     mprintf( '          %f', P_T(i));
25     mprintf( '          %f', P_D(i));
26     mprintf( '          %f', P_s(i));
27 end
28
29 //(2) Calculation of bubble point and comparison of
    values
30 clf;
31 plot(t, P_s);
32 xtitle("t vs P_s", "t", "P_s");
33 T = interp1n([P_s'; t'], 686);
34 P = 686; //pressure of solution in mm Hg
35 y_T_e = 0.912; //experimental value of mole fraction
    of toluene
36 //From the graph we found that the temperature at P
    = 686 mm Hg is
37 //t = 105.3; //in deg cel
38 mprintf( '\n\n(2) The bubble point is %f deg cel', T);
39 //From equation (a) (page no 260)
40 P_T = 10^(6.95464 - (1344.8 / (219.482 + T))); //vapour
    pressure of Toluene in mmHg
41 //From equation 13.27 (page no 245)
42 y_T_c = (x_T * P_T) / P;
43 y_D_c = 1 - y_T_c;
44 mprintf( '\n The vapour composition of toluene is %f
    ', y_T_c);
45 mprintf( '\n The vapour composition of 1,2-
    dichloroethane is %f', y_D_c);
46 e = ((y_T_e - y_T_c) / y_T_e) * 100;
47 mprintf( '\n The percentage error is %f percent', e);
48
49 //(3) Calculation of free energy
50 del_F = R * (T + 273) * ((x_T * log(x_T)) + (x_D * log(x_D)));
51 mprintf( '\n\n(3) The free energy of mixing is %f Kcal
    /Kgmole', del_F);
52 //end

```


Scilab code Exa 13.8 To Calculate the heating load required for the process

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.8
6 clear all;
7 clc;
8
9 //Given
10 //Consider the diagram shown in page no 263
11 w1 = 100; //weight of LiBr entered as feed in the
    evaporator per hour in Kg
12 x1 = 0.45; //weight fraction of LiBr entered as feed
13 x2 = 0; //weight fraction of steam in the LiBr soln
14 x3 = 0.65; //weight fraction of LiBr formed as
    product
15 H1 = -39; //Enthalpy of 45% solution at 25 deg cel in
    Kcal/Kg
16 H3 = -4.15; //Enthalpy of 65% solution at 114.4 deg
    cel in Kcal/Kg
17 H2 = 649; //Enthalpy of superheated steam at 100 mmHg
    and 114.4 deg cel in Kcal/Kg
18
19 //To Calculate the heating load required for the
    process
20 //According to material balance
21 w3 = (w1*x1)/x3; //weight of LiBr solution formed
    after evaporation per hour in Kg
22 w2 = w1-w3; // weight of steam formed in Kg/hr
23 //According to energy balance
24 Q = (w2*H2)+(w3*H3)-(w1*H1);
```

```
25 mprintf('The heat that has to be supplied for this
    concentration process is %f Kcal/hr ',Q);
26 //end
```

Scilab code Exa 13.9 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.9
6 clear all;
7 clc;
8
9 //Given
10 // In the given example, all the values were
    determined from the graph given as figure 13.9
    and it does not involve any numerical computation
11 //end
```

Scilab code Exa 13.10 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.10
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and
    does not involve any numerical computation
```

```
11 //end
```

Scilab code Exa 13.11 Theoretical problem

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.11
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and
    does not involve any numerical computation
11 //end
```

Scilab code Exa 13.12 To Calculate the partial pressure of toluene in the solution and check with the experimental value

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.12
6 clear all;
7 clc;
8
9 //Given
10 x_A = [0 0.0435 0.0942 0.1711 0.2403 0.3380 0.5981];
    //mole fraction of acetic acid
11 p_A = [0 17.2 30.5 46.5 57.8 69.3 95.7]; //partial
    pressure of acetic acid in mmHg
```

```

12 P_T1 = 202; //vapour pressure of toluene in mmHg
13 P_T2_ex = 167.3; //experimental partial pressure in
    mmmHg
14
15 //To Calculate the partial pressure of toluene in
    the solution and check with the experimental
    value
16 //From the equation 13.95,
17 //ln(P_T2/P_T1) = -intg(x_A/((1-x_A)*p_A))
18 for i = 1:7
19     if (p_A(i) ~= 0)
20         x(i) = (x_A(i)/((1-x_A(i))*p_A(i)))*10^4
21     end
22 end
23 plot(x,p_A);
24 xtitle(" ", "(x_A/((1-x_A)*p_A))*10^4", "p_A");
25 //Area of the graph drawn is
26 A = -0.138;
27 P_T2 = (%e^A)*P_T1;
28 e = ((P_T2-P_T2_ex)*100)/P_T2_ex;
29 mprintf('The partial pressure of toluene is %f mmHg'
    ,P_T2);
30 mprintf('\n This deviates %i percent from the
    reported value ',e);
31 //end

```

Scilab code Exa 13.13 To Check whether the activity coefficient of the solution can be represented by the Margules equation

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.13
6 clear all;

```

```

7  clc;
8
9  //Given
10 P = 760; //pressure at maximum boiling azeotrope of A
    and B in mmHg
11 x_A = 0.6; //mole fraction of A in liquid phase
12 x_B = 0.4; //mole fraction of B in liquid phase
13 p_A = 600; //vapour pressure of A at 90 deg cel
14 p_B = 300; //vapour pressure of B at 90 deg cel
15
16 //To Check whether the activity coefficient of the
    solution can be represented by the Margules
    equation
17 y_A = P/p_A; //Activity coefficient of A
18 y_B = P/p_B; //Activity coefficient of B
19 //From the Margules equation or equation (a) & (b)
20 U = [((x_B^2) - (2*(x_B^2)*x_A)) (2*(x_B^2)*x_A); (2*(
    x_A^2)*x_B) ((x_A^2) - (2*(x_A^2)*x_B))];
21 V = [log(y_A); log(y_B)];
22 W = U\V;
23 //Now the value of constants A and B in equations(a)
    &(b) are given as
24 A = W(1);
25 B = W(2);
26 //let us assume
27 x_A = [0.0 0.2 0.4 0.6 0.8 1.0];
28 x_B = [1.0 0.8 0.6 0.4 0.2 0.0];
29 //C = lny_A; D = lny_B; E = ln(y_A/y_B)
30 for i = 1:6
31     C(i) = (x_B(i)^2)*(2*(B-A)*x_A(i)+A);
32     D(i) = (x_A(i)^2)*(2*(A-B)*x_B(i)+B);
33     E(i) = C(i)-D(i);
34 end
35 clf;
36 plot(x_A,E);
37 xtitle(" ", "x_A", "ln(y_A/y_B)");
38 a = get("current_axes");
39 set(a, "x_location", "origin");

```

```

40 //Since the graph drawn is approximately symmetrical
    .Thus it satisfies the Redlich–Kister Test
41 mprintf('The activity coefficients of the system can
    be represented by Margules equation');
42 //end

```

Scilab code Exa 13.14 To Calculate the composition of the vapour evolved

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.14
6 clear all;
7 clc;
8
9 //Given
10 P = 760; //Total pressure of the mixture in mmHg
11 T = [80 90 95 100]; //Temperature in deg celsius
12 P1 = [87.4 129.0 162.0 187.0]; //vapour pressure of
    1,1,2,2-tetrachloroethane in mmHg
13 P2 = [356 526 648 760]; //Vapour pressure of water in
    mmHg
14
15 //To Calculate the composition of the vapour evolved
16 clf;
17 plot2d(T,P1,style=3);
18 plot2d(T,P2,style=5);
19 xtitle(" ", "Temp in deg cel", "Vapour pressure in
    mmHg");
20 legend("1,1,2,2-tetrachloroethane", "Water");
21 //From the graph we conclude that at 93.8 deg cel
22 P1 = 155; //in mm Hg
23 P2 = 605; //in mm Hg
24 y_1 = P1/P;

```

```

25 y_2 = P2/P;
26 mprintf('Mole fraction of 1,1,2,2-tetrachloroethane
    in vapour is %f',y_1);
27 mprintf('\n Mole fraction of water in vapour is %f',
    y_2);
28 //end

```

Scilab code Exa 13.15 To plot a graph between temperature and vapour phase composition

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.15
6 clear all;
7 clc;
8
9 //Given
10 T = [146.2 142.3 126.1 115.9 95.0 98.0 100]; //
    Temperature in deg cel
11 P1 = [760.0 685.0 450.3 313.0]; //Vapour pressure of
    1,1,2,2-tetrachloroethane at the coressponding
    temperature in mm Hg
12 P2_5 = 648.0; //Vapour pressure of water at 95 deg
    cel in mm Hg
13 P2_6 = 711.0; //Vapour pressure of water at 98 deg
    cel in mm Hg
14 P = 760; //Total pressure of mixture in mm Hg
15
16 x1 = [0 0 0 0 0 0 0];
17 //To plot a graph between temperature and vapour
    phase composition
18 for i = 1:4
19     x1(i) = P1(i)/P; //mole fraction of 1,1,2,2-

```

```

                tetrachloroethane
20 end
21 x2_5 = P2_5/P; //mole fraction of water at 95 deg cel
22 x2_6 = P2_6/P; //mole fraction of water at 98 deg cel
23 x1(5) = 1-x2_5;
24 x1(6) = 1-x2_6;
25
26 clf;
27 plot(x1,T);
28 xtitle("","mole fraction of 1,1,2,2-
        tetrachloroethane","Temperature in deg cel");
29 mprintf('The required graph has been plotted in the
        graphic window');
30 //end

```

Scilab code Exa 13.16 To Calculate the heat of vapourization of toluene by using ideal gas law and second virial coefficient but neglecting v_l and including v_l

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.16
6 clear all;
7 clc;
8
9 //Given
10 //B = -(1.203*10^10)*(T^2.7); second virial
    coefficient, T is in K
11 //log P = 6.95464-(1344.8/(219.482+t)) ... (a); Vapour
    pressure of toluene
12 t = 107.2; //Temperature in deg cel
13 T = t+273.16; //in K
14 H_ex = 7964; //experimental value of heat of

```



```

    vapourisation in Kcal/Kgmole
15 d = 800; //density of liquid toluene in Kg/cubic
    meter
16 R = 1.98; //gas constant in Kcal/Kgmole K
17 M = 92.14; //molecular weight of toluene
18
19 //To Calculate the heat of vapourization of toluene
    by using ideal gas law, second virial coefficient
    but neglecting vl and including vl
20 //From equation (a), let  $K = d\log P/dT$ 
21  $K = 1344.8/(219.482+t)^2$ ;
22 //(i)Using ideal gas behaviour
23 //From equation 13.112(page no 286)
24  $H_c = (2.303*R*(T^2))*K$ ;
25 mprintf('(i)The heat of vapourization using ideal
    gas behaviour is %f Kcal/Kgmole',H_c);
26  $D = ((H_c-H_{ex})/H_c)*100$ ;
27 mprintf('\\n    The deviation is %f percent',D);
28
29 //(ii)Using second virial coeff but neglecting vl
30 //From equation(a)
31  $P = 10^{(6.95464-1344.8/(219.482+t))}$ ; //in mm Hg
32  $P1 = P*1.033*10^4/760$ ; //in Kgf/sq m
33  $B = -((1.203*10^{10})/(T^{2.7}))*10^{-3}$ ; //in cubic meter/
    Kgmole
34 //From equation 13.111 (page no 286) neglecting vl,
35  $l = (R*T)+((B*P1)/427)$ ; //in Kcal/Kgmole
36  $H_c = K*2.303*T*1$ ;
37 mprintf('\\n\\n(ii)The heat of vapourisation using
    second virial coefficient but neglecting vl is %f
    Kcal/Kgmole',H_c);
38  $D = ((H_c-H_{ex})/H_c)*100$ ;
39 mprintf('\\n    The deviation in this case is %f
    percent',D);
40
41 //(iii)Using second virial coeff including vl
42  $vl = M/d$ ; //Liquid specific volume in cubic meter/
    Kgmole

```

```

43 n = P1*v1/427; //in Kcal/Kgmole
44 H_c = K*2.303*T*(1-n);
45 mprintf('\n\n(iii)The heat of vapourisation using
    second virial coefficient including v1 is %f Kcal
    /Kgmole',H_c);
46 D = ((H_c-H_ex)/H_c)*100;
47 mprintf('\n    The deviation in this case is %f',D)
    ;
48 //end

```

Scilab code Exa 13.17 To Calculate the heat of vapourisation of water by Vishwanath and Kuloor method and by Riedel method and compare with the experimental value

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.17
6 clear all;
7 clc;
8
9 //Given
10 H_ex = 539; //Heat of vapoization of water in Kcal/Kg
11 Tc = 647; //Critical temperature in K
12 Pc = 218; //Critical pressure in atm
13 Tb = 373; //Boiling point of water in K
14 t = 100; //temperature in deg cel
15 M = 18; //Molecular weight of water
16 P = 1; //pressure at boiling point in atm
17 P1 = 1.033*10^4; //pressure in Kgf/sq m
18
19 //To Calculate the heat of vapourisation of water by
    Vishwanath and Kuloor method and by Riedel's
    method and compare with the experimental value

```

```

20 // (i) Using Vishwanath and Kuloor method
21 H_c = (4.7*Tc*((1-(P/Pc))^0.69)*log(P/Pc))/((1-(Tc/
    Tb))*18);
22 mprintf('(i)The heat of vapourisation of water using
    Vishwanath and Kuloor method is %f Kcal/Kg',H_c)
    ;
23 D = (H_c-H_ex)*100/H_c;
24 mprintf('\n    The deviation occurs using this
    method is %f percent',D);
25
26 //(ii)Using Riedel's method
27 H_c = (Tb*2.17*(log(218)-1))/((0.93-(Tb/Tc))*18);
28 mprintf('\n\n(ii)The heat of vapourisation of water
    using Riedel method is %f Kcal/Kg',H_c);
29 D = (H_c-H_ex)*100/H_c;
30 mprintf('\n    The deviation occurs using this
    method is %f percent',D);
31
32 //(iii)By using given vapour equation; logP =
    8.2157-(2218.8537/(273.16+t)), t is in deg cel
33 //From steam table,
34 Vv = 1.673;//in cubic meter/Kg
35 V1 = 0.001;//in cubic meter/Kg
36 H_c = (2218.8/(273.16+t)^2)*(2.3*Tb*P1*(Vv-V1)/427);
37 mprintf('\n\n(iii)The heat of vapourisation using
    the given vapour equation is %f Kcal/Kg',H_c);
38 D = (H_c-H_ex)*100/H_c;
39 mprintf('\n    The deviation occurs using this
    method is %f percent',D);
40 //end

```

Scilab code Exa 13.18 To Calculate the latent heat of saturated ethane at 0 deg cel

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.18
6 clear all;
7 clc;
8
9 //Given
10 T1 = 273-87;//temp in K
11 T2 = 273;//temp in K
12 H1 = 115;//Latent heat of saturated ethane at 1 atm
    and -87 deg cel in Kcal/Kg
13 H2_ex = 72.44;//Experimental value of latent heat at
    0 deg cel in Kcal/Kg
14 Tc = 306;//Critical temperature in K
15 M = 30;//Molecular weight of ethane
16
17 //To Calculate the latent heat of saturated ethane
    at 0 deg cel
18 Tr1 = T1/Tc;//reduced temp in K
19 Tr2 = T2/Tc;//reduced temp in K
20 //(i)Using Watson's method:
21 H2_c = H1*((1-Tr2)/(1-Tr1))^0.38;
22 mprintf('(i)The latent heat of saturated ethane at 0
    deg cel using Watson method is %f Kcal/Kg',H2_c);
23 D = (H2_ex-H2_c)*100/H2_ex;
24 mprintf('\n The deviation occurs using this method
    is %f percent',D);
25
26 //(ii)Using Vishwanath and Kuloor method
27 //From equation 13.117 (page no 289)
28 n = (0.00133*(H1*M/T1)+0.8794)^(1/0.1);
29 H2_c = H1*((1-Tr2)/(1-Tr1))^n;
30 mprintf('\n\n(ii)The latent heat of saturated ethane
    at 0 deg cel using Vishwanath and Kuloor method
    is %f Kcal/Kg',H2_c);
31 D = (H2_ex-H2_c)*100/H2_ex;

```

```

32 mprintf('\n The deviation occurs using this method
    is %f percent ',D);
33 //end

```

Scilab code Exa 13.19 To calculate the latent heat of the solution and compare it with the one which calculated from the given vapour pressure equation

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 13
3 //Thermodynamics in Phase Equilibria
4
5 //Example 13.19
6 clear all;
7 clc;
8
9 //Given
10 H_s_ex = 32.7; //experimental value of latent heat of
    the solution in KJ/mole
11 x1 = 0.536; //mole percent of toluene in the solution
12 x2 = 1-0.536; //mole percent of 1,1,1-trichloroethane
    in the solution
13 H1 = 33.34; //Latent heat of toluene in KJ/gmole
14 H2 = 29.72; //Latent heat of 1,1,1-trichloroethane in
    KJ/gmole
15 He = 0; //excess enthalpy is neglected
16 Cp1 = 39.55; //Specific heat of toluene in cal/gmole
    deg cel
17 Cp2 = 24.62; //Specific heat of 1,1,1-trichloroethane
    in cal/gmole deg cel
18 T_D = 100; //dew point temperature in deg cel
19 T_B = 92.6; //bubble point temperature in deg cel
20
21 //To calculate the latent heat of the solution and
    compare it with the one which calculated from the

```

```

        given vapour pressure equation
22 // (i) Calculation of latent heat of the solution
23 // From equation 13.118 (page no 291)
24 H_s = H1*x1+H2*x2+He+(Cp1*x1+Cp2*x2)*10^-3*4.17*(T_D
    -T_B);
25 fprintf('(i)The latent heat of the solution is %f KJ
    /gmole ',H_s);
26 D = ((H_s_ex-H_s)*100)/H_s_ex;
27 fprintf('\n    The deviation occurs using this
    method is %f percent ',D);
28
29 // (ii) Calculation of latent heat from the vapour
    pressure equation
30 // From equation (a) (page no 291)
31 K = 1657.599/((273.16+5)^2);
32 H_s = (K*2.303*8.314*(273.16+5)^2)*10^-3;
33 fprintf('\n\n(ii)The latent heat of the solution is
    %f KJ/gmole ',H_s);
34 D = ((H_s_ex-H_s)*100)/H_s_ex;
35 fprintf('\n    The deviation occurs using this
    method is %f percent ',D);
36 //end

```

Chapter 14

Thermodynamics of Chemical Reactions

Scilab code Exa 14.1 To Calculate the standard heats of reaction at 25 deg celsius

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.1
6 clear all;
7 clc;
8
9 //Given
10 H_f_C2H4 = 12500; //Standard heat of formation of
    ethylene at 25 deg cel in Kcal/Kgmole
11 H_f_C2H4O = -11667; //Standard heat of formation of
    ethylene oxide at 25 deg cel in Kcal/Kgmole
12
13 //To Calculate the standard heats of reaction at 25
    deg celsius
14 //The reaction is: C2H4 + (1/2)O2 -> C2H4O
15 del_H_rxn = H_f_C2H4O - H_f_C2H4; //Since , Standard
```

```

    heat of formation of O2 is zero
16 mprintf('The standard heats of reaction at 25 deg
    celsius is %d Kcal/Kgmole',del_H_rxn);
17 //end

```

Scilab code Exa 14.2 To Calculate the sensible heat required

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.2
6 clear all;
7 clc;
8
9 //Given
10 T1 = 25+273;//Initial temperature in K
11 T2 = 450+273;//Final temperature in K
12 //Specific heat of sulphur dioxide is given by the
    relation:
13 //Cp = 7.116+9.512*10-3*T+(3.511*10-6)*T2
14
15 //To Calculate the sensible heat required
16 //Basis: 1 Kgmole of sulphur dioxide
17 Q = 7.116*(T2-T1)+(9.512*10-3*(T22-T12)/2)
    +((3.51*10-6)*(T23-T13)/3);
18 mprintf('Sensible heat required is %d Kcal/Kgmole',Q
    );
19 //end

```

Scilab code Exa 14.3 To Calculate the heat must be removed if the product temperature should not exceed 260 deg cel


```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.3
6 clear all;
7 clc;
8
9 //Given
10 H_C2H4 = 12500; //Standard heat of formation of
    ethylene at 25 de cel
11 H_C2H4O = -12190; //Standard heat of formation of
    ethylene oxide at 25 deg cel
12 H_CO2 = -94052; //Standard heat of formation of CO2
    at 25 deg cel
13 H_H2O = -57798; //Standard heat of formation of H2O
    at 25 deg cel
14 T1 = 200; //temperature at which mixture entered in
    deg cel
15 Ti = 25; //intermediate temperature in deg cel
16 T2 = 260; //product temperature in deg cel
17 Cp_air_a = 7; //Mean specific heat for 25 to 200 deg
    cel in Kcal/Kgmole
18 Cp_C2H4_a = 18; //Mean specific heat for 25 to 200
    deg cel in Kcal/Kgmole
19 //Mean specific heat for 25 to 260 deg cel in Kcal/
    Kgmole are given as:
20 Cp_C2H4_b = 19;
21 Cp_C2H4O_b = 21;
22 Cp_O2_b = 7.30;
23 Cp_N2_b = 7.00;
24 Cp_CO2_b = 10.00;
25 Cp_H2O_b = 8.25;
26 //Basis: 1 Kgmole of ethylene as feed
27 n_air = 9; //Kgmoles
28 n_C2H4 = 1; //Kgmoles
29 n_C2H4_1 = 0.6 //ethylene consumed while converting
    in C2H4O in Kgmoles (Rxn 1)

```

```

30 n_C2H4_2 = 0.3; //ethylene burnt completely to CO2 in
    Kgmoles (Rxn 2)
31
32 //To Calculate the heat must be removed if the
    product temperature should not exceed 260 deg cel
33 n_O2 = n_air*0.21; //Kgmoles of O2 fed
34 n_N2 = n_air-n_O2; //Kgmoles of N2 fed
35 //Rxn 1: (0.6)C2H4 + (0.3)O2 - (0.6)C2H4O;...( i) 60%
    of C2H4 is converted to C2H4O
36 n_O2_1 = n_C2H4_1/2; //Kgmoles of oxygen consumed
37 n_C2H4O_1 = n_C2H4_1; //C2H4O formed in Kgmoles
38 //Rxn 2: (0.3)C2H4 + (0.9)O2 - (0.6)CO2+ (0.6)H2O
    ;...( ii) 30%conversion
39 n_O2_2 = 3*n_C2H4_2; //Kgmoles of O2 reacted
40 n_CO2_2 = 2*n_C2H4_2; //Kgmoles of CO2 formed
41 n_H2O_2 = 2*n_C2H4_2; //Kgmoles of H2O formed
42 n_C2H4_r = n_C2H4 - n_C2H4_1 - n_C2H4_2; //unreacted
    ethylene in Kgmoles
43 n_O2_r = n_O2 - n_O2_1-n_O2_2; //unreacted O2 in
    Kgmoles
44 //The overall rxn is given by (i)&(ii),
45 //(0.9)C2H4 + (1.2)O2 - (0.6)C2H4O + (0.6)CO2 +
    (0.6)H2O...( iii)
46 del_H = (0.6*H_C2H4O)+(0.6*H_CO2)+(0.6*H_H2O)-(0.9*
    H_C2H4); //since ,standard enthalpy of O2 is zero;
    Standard heat of rxn in Kcal/Kgmole
47 Q1 = (n_C2H4*Cp_C2H4_a + n_air*Cp_air_a)*(Ti-T1); //
    Sensible heat in feed in Kcal
48 Q2 = (n_C2H4_r*Cp_C2H4_b + n_C2H4O_1*Cp_C2H4O_b +
    n_CO2_2*Cp_CO2_b + n_H2O_2*Cp_H2O_b + n_O2_r*
    Cp_O2_b + n_N2*Cp_N2_b)*(T2-Ti); //Sensible heat
    in product in Kcal
49 Q = Q1+Q2+del_H;
50 mprintf('The heat to be removed is %f Kcal so that
    the product temperature is 260 deg celsius ',-Q);
51 //end

```

Scilab code Exa 14.4 To Calculate the theoretical flame temperature when both air and CO₂ enter at 95 deg celsius

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.4
6 clear all;
7 clc;
8
9 //Given
10 //Basis: 1Kgmole of C0
11 //CO + (1/2)O2 - CO2
12 //When mixture entered ,their compositions are given
    as:
13 n_C0 = 1; //Kgmole
14 del_H = -67636; //Standard heat of reaction in Kcal/
    Kgmole at 25 deg cel
15 T1 = 95; //Temperature at which mixture entered in
    deg celsius
16 T2 = 25; //Intermediate temperature in deg celsius
17 //Mean specific heat values for the temperature
    between 25 and 95 deg celsius in Kcal/Kgmole are
    given as (from figure 14.4)(page no 303)
18 Cpm_CO = 6.95;
19 Cpm_O2 = 7.1;
20 Cpm_N2 = 6.95;
21
22 //To Calculate the theoretical flame temperature
    when both air and CO2 enter at 95 deg celsius
23 n_O2 = 1; //Kgmole, as 100% excess air is given
24 n_N2 = n_O2*(0.79/0.21); //Kgmole
25 //After the rxn:
```

```

26 n_CO2 = n_CO; //Kgmole
27 n_O2_r = n_O2-(n_CO/2); //remaining Kgmole of O2
28 //In equation 14.18 (page no 307) say: H2-HR = Ha,
    HP-H3 = Hb, Hc = del_H+Ha & Ht = Hc+Hb
29 Ha = (n_CO*Cpm_CO + n_O2*Cpm_O2 + n_N2*Cpm_N2)*(T2-
    T1); //in Kcal/Kgmole
30 Hc = del_H+Ha; //in Kcal/Kgmole
31 //For calculating Hb let us assume the temperature
    as
32 T = [530 1000 1650]; //in deg celsius
33 Cpm_CO2 = [10.85 12 12.75]; //Mean specific heat of
    CO2 at the coresspondig temperature (from figure
    14.4)
34 Cpm_O2 = [7.55 7.8 8.3]; //Mean specific heat of O2
    at the coresspondig temperature (from figure
    14.4)
35 Cpm_N2 = [7.15 7.5 7.85]; //Mean specific heat of N2
    at the coresspondig temperature (from figure
    14.4)
36 for i = 1:3
37     Hb(i) = (n_CO2*Cpm_CO2(i)+n_O2_r*Cpm_O2(i)+n_N2*
        Cpm_N2(i))*(T(i)-T2); //in Kcal/Kgmole
38     Ht(i) = Hc+Hb(i); //in Kcal/Kgmole
39 end
40 clf;
41 plot(T,Ht);
42 xtitle(" ", "Temperature, deg celsius", "Ht in Kcal/
    Kgmole");
43 a = get("current_axes");
44 set(a, "x_location", "origin");
45 Tf = interp1n([Ht';T],0);
46 mprintf('The adiabatic temperature is read as %d
    degree celsius ',Tf);
47 //end

```

Scilab code Exa 14.5 To Calculate the standard free energy for the reaction

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.5
6 clear all;
7 clc;
8
9 //Given
10 T = 298; //Temperature in Kelvin
11 //Standard enthalpy in Kcal/Kgmole of the following
    components at 298 K are given as
12 H_SO2 = -70960;
13 H_SO3 = -94450;
14 H_O2 = 0;
15 //Standard entropy in Kcal/Kgmole K of the following
    components at 298 K are given as
16 S_SO2 = 2.48;
17 S_SO3 = -19.7
18 S_O2 = 0;
19 //Basis: 1 Kgmole of SO2
20 //SO2 +(1/2)O2 - SO3
21
22 //To Calculate the standard free energy for the
    reaction
23 n_SO2 = 1; //Kgmole of SO2 fed
24 n_O2 = (1/2)*2; //Kgmole of O2 fed as 100% excess O2
    is given
25 n_SO3 = n_SO2; //Kgmole of SO3 formed
```

```

26 //From equation 14.38 (page no 312)
27 del_F = (H_S03-(T*S_S03))-(H_S02-(T*S_S02))-(H_O2-(T
    *S_O2));
28 mprintf('The standard free energy for the reaction
    at 25 degree celsius is %f Kcal/Kgmole',del_F);
29 //end

```

Scilab code Exa 14.6 To show the variation of the standard heats of reaction with temperature and the equilibrium constant with temperature graphically in the given temperature range

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.6
6 clear all;
7 clc;
8
9 //Given
10 //SO2 + (1/2)O2 - SO3
11 //Basis: 1 Kgmole of SO2
12 n_S02 = 1; // SO2 fed in Kgmole
13 //From table 14.1 (page no 301)
14 //alpha values for the following components are
    given as
15 a_S02 = 7.116;
16 a_O2 = 6.148;
17 a_S03 = 6.077;
18 //beta values for the following components are given
    as
19 b_S02 = 9.512*10^-3;
20 b_O2 = 3.102*10^-3;
21 b_S03 = 25.537*10^-3;
22 //Standard enthalpy of the following components at

```

```

    25 deg cel in Kcal/Kgmole are given as
23 H_S02 -70960;
24 H_O2 = 0;
25 H_S03 = -94450;
26 //Standard free energy of the following components
    at 25 deg cel in Kcal/Kgmole K are given as
27 F_S02 = -71680;
28 F_O2 = 0;
29 F_S03 = -88590;
30 n_O2 = n_S02; //O2 fed in Kgmole; since 50 mole
    percent mixture of SO2 & O2 is fed
31 n_S03 = n_S02; //SO3 formed in Kgmole
32 n_O2_e = n_O2 - (n_O2/2); //Kgmoles of O2 in exit gas
33 n_O2_r = n_O2/2; //Kgmoles of O2 reacted
34 R = 1.98; //gas constant in Kcal/Kgmole K
35
36 //To show the variation of the standard heats of
    reaction with temperature and the equilibrium
    constant with temperature graphically in the
    given temperature range
37 //(i) Variation of the standard heats of reaction
    with temperature
38 del_H = (n_S03*H_S03) - (n_O2_r*H_O2) - (n_S02*H_S02); //
    in Kcal/Kgmole
39 del_F = (n_S03*F_S03) - (n_O2_r*F_O2) - (n_S02*F_S02); //
    in Kcal/Kgmole
40 //From equation 14.10 (page no 301)
41 del_a = (n_S03*a_S03) - (n_O2_r*a_O2) - (n_S02*a_S02);
42 del_b = (n_S03*b_S03) - (n_O2_r*b_O2) - (n_S02*b_S02);
43 //In equation 14.11 (page no 302), substituting
    del_H at
44 T = 298; //in deg cel
45 I = del_H - del_a*T - (del_b*(T^2)/2); // integrating
    constant
46 mprintf('(i)The standard heat of reaction at any
    temperature can be calculated by the relation:')
    ;
47 mprintf('\n    del_Ht = %fT + %fT^2 %f', del_a, del_b

```

```

    /2,I);
48
49 //(ii)Variation of the equilibrium constant with
    temperature
50 //K1 = lnKa (say)
51 K1 = -del_F/(R*T);
52 //From equation 14.42 (page no 316); M1 = M/R (say)
53 M1 = K1-(del_a/R)*log(T)-(del_b/(2*R))*T+(I/(T*R));
54 //Let us assume the temperature in the range 800K to
    1500K as
55 Ta = [700 800 825 850 900 1000 1100 1300 1500];
56 for i = 1:9
57     Ka(i) = %e^((del_a/R)*log(Ta(i))+(del_b*Ta(i)
        /(2*R))-(I/(Ta(i)*R))+M1);
58 end
59 clf;
60 plot(Ta,Ka);
61 xtitle(" ", "Temperature in K", "equilibrium constant
    K");
62 mprintf('\n\n(ii)From the graph it can be seen that
    as temperature increases Ka decreases
    exponentially,so the reaction is exothermic. ');
63 //end

```

Scilab code Exa 14.7 To Calculate the conversion of SO₂ to SO₃ at 1atm and at various temperature

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.7
6 clear all;
7 clc;
8

```



```

9 //Given
10 //SO2 + (1/2)O2 - SO3
11 //Basis: 1 Kgmole of SO2
12 n_SO2 = 1; // SO2 fed in Kgmole
13 n_O2 = n_SO2; //O2 fed in kgmole
14
15 //To Calculate the conversion of SO2 to SO3 at 1atm
    and at various temperature
16 //(1) Calculate the conversion of SO2 to SO3
17 P = 1; //Pressure in atm
18 T = 850; //Temperature in K
19 m = 1-1-(1/2);
20 //From example 14.6
21 Ta = [700 800 825 850 900 1000 1100 1300 1500];
22 Ka = [395.40 52.51 34.60 23.44 11.59 3.527 1.48
    0.398 0.0016];
23 clf;
24 xset('window',2);
25 plot2d(Ta,Ka,style=3);
26 xtitle("Equilibrium constant vs Temperature",
    Temperature in K","Ka");
27 Ka1 = interp1n([Ta;Ka],850);
28 //Let Nc be the moles of SO3 at equilibrium
29 Nc = [0.1 0.2 0.3 0.4 0.5 0.7 0.8 0.9 0.930 0.95
    0.98 0.988 0.989 0.9895 0.9897 0.9899 0.9900];
30 //From equation 14.49 (page no 320) and using the
    given data ,we got equation (b) (page no 323)
31 for i = 1:17
32     Ka(i) = (((n_SO2+n_O2-0.5*Nc(i))/(n_O2-0.5*Nc(i))
        )^(1/2))*(Nc(i)/(n_SO2-Nc(i)));
33 end
34 xset('window',1);
35 plot2d(Nc,Ka,style=2);
36 xtitle("Equilibrium constant vs Kgmole of SO3",
    moles of SO3","Ka");
37 Nc1 = interp1n([Ka;Nc],Ka1);
38 C = Nc1*100/n_SO2;
39 mprintf('(1)The conversion of SO2 to SO3 at 1atm and

```

```

850K is %f percent ',C);
40
41 //(2) Calculation of conversion at 1 atm and 850 K
    under the following conditions
42 //(i) Given:
43 n_N2 = 3.75; //Kgmol of N2 fed
44 //Let Nc be the moles of SO3 at equilibrium
45 Nc = [0.85 0.87 0.90];
46 //From equation 14.49 (page no 320) and using the
    given data ,we got equation (c) (page no 324)
47 for i = 1:3
48     Ka2(i) = (((+n_N2+n_SO2+n_O2-0.5*Nc(i))/(n_O2
        -0.5*Nc(i)))^(1/2))*(Nc(i)/(n_SO2-Nc(i)));
49 end
50 xset('window',1);
51 plot2d(Nc,Ka2,style=5);
52 Nc2 = interp1n([Ka2';Nc],Ka1);
53 C2 = Nc2*100/n_SO2;
54 mprintf('\n\n (2)(i)The conversion of SO2 to SO3 at
    1 atm and 850 K when inert gas is also added is
    %f percent ',C2);
55
56 //(ii)SO3 is also sent along the original feed
57 n_SO3 = 1; //Kgmol of SO3 fed
58 //Let Nc be the moles of SO3 at equilibrium
59 Nc = [0.80 0.86 0.92];
60 //From equation 14.49 (page no 320) and using the
    given data ,we got equation (d) (page no 326)
61 for i = 1:3
62     Ka3(i) = (((+n_SO3+n_SO2+n_O2-0.5*Nc(i))/(n_O2
        -0.5*Nc(i)))^(1/2))*((n_SO3+Nc(i))/(n_SO2-Nc(
        i)));
63 end
64 xset('window',1);
65 plot2d(Nc,Ka3,style=6);
66 Nc3 = interp1n([Ka3';Nc],Ka1);
67 C3 = Nc3*100/n_SO2;
68 mprintf('\n    (ii)The conversion of SO2 to SO3 at 1

```

```

        atm and 850 K when SO3 is also added along the
        original feed is %f percent',C3);
69
70 //(iii)Variation of SO2 to O2 ratio:
71 //(a)SO2:O2 = 1:1 ; This has been worked out in part
    1
72 mprintf('\\n    (iii)(a)The conversion of SO2 to SO3
        at 1atm and 850K when SO2:O2 = 1:1 is %f percent'
        ,C);
73 Xc = Nc1/(n_SO2+n_O2-0.5*Nc1);
74
75 //(b)SO2:O2 = 1.1:0.5 ,Now
76 n_SO2 = 1.1;//Kgmol of SO2 fed
77 n_O2 = 0.5;//Kgmol of O2 fed
78 //Let Nc be the moles of SO3 at equilibrium
79 Nc = [0.9 0.91 0.92];
80 //From equation 14.49 (page no 320) and using the
        given data ,we got equation (e) (page no 327)
81 for i = 1:3
82         Ka4(i) = (((n_SO2+n_O2-0.5*Nc(i))/(n_O2-0.5*
                Nc(i)))^(1/2))*(Nc(i)/(n_SO2-Nc(i)));
83 end
84 xset('window',1);
85 plot2d(Nc,Ka4,style=1);
86 Nc4 = interpl([Ka4';Nc],Ka1);
87 C4 = Nc4*100/n_SO2;
88 mprintf('\\n    (iii)(b)The conversion of SO2 to SO3
        at 1atm and 850K when SO2:O2 = 1.1:0.5 is %f
        percent',C4);
89 Xc1 = Nc4/(n_SO2+n_O2-0.5*Nc4);
90
91 //(c)SO2:O2 = 1:0.5
92 n_SO2 = 1;//Kgmol of SO2 fed
93 n_O2 = 0.5;//Kgmol of O2 fed
94 //Let Nc be the moles of SO3 at equilibrium
95 Nc = [0.8 0.85 0.86 0.87];
96 //From equation (a)
97 for i = 1:4

```

```

98     Ka5(i) = (((n_SO2+n_O2-0.5*Nc(i))/(n_O2-0.5*Nc(i)
          )))^(1/2))*(Nc(i)/(n_SO2-Nc(i)));
99 end
100 xset('window',1);
101 plot2d(Nc,Ka5,style=4);
102 Nc5 = interp1n([Ka5';Nc],Ka1);
103 C5 = Nc5*100/n_SO2;
104 mprintf('\n    (iii)(c)The conversion of SO2 to SO3
          at 1atm and 850K when SO2:O2 = 1:0.5 is %f
          percent',C5);
105 Xc2 = Nc5/(n_SO2+n_O2-0.5*Nc5);
106
107 if(Xc2>Xc) and (Xc2>Xc1)
108     mprintf('\n          SO2:O2 = 1:0.5 gives the
          maximum concentration of SO3 at equilibrium.'
          );
109 else
110     if(Xc1>Xc) and (Xc1>Xc2)
111         mprintf('\n          SO2:O2 = 1.1:0.5 gives
          the maximum concentration of SO3 at
          equilibrium');
112     else
113         if(Xc>Xc1) and (Xc>Xc2)
114             mprintf('\n          SO2:O2 = 1:1 gives
          the maximum concentration of SO3 at
          equilibrium');
115         end
116     end
117 end
118
119 //(3) Conversion of SO2 to SO3 at 50 atm and 850 K
          when SO2:O2 = 1:1
120 n_SO2 = 1;//Kgmole of SO2 fed
121 n_O2 = 1;//Kgmoles of O2 fed
122 P = 50;//Pressure in atm
123 //From figure A.2.9
124 phi_SO2 = 0.99;
125 phi_SO3 = 0.972;

```

```

126 phi_02 = 1;
127 //From equation 14.48 (page no320), Ka = Ky*(P^m)*
      K_phi
128 K_phi = phi_SO3/(phi_SO2*(phi_02^2));
129 //Let Nc be the moles of SO3 at equilibrium
130 Nc = [0.99 0.985 0.97 0.96];
131 for i = 1:4
132     Ka6(i) = K_phi*(P^m)*(((n_SO2+n_O2-0.5*Nc(i))/(
          n_O2-0.5*Nc(i)))^(1/2))*(Nc(i)/(n_SO2-Nc(i)))
          );
133 end
134 xset('window',1);
135 plot2d(Nc,Ka6,style=3);
136 Nc6 = interpln([Ka6';Nc],Ka1);
137 C = Nc6*100/n_SO2;
138 mprintf('\n\n (3)The conversion of SO2 to SO3 at 50
          atm and 850K when SO2:O2 = 1:1 is %f percent',C)
          ;
139 legend("1 part", "2.(i) part", "2.(ii)part", "2.(iii).(
          b)part", "2.(iii).(c)part", "3 part");
140 //end

```

Scilab code Exa 14.8 Theoretical problem

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.8
6 clear all;
7 clc;
8
9 //Given
10 //The given example is a theoretical problem and it
      does not involve any numerical computation.

```

11 //end

Scilab code Exa 14.9 To find out the equilibrium has been attained or not
If not then calculate the equilibrium composition and also find out whether
the equilibrium composition will change or not if pressure were increased to
3 atm

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.9
6 clear all;
7 clc;
8
9 //Given
10 //2A(g) - B(g)+C(g)
11 T = 400; //Temperature in Kelvin
12 P = 1; //Pressure in atm
13 R = 1.98; //gas constant in Kcal/Kgmole K
14 del_Fo = 3000; //Standard free energy of the reaction
    in Kcal/Kgmole
15 n_A = 1; //Kgmoles of A
16 n_B = 0.1; //Kgmoles of B
17 n_C = 0.1; //Kgmoles of C
18
19 //To find out the equilibrium has been attained or
    not. If not then calculate the equilibrium
    composition and also find out whether the
    equilibrium composition will change or not if
    pressure were increased to 3 atm.
20 //(1)To find out the equilibrium has been attained
    or not. If not then calculate the equilibrium
    composition
21 //P_B/P_C = 1 (Given)
```

```

22 n_T = n_A+n_B+n_C; //Total Kgmoles of the component
23 p_A = (n_A/n_T)*P; //Partial pressure of A
24 p_B = (n_B/n_T)*P; //Partial pressure of B
25 p_C = (n_C/n_T)*P; //Partial pressure of C
26 //Using the relation 14.36 (page no 312)
27 del_F = del_Fo + (R*T)*log((p_B*p_C)/(p_A^2));
28 if del_F == 0;
29     then mprintf('1.Equilibrium has been attained.')
        ;
30 else
31     mprintf('1.Equilibrium has not been attained.');
```

```

32 end
33 //Equilibrium composition
34 //At equilibrium del_F = 0
35 //From equations 14.35(page no 312) and 14.49(page
    no 320), we got the relations (a),(b)(page no
    331) &(c)(page no 332) and
36 //ln(p_C^2/(P-(2*p_C^2)))= -del_Fo/(R*T);
37 Kp = %e^(-del_Fo/(R*T)) //equilibrium constant in
    terms of pressure
38 p_C = (Kp^(1/2))/(1+2*(Kp^(1/2))); //Partial pressure
    of C at equilibrium in atm
39 p_B = p_C; //as p_B/p_C = 1
40 p_A = P-(2*p_C); //Partial pressure of A at
    equilibrium in atm
41 N_A = p_A*P*100;
42 N_B = p_B*P*100;
43 N_C = p_C*P*100;
44 mprintf('\n Equilibrium composition of A,B and C
    are %f,%f and %f mole percent respectively.',N_A,
    N_B,N_C);
45
46 //2. Calculation of composition at 400 K and 3 atm
    and vapour pressure of C at 400 K is 0.3 atm
47 P = 3; //Pressure in atm
48 P_C = 0.3; //Vapour pressure of C in atm
49 //Since m=0, pressure will not have an effect on
    equilibrium compositions.
```

```

50 mprintf('\n\n 2.The compositions will be the same as
    above on increasing the pressure. ');
51 p_B1 = p_B*P; //Partial pressure of B in atm
52 p_C1 = p_B1; //Partial pressure of C in atm
53 p_A1 = p_A*P; //Partial pressure of A in atm
54 if P_C < p_C1
55 p_A2 = ((p_B1*P_C)/Kp)^(1/2); //decreased partial
    pressure of A in atm
56 mprintf('\n  The partial pressure of A drops from
    %f to %f to compensate for the amount of C
    condensed. ', p_A1, p_A2);
57 //end

```

Scilab code Exa 14.10 To Calculate the final temperature for various conversions and the maximum conversion that can be attained in a single reactor operating adiabatically

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.10
6 clear all;
7 clc;
8
9 //Given
10 //SO2(A) + (1/2)O2 (B) - SO3(C)
11 //Basis: 1 Kgmole SO2
12 n_A = 1; //Kgmole of SO2 fed
13 n_B = n_A; //Kgmole of O2 fed
14 T1 = 273+400; //Temperature in K at which reactants
    enter
15 To = 298; //room temperature in K
16 del_H = -23490; //Standar heat of reaction at 25 deg
    cel from example 14.6 in Kcal/Kgmole

```



```

17
18 //At T1,
19 C_A_T1 = 11.0; C_B_T1 = 7.4; //in Kcal/Kgmole
20 //Assume the various temperature be
21 T = [913 1073 1373 1573]; //in K
22 //Mean specific heats of the components A,B & C at
    various temperature are given below in Kcal/
    Kgmole K
23 C_A = [11.6 11.8 12.3 12.5];
24 C_B = [7.7 7.8 8.0 8.2];
25 C_C = [ 16.6 17.2 18.2 18.6];
26
27 //To Calculate the final temperature for various
    conversions and the maximum conversion that can
    be attained in a single reactor operating
    adiabatically
28 //In equation 14.18 (page no 307),  $H_2-H_r = K$  &  $(H_p-
    H_3) = L(\text{say})$ 
29  $K = ((n_A * C_{A\_T1}) + (n_B * C_{B\_T1})) * (T_o - T_1)$ ; //in Kcal/
    Kgmole
30 mprintf('Adiabatic reaction temp in K
    percentage conversion of SO2');
31 for i = 1:4
32      $n_C(i) = (-K - (C_A(i) * (T(i) - T_o)) - (C_B(i) * (T(i) - T_o)$ 
         $)))/((T(i) - T_o) * (C_C(i) - C_A(i) - 0.5 * C_B(i)) +$ 
        del_H);
33 mprintf(' \n    %d', T(i));
34 mprintf('
        %f',
        n_C(i) * 100);
35 end
36
37 clf;
38 //plot(T, n_C * 100);
39 plot2d(T, n_C * 100, style = 2);
40 //Now equilibrium conversion at various temperature
    taken from figure 14.7 (page no 325) are given as
41 Ta = [850 900 1000 1100 1200 1300 1400];

```

```

42 n_C1 = [93.5 88.2 69.0 49.0 37.0 21.5 6.25];
43 plot2d(Ta,n_C1,style=3);
44 xtitle("Temperature vs Percentage Conversion",
        "Temperature in K", "% Conversion");
45 //From the graph, it can be seen that the curve cut
        each other approximately at the temp
46 T1 = 1140;//in Kelvin
47 C = interp1n([Ta;n_C1],T1);
48 mprintf('\n\n The maximum conversion that can be
        attained is %d percent ',C);
49 //end

```

Scilab code Exa 14.11 To Calculate the conversion of benzene at 25 degree celsius and 1 atm

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.11
6 clear all;
7 clc;
8
9 //Given
10 //Basis: 1 Kgmole of benzene
11 //C6H6 (A) + HNO3 (B) - C6H5NO2 (C) + H2O (D)
12 T = 298;//Temperature in K
13 R = 1.98;//gas constant in Kcal/Kgmole K
14 //Standard enthalpy in Kcal/Kgmole at 25 deg celsius
        of the above components are given as
15 H_A = 11718;
16 H_B = -41404;
17 H_C = -68371;
18 H_D = 3800;
19 //Standard entropy in Kcal/Kgmole K at 25 deg

```

```

        celsius of the above components are given as
20 S_A = 41.30;
21 S_B = 37.19;
22 S_C = 16.72;
23 S_D = 53.60;
24
25 //To Calculate the conversion of benzene at 25
    degree celsius and 1 atm
26 del_F = (H_C+H_D-(T*(S_C+S_D)))-(H_A+H_B-(T*(S_A+S_B
    )));
27 Ka = %e^(-del_F/(R*T)); //Equilibrium constant
28 x = (Ka^(1/2)/(1+(Ka^(1/2))));
29 mprintf('The conversion is almost %f percent for
    this reaction.',x*100);
30 //end

```

Scilab code Exa 14.12 To Calculate the maximum CH₄ concentration under the condition of 2 atm and the quantity of methane obtained if pressure is 1 atm

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.12
6 clear all;
7 clc;
8
9 //Given
10 //C + 2H2 - CH4
11 //Basis: 1 Kgmole of C fed
12 T = 1000; //Temperature in K
13 P1 = 2; //Pressure in atm
14 del_F = 4580; //Standard free energy in Kcal/Kgmole
15

```

```

16
17 //To Calculate the maximum CH4 concentration under
    the condition of 2 atm and the quantity of
    methane obtained if pressure is 1 atm
18 Ka = %e^(-del_F/(R*T)); //Equilibrium constant
19 //In relation (d) (page no 339) p_H2 = p (say)
20 p = poly(0, 'p');
21 q = Ka*(p^2)+p-P1;
22 r = roots(q);
23 p_H2 = r(2); //partial pressure of H2
24 p_CH4 = P1-p_H2; //partial pressure of CH4
25 X_H2 = p_H2*100/P1; //mole percent of H2
26 X_CH4 = p_CH4*100/P1; //mole percent of CH4
27 mprintf('Under the conditions of 2 atm and 1000 K,
    the maximum CH4 concentration is %f percent and
    further increase is not possible', X_CH4);
28 //Now. pressure has become
29 P2 = 1; //in atm
30 q = Ka*(p^2)+p-P2;
31 r = roots(q);
32 p_H2 = r(2); //partial pressure of H2
33 p_CH4 = P2-p_H2; //partial pressure of CH4
34 X_H2 = p_H2*100/P2; //mole percent of H2
35 X_CH4 = p_CH4*100/P2; //mole percent of CH4
36 mprintf('\n\n Under the conditions of 1 atm and 1000
    K, Methane = %f percent and Hydrogen = %f percent
    ', X_CH4, X_H2);
37 //end

```

Scilab code Exa 14.13 To Calculate the partial pressure of CO₂ required for decomposition and thus determine whether Ag₂CO₃ will decomposes or not at the given pressure and temperature

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14

```

```

3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.13
6 clear all;
7 clc;
8
9 //Given
10 T1 = 273+110; //Temperature in K
11 T = 298; //Room temperature in K
12 P = 1; //Pressure in atm
13 R = 1.98; //gas constant in Kcal/Kgmole
14 //Ag2CO3(s) (A) = Ag2O(s) (B) + CO2(g) (C)
15 a = 1; //Stoichiometry coefficient of A
16 b = 1; //Stoichiometry coefficient of B
17 c = 1; //Stoichiometry coefficient of C
18 //Standard entropy of the above components in Kcal/
    Kgmole K at 25 deg cel are given as
19 S_A = 40.17;
20 S_B = 29.09;
21 S_C = 51.08;
22 //Standard enthalpy of the above components in Kcal/
    Kgmole at 25 deg cel are given as
23 H_A = -119900;
24 H_B = -6950;
25 H_C = -94036;
26 //Specific heat (assumed constant) of the above
    components in Kcal/Kgmole K are given as
27 C_A = 26.1;
28 C_B = 16.5;
29 C_C = 9.6;
30
31 //To Calculate the partial pressure of CO2 required
    for decomposition and thus determine whether
    Ag2CO3 will decomposes or not at the given
    pressure and temperature
32 del_H = H_C+H_B-H_A; //Standard heat of reaction at
    25 deg cel in Kcal/Kgmole
33 del_C = b*C_B+c*C_C-a*C_A;

```

```

34 //From equation 14.15 (page no 340)
35 del_Ht = del_H +del_C*(T1-T);
36 del_F = del_H-(T*(S_B+S_C-S_A)); //Standard free
    energy in Kcal/Kgmole
37 Ka1 = %e^(-del_F/(R*T)); //Equilibrium constant at
    temperature T
38 //Since del_Ht is constant(as del_C = 0),Ka2 can be
    calculated by equation 14.43 (page no 316)
39 Ka2 = Ka1* %e^((del_Ht/R)*(1/T1-1/T));
40 p_CO2 = Ka2;
41 mprintf('The partial pressure of CO2 required for
    decomposition is %4.3e atm',p_CO2);
42 if p_CO2 < P
43     mprintf('\n Silver carbonate will not decompose
        at 110 deg celsius as the pressure given is 1
        atm');
44 else
45     mprintf('\n Silver carbonate will decompose at
        110 deg celsius');
46 end
47 //end

```

Scilab code Exa 14.14 Theoretical problem

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.14
6 clear all;
7 clc;
8
9 //Given

```

```

10 //The given example is an theoretical problem and it
    does not involve any numerical computation.
11 //end

```

Scilab code Exa 14.15 To Calculate the equilibrium composition of the mixture

```

1 //Chemical Engineering Thermodynamics
2 //Chapter 14
3 //Thermodynamics of Chemical Reactions
4
5 //Example 14.15
6 clear all;
7 clc;
8
9 //Given
10 //C3H8 = C3H6 + H2... (i)
11 //C3H8 = C2H4 +CH4...(ii)
12 Kp1 = 7.88; //Equilibrium constant of equation (i)
13 Kp2 = 775; //Equilibrium constant of equation (ii)
14 T = 760+273; //Temperature in K
15
16 //To Calculate the equilibrium composition of the
    mixture
17 //Basis: 1 mole of C3H8 in feed
18 //From the equations (a) &(b) (page no 343); y/x = z
    (say)
19 z = (Kp2/Kp1)^(1/2);
20 //Substituting y = z*x in equation(a), we got the
    equation p:
21 x = poly(0, 'x')
22 p = (1+Kp1+Kp1*(z^2)+2*Kp1)*x^2 - Kp1;
23 q = roots(p);
24 x = q(1);
25 y = z*x;

```

```
26 mprintf('Moles of H2, C3H6, C2H4 and CH4 formed at  
    equilibrium are %f %f %f %f respectively.',x,x,y,  
    y);  
27 //end
```

Chapter 15

Fuel Cells

Scilab code Exa 15.1 To Calculate the emf of the cell and the cell efficiency and heat to be removed to maintain isothermal conditions

```
1 //Chemical Engineering Thermodynamics
2 //Chapter 15
3 //Fuel Cells
4
5 //Example 15.1
6 clear all;
7 clc;
8
9 //Given
10 del_F = -56.29; //Standard free energy change in Kcal/
    //Kgmole
11 del_H = -68.317; //Standard heat of reaction in Kcal/
    //kgmole
12 F = 23.06; //Electro-chemical equivalent in Kcal/volt
13 J = 2; //Valance for H2
14
15 //To Calculate the emf of the cell , cell efficiency
    //and heat to be removed to maintain isothermal
    //conditions
16 //Basis: 1 Kgmole of H2
```

```
17 //From equation 15.4 (page no 355)
18 E = -del_F/(F*J);
19 mprintf('1.The emf of the cell is %f volt.',E);
20 n = del_F/del_H*100;
21 mprintf('\n 2.The cell efficiency is %f percent.',n)
    ;
22 Q = del_H-del_F;
23 mprintf('\n 3.The heat to be removed is %f Kcal to
    maintain the temperature at 25 degree celsius.',Q
    );
24 //end
```
