Scilab Textbook Companion for Chemical Engineering Thermodynamics by S. Sundaram[1]

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Book Description

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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

Chapter 1

Introduction

Scilab code Exa 1.1 To determine the force exerted

```
//Chemical Engineering Thermodynamics
//Chapter 1
//Introduction

//Example 1.1
clear;
clc;

//Given
m = 100;//m is the mass of the object in kg
a = 10;//a is the acceeleration due to gravity in m/s^2

//To determine the force exerted
F = m*a;//F is the force exerted by the object in kg
mprintf('Force exerted by the object= %f N',F);
F = (1/9.8065)*m*a;//F is the force exerted by the object in kgf
mprintf('\n Force exerted by the object= %f N',F);
//end
```

Scilab code Exa 1.2 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter
//Introduction

//Example 1.2
clear;
clc;

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

Scilab code Exa 1.3 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter
//Introduction

//Example 1.3
clear;
clc;

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

Scilab code Exa 1.4 To determine the mass of water required

```
//Chemical Engineering Thermodynamics
//Chapter 1
//Introduction

//Example 1.4
clear;
clc;

//Given
h = 100;//h is the height of the water fall in m
n = .855;//n is the efficiency of the turbine
g = 9.8;//g is the acceleration due to gravity in m/(s^2)
E = 100*10*3600;//E is the potential enery of water available to the bulb for 10 hours in watt or J/s

//To determine the mass of water required
m = (E/(g*h*n));//m is the mass of water required for lighting the bulb for 10 hours in Kg
mprintf('Mass of water required for lighting the bulb for 10 hours in Kg= %f Kg',m);
mprintf('\n Mass of water required for lighting the bulb for 10 hours in tonnes= %f Kg',m/907.2);
//end
```

Scilab code Exa 1.5 To Calculate the work obtained

```
//Chemical Engineering Thermodynamics
//Chapter 1
//Introduction

//Example 1.5
clear;
```

```
clc;

//Given
n = 1;//n is the Kg mole of an ideal gas
P = 700*(10^4);//P is the pressure of the system in N/(m^2)
W = 45;//W is the weight of the mass in Kg
M = 20;//M is the weight of the piston and piston rod together in Kg
T = 300;//T is the constant temperature of the bath in K
h = .4;//h is the height difference of the piston after expansion in m

//To calculate the work obtained
a = (10^-4);//a is the cross sectional area of the cylinder in m^2
V = h*a;//V is the volume changed as gas expands in m^3

//(i). If gas alone is the system
//1Kgf = 9.8065Nm
P1 = ((W+M)*9.8065)/(10^-4);//P1 is the resisting pressure when the gas confined in the cylinder taken as a system
W1 = P1*V;//W1 is the work done if the gas confined in the cylinder us taken as system
mprintf('Work done by the system if the gas confined in the cylinder is taken as a system is %f Nm',W1);

//(ii). If gas + piston + piston rod is a system
P2 = ((W*9.8065)/(10^-4));//P2 is the resisting pressure when the gas plus piston plus piston rod is taken as a system
W2 = P2*V;//W2 is the Work done by the system if the gas plus piston plus piston rod is taken as a system
```

```
mprintf('\n Work done by the system if the gas plus piston plus piston rod is taken as system is %f Nm',W2);

//(iii). If gas + piston + piston rod +weight is system
P3 = 0;//P3 is the resisting pressure when the gas plus piston plus piston rod plus weight is taken as a system
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
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);
//end
```

Scilab code Exa 1.6 To Calculate the work done

```
//Chemical Engineering Thermodynamics
//Chapter 1
//Introduction

//Example 1.6
clear;
clc;

//Given
n = 1;//n is the Kg mole of ideal gas.
P1 = 700*(10^4);//P1 is the initial pressure of the system in N/(m^2)
P2 = 638*(10^4);//P2 is the final pressure of the system in N/(m^2)
T = 300;//T is temperature of the system in K
R = 8314.4;//R is gas constant in Nm/Kgmole deg K
```

```

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

Chapter 2

P V T Relations

Scilab code Exa 2.1 To determine the temperature required

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P–V–T Relations

//Example 2.1
clear;
clc;

//Given
m = 140;//m is the mass of N2 in Kg
P = 4.052*(10^5);//P is the pressure of the system
    in Pa
V = 30;//V is the volume of the system in m^3
R = 8314.4;// R is the gas constant

//To determine temperature required
T = P*V/((m/28)*R);//T is the temperature of the
    system in K
mprintf('Temperature of the system is %f K',T);
//end
```

Scilab code Exa 2.2 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P—V—T Relations

//Example 2.2
clear;
clc;

//Given
//This example is a theoretical problem and does not
    involve any numerical computation
//end
```

Scilab code Exa 2.3 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P—V—T Relations

//Example 2.3
clear;
clc;

//Given
//This example is a theoretical problem and does not
    involve any numerical computation
//end
```

Scilab code Exa 2.4 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P-V-T Relations

//Example 2.4
clear;
clc;

//Given
//This example is a theoretical problem and does not
    involve any numerical computation
//end
```

Scilab code Exa 2.5 To calculate the volume of Methane

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P-V-T Relations

//Example 2.5
clear;
clc;

//Given
n = 1;//n is Kg moles of methane
T = 423;//T is the temperatue of the system in
   kelvin
P = 100;//P is the pressure of the system in atm
Tc = 191;//Tc is the critical temperature of the
   system in K
Pc = 45.8;//Pc is the critical pressure of the
   system in atm
R = 0.08206;//R is the gas constant in (m^3 atm/Kg
```

```
mole K)

//To calculate the volume of methane
//(i)Using ideal gas equation
V1 = (n*R*T)/P;//V1 is the volume of the gas in m^3
mprintf('(i)Volume of the gas using ideal gas equation is %f cubic meter',V1);

//(ii)Using Vander Waals' equation
a = (27*(R^2)*(Tc^2))/(64*Pc);//Vander Waais constant
b = (R*Tc)/(8*Pc);//Vander Waais constant
v = poly(0, 'v');
q = -((a*b)/P)+(a/P)*v-(((R*T)+(b*P))/P)*v^2+(v^3);//According to Vander Waals equation
r = roots(q);
mprintf('\n (ii)Volume of the gas using Vander Waals equation is %f cubic meter',r(1));

//(iii)Using generalized Z chart
Tr = T/Tc;//Tr is the reduced temperatue
Pr = P/Pc;//Pr is the reduced pressure
//From the figure A.2.2,
Z = 0.97;//Z is the compressibility factor
V = (Z*R*T)/P;
mprintf('\n (iii)Volume of the gas using Z chart is %f cubic meter',V);

//(iv)Using molar polarisation method
//From Table 2.2
Pmc = 6.82;//Pmc is the molar polarisation for methane
//From figure A.2.4
Z0 = .965;
Z1 = 14.8*(10^-4);
Z = Z0+(Z1*Pmc);
V = (Z*R*T)/P;
mprintf('\n (iv)Volume of the gas using molar
```

```
   polarisation method is %f cubic meter',V);

//(v)From experiment
//Given
Z = 0.9848;
V = (0.9848*n*R*T)/P;
mprintf('\n (v)Volume of the gas calculated by
   experimental Z value is %f cubic meter',V);
//end
```

Scilab code Exa 2.6 To calculate the final pressure acheived

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P–V–T Relations

//Example 2.6
clear;
clc;

//Given
P1 = 266;
T1 = 473.16;//Initial temperature in Kelvin
T2 = 273.16;//Final temperature in Kelvin
V1 = 80; V2 = 80;//Initial & final volume in litres
N1 = (14.28/28); N2 = (14.28/28);//Initial and final
    Kg moles are equal
Tc = 126;//Critical temperature of N2 in K
Pc = 33.5;//Critical pressure of N2 in atm

//To calculate the final pressure achieved
//(i)Using ideal gas law
p2 = (P1*V1*N2*T2)/(V2*N1*T1);
mprintf('(i)Final pressure of N2  using ideal gas
   law is %f atm',p2);
```

```

//(ii)Using generalized Z chart
Tr1 = T1/Tc;//reduced initial temp in k
Pr1 = P1/Pc;//reduced initial press in K
//From the Z–chart compressibility factor coressponding to the above Tr1 &Pr1 is
Z1 = 1.07;
P2 = [125,135,150];
Z2 = [0.95, 0.96, 0.98];
F = [0,0,0];
for i = 1:3
    F(i) = (P2(i)/(Z2(i)*T2))-(P1/(Z1*T1));
end
clf;
plot(P2,F);
xtitle(”P2 vs F”,”P2”,”F”);
P3 = interpln([F;P2],0);
mprintf(’\n (ii)Final pressure of N2 from Z chart is %f atm’,P3);

//(iii)Using Pseudo reduced density chart
R = 0.082;//gas constant
v = V1/N1;//Volume per moles of nitrogen in m^3/Kg mole
Dr = (R*Tc)/(Pc*v);
Tr2 = T2/Tc;//final reduced temp in K
//From figure A.2.1, reduced pressure coressponding to this Dr and Tr2 is
Pr2 = 4.1//final reduced pressure in atm
p2_ = Pr2*Pc;
mprintf(’\n (iii)Final pressure achieved using Dr chart is %f atm’,p2_);
//end
```

Scilab code Exa 2.7 To compute the work required

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P–V–T Relations

//Example 2.7
clear;
clc;

//Given
n = 1;//n is the Kg mole of methane gas
T = 298;//T is the constant temperature in K
P1 = 1;//P1 is the initial pressure of the system
P2 = 100;//P2 is the final pressure of the system
R = 8314.4;//R is the gas constant in Nm/Kgmole deg K

//To compute the work required
//(i)Using ideal gas law
W = R*T*log(P1/P2);
mprintf('(i)Work done by the system if the gas obeys ideal gas law is %4.2e Nm',W);

//(ii)Using Vander Waals' equation
//Given
//For methane
a = 2.32*(10^5);//Vander Wals' constant a in N/m^2
b = 0.0428;//Vanderwaals' constant b in m^3
//V1 and V2 are evaluated by trial and error using Vanderwaals' equation as P1 and P2 are known
V1 = 11.1;//initial volume of the gas in m^3
V2 = 0.089;//final volume of the gas in m^3
W = (R*T*log((V2-b)/(V1-b)))+(a*((1/V2)-(1/V1)))
mprintf('\n (ii)Work done by the system if the gas obeys Vander Waals equation is %4.2e Nm',W);
//end
```

Scilab code Exa 2.8 To determine the vapour pressure of Chlorine

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P–V–T Relations

//Example 2.8
clear;
clc;

//Given
V = 27*(10^-3);//Volume of the container in m^3
n = (15/70.91);//n is the Kg moles of chlorine
T = 293;//T is the temperature in K
R = 0.08206;
P = 10^(4.39-(1045/293));//P is the vapour pressure of chlorine
Pc = 76.1;//Critical pressure of Chlorine
Tc = 417;//Critical temperature of Chlorine
Pr = P/Pc;//Reduced pressure of Chlorine
Tr = T/Tc;//Critical temperature of Chlorine
M = 70.91;//Molecular weight of the Chlorine

//To determine the vapour pressure of chlorine, amount of liquid Cl2 and temperature required
//(i)Specific volume of liquid Chlorine
//From figure A.2.2
Zg = 0.93;
//From figure A.2.6
Zl = 0.013;
vl = ((Zl*R*T)/P);
mprintf('(i)Specific volume of liquid Chlorine from compressibility chart is %f cubic meter /Kgmole',vl);
```

```

//From Francis relation , taking the constants from Table 2.3
D = (1.606-(216*(10^-5)*20)-(28/(200-20)))*10^3;//Density of liq Cl2 in Kg/m^3
Vl = M/D;
mprintf('\n   Specific volume of liquid Chlorine from Francis relation is %f cubic meter /Kgmole',Vl);

//(ii)Amount of liquid Cl2 present in the cylinder
vg = ((Zg*R*T)/P);
V1 = V-vg;//V1 is the volume of liquid Chlorine
Vct = 0.027;//volume of the container
Vg = (0.212-(Vct/vl))/((1/vg)-(1/vl));//By material balance
W = ((V-Vg)*70.9)/vl;
mprintf('\n\n (ii)Weight of Chlorine at 20deg cel is %f Kg',W);

//(iii)Calculation of temperature required to evaporate all the liquid chlorine
//log P' = 4.39 - 1045/T (given)
//Assume the various temperature
Ng = 0.212;//total Kg moles of gas
Ta = [413 415 417];
N = [0,0,0];
for i = 1:3
    Tr(i) = Ta(i)/Tc;//reduced temperature in K
    P(i) = 10^(4.39-(1045/Ta(i)));
    Pr(i) = P(i)/Pc;//reduced pressure in K
//From the compressibility factor chart,Z values coressponding to the above Tr &Pr are given as
Z = [0.4 0.328 0.208];
N(i) = (P(i)*Vct)/(Z(i)*R*Ta(i));
end

clf;
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P–V–T Relations

//Example 2.9
clear;
clc;

//Given
N1 = 0.7;//Kg mole of CH4
N2 = 0.3;//Kg mole of N2
R = 0.08206;//Gas constant
T = 323;//Temperature in Kelvin
V = 0.04;//Volume in m^3
a1 = 2.280; b1 = 0.0428;//Vanderwaals constants for CH4
a2 = 1.345;b2 = 0.0386;//Vanderwaals constants for N2
Tc1 = 191; Pc1 = 45.8;//Critical temperature in K and pressure of CH4 in atm
Tc2 = 126;Pc2 = 33.5;//Critical temperature in K and pressure of N2 in atm

//To find Approx Value
function[A]=approx(V,n)
```

```
  A=round(V*10^n)/10^n;//V-Value  n-To what place
  funcprot(0)
endfunction

//To calculate the pressure exerted by the gas mixture
//(i)Using ideal gas law
P = (N1+N2)*((R*T)/V);
mprintf('(i) Pressure exerted by the gas mixture using ideal gas law is %d atm',P);

//(ii)Using Vander waal equation
P1 = ((N1*R*T)/(V-(N1*b1)))-((a1*(N1^2))/(V^2));//Partial pressure of CH4
P2 = ((N2*R*T)/(V-(N2*b2)))-((a2*(N2^2))/(V^2));//Partial pressure of N2
Pt = P1+P2;
mprintf('\n(ii) Pressure exerted by the gas mixture using Vander waal equation is %f atm', Pt);

//(iii)Using Zchart and Dalton's law
Tra = T/Tc1;//reduced temperature of CH4
Trb = T/Tc2;//reduced temperature of N2
//Asssume the pressure
P = [660 732 793 815 831];
for i = 1:5
    Pa(i) = N1*P(i);// partial pressure of CH4 for the ith total pressure
    Pb(i) = N2*P(i);// partial pressure of N2 for the ith total pressure
    Pra(i) = Pa(i)/Pc1;//reduced pressure of CH4 for the ith total pressure
    Prb(i) = Pb(i)/Pc2;//reduced pressure of N2 for the ith total pressure
end

//For the above Pr and Tr values compressibility factors  from the figure A.2.3 are given as
```

```
Za = [1.154 1.280 1.331 1.370 1.390];//Z values of CH4
Zb = [1 1 1 1 1];//Z values of N2
V3 = 0.0421;
for i = 1:5
    Pa(i) = Za(i)*N1*((R*T)/V);//partial pressure of CH4 coressponding to the ith total presure
    Pb(i) = Zb(i)*N2*((R*T)/V);//partial pressure of N2 coressponding to the ith total pressure
    Pt(i) = Pa(i)+Pb(i);//total pressure of the gas mixture
    if Pt(i)-P(i) < 15
    mprintf('\n(iii) pressure exerted by the gas mixture using Z chart and Dalton Law is %d atm',Pt(i));
    else
    end
end

//(iv)Using Amagat's law and Z chart
P = [1000 1200 1500 1700];
for i=1:4
    Pra(i) = P(i)/Pc1;
    Prb(i) = P(i)/Pc2;
end
//For the above Pr and Tr values compressibility factors from the figure A.2.3 are given as
Za = [1.87 2.14 2.52 2.77];
Zb = [1.80 2.10 2.37 2.54];
for i = 1:4
    Va(i) = approx((N1*Za(i)*((R*T)/P(i))),4);
    Vb(i) = approx((N2*Zb(i)*((R*T)/P(i))),4);
    V1(i) = approx((Va(i)+Vb(i)),4);
    if V1(i)-V <= 0.003
     mprintf('\n(iv) Pressure exerted by the gas mixture using Amagat law and Zchart is %d atm ',P(i));
    else
```

```
end
end
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 2
//P–V–T Relations

//Example 2.10
clear;
clc;

//Given
yN2 = 1/4;//mole faction of N2 in the mixture
yH2 = 3/4;//mole fraction of H2 in the mixture
V = 5.7;//V is the rate at which mixture enters in m^3 in 1 hour
P = 600;//P is in atm
T = 298;//T is in K
TcN2 = 126;//critical temp of N2 in K
TcH2 = 33.3;//critical temp of H2 in K
TcNh3 = 406.0;//critical temp of NH3 in K
PcN2 = 33.5;//critical pressure of N2 in atm
PcH2 = 12.8;//critical pressure of H2 in atm
PcNH3 = 111.0;//critical pressure of NH3 in atm
R = 0.082;//gas constant

//To calculate the amount of ammonia leaving the reactor and the velocity of gaseous product leaving the reactor
```

```
//(i)Calculation of amount of NH3 leaving the reactor
Tcm = (TcN2*yN2)+(TcH2*yH2);//critical temperature of the mixture
Pcm = (PcN2*yN2)+(PcH2*yH2);//critical pressure of the mixture
Trm = T/Tcm;
Prm = P/Pcm;
//From figure A.2.3
Zm = 1.57;//compressibility factor of the mixture
N = (P*V)/(Zm*R*T);//Kg mole of the mixture
N1 = 0.25*N;//Kg mole of N2 in feed
//N2+3H2 - 2NH3
W = 2*0.15*N1*17;
mprintf('(i)Ammonia formed per hour is %f Kg',W);

//(ii)Calculation of velocity
N1 = 0.25*N-(0.25*N*0.15);//Kg mole of N2 after reactor
N2 = 0.75*N-(0.75*N*0.15);//Kg mole of H2 after reactor
N3 = 0.25*N*2*0.15;//Kg mole of NH3 after reactor
Nt = N1+N2+N3;//total Kg moles after reactor
y1NH3 = N3/Nt;//mole fraction of NH3 after reactor
y1N2 = N1/Nt;//mole fraction of N2 after reactor
y1H2 = N2/Nt;//mole fraction of H2 after reactor
T1cm = (TcN2*y1N2)+(TcH2*y1H2);
P1cm = (PcN2*y1N2)+(PcH2*y1H2);
T1 = 448;//in K
P1 = 550;//in atm
T1rm = T1/T1cm;
P1rm = P1/P1cm;
//From Figure A.2.2
Zm1 = 1.38;
V1 = (Zm1*Nt*R*T1)/P1;
d = 5*(10^-2);//diameter of pipe
v = V1/((%pi/4)*(d^2)*3600);
mprintf('\n (ii)Velocity in pipe is %f m/sec',v);
```

```
//end
```

Chapter 3

First Law of Thermodynamics

Scilab code Exa 3.1 To calculate the change in internal energy

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.1
clear;
clc;

//Given
W = -((2*745.6*(10^-3)/4.18)*3600);//work added to
    the system in Kcal/hr
m = 10;//Amount of fluid in tank in Kg
Q = -378;//Heat losses from the system in Kcal/hr

//To calculate the change in internal energy
delE=(Q-W)/m;// Change in internal energy in Kcal/hr
    kg
mprintf('Change in Internal energy is %f Kcal/hr Kg'
    ,delE);
//end
```

Scilab code Exa 3.2 To calculate the change in internal energy

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.2
clear;
clc;

//Given
n = 1;//kg moles of a gas
Cv = 5;//specific heat in Kcal/Kgmole
delT = 15;//increase in temperature in deg celsius

//To calculate the change in internal energy
Q = n*Cv*delT;//heat given to the system in Kcal
W = 0;//work done
delE = Q-W;//Change in internal energy
mprintf('Change in internal energy is %f Kcal',delE)
    ;
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.3
clear;
```

```
clc;

//Given
P = 1;//constant pressure throughout the process in atm
T1 = 273;//Initial temperature in K
T2 = 373;//Final temperature in K
V1 = 0;//Volume of liquid water or initial volume
V0 = 22.4;//volume of vapour at standard condition in cubic meter
Q = 9.7//Heat of vapourisation in Kcal

//To calculate the work done by the expanding gas and increase in internal energy
//(i)Calculation of work done
V2 = 22.4*(T2/T1)*(P)*(10^-3);//Volume of final vapour in cubic meter
w = P*(V2-V1);//Work done in atm cubic meter
W = w*(1.03*10^4)/427;//Work done in Kcal
mprintf('(i)Work done by the expanding gas is %f Kcal',W);

//(ii)Calculation of change in internal energy
delE = Q-W;
mprintf('\n\n (ii)Increase in internal energy is %f Kcal',delE);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

```

```
//Example 3.4
clear;
clc;

//Given
W = 0;//work done during the process
P1 = 1;//Initial pressure in atm
P2 = 10;//Final pressure in atm
V2 = V1;//Initial & final volume are equal
Cv = 0.23//specific heat at constant volume in Kcal/Kg deg K
//(delQ/delT)=Q
Q = 1.3;//Rate of heat addition in Kcal/min
m = 2.5//Weight of an ideal gas in Kg
T1 = 298//Initial temperature in Kelvin

//To calculate the time taken for the gas to attain 10 atm
//Q = m*Cv*(delT/delt)=1.3
T2 = (P2*T1)/(P1);//Final temperature in Kelvin
t = ((m*Cv)/1.3)*(T2-T1);//time taken in minutes
mprintf('The time taken to attain a pressure of 10 atm is %f hrs',t/60);
//end
```

Scilab code Exa 3.5 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.5
clear;
clc;

```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.6
clear;
clc;

//Given
R = 1.98;//gas constant in kcal/Kgmole deg K
T = 293;//Temperature in K
M = 29;//Molecular weight of air

//To calculate the flow work per kg of air
//W=(P*V)=(R*T)
W = R*T;//Flow work in Kcal/Kg mole
W1 = W/M;
mprintf('Flow work is %f Kcal/Kg',W1);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

```

```
//Example 3.7
clear;
clc;

//Given
m = 5000;//Amount of steam recived per hour in Kg
H1 = 666;//Specific enthalpy when steam entered in the turbine in Kcal/Kg
H2 = 540;//Specific enthalpy when steam left the turbine in Kcal/Kg
u1 = 3000/60;//velocity at which steam entered in m/sec
u2 = 600/60;//velocity at which steam left in m/sec
Z1 = 5;//height at which steam entered in m
Z2 = 1;//height at which steam left in m
Q = -4000;//heat lost in Kcal
g = 9.81;

//To calculate the horsepuwer output of the turbine
delH = H2-H1;//change in enthalpy in Kcal
delKE = ((u2^2)-(u1^2)/(2*g))/(9.8065*427);//change in kinetic energy in Kcal; 1kgf = 9.8065 N
delPE = ((Z2-Z1)*g)/(9.8065*427);//change in potential energy in Kcal
W = -(m*(delH+delKE+delPE))+Q;//work delivered in Kcal/hr
W1 = W*(427/(3600*75));//work delivered by turbine in hp
mprintf('Work delivered by turbine is %f hp',W1);
//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

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.8
clear;
clc;

//Given
m = 183;//rate of water flow in Kg/min
H1 = 95;//enthalpy of storage tank 1 in Kcal/Kg
h = 15;//height difference between two storage tanks in m
Q = -10100;//extraced heat from storage tank 1 in a heat exchanger in Kcal/min
W = -2;//work delivered by motor in hp

// To find out the  enthalpy of water tank2 and the temperature of water in the second tank
delPE = h/427;//change in potential energy in Kcal/Kg
delKE = 0;//change in kinetic energy
W1 = W*(75/427);//work delivered by motor in Kcal/sec
W2 = W1*60;//work delivered by motor in Kcal/min
H2 = ((Q+W2)/m)-delKE-delPE+H1;//enthalpy of storage tank 2 in Kcal/Kg
mprintf('The enthalpy of storage tank 2 is %f Kcal/Kg',H2);

//The enthalpy H2=39.66 corresponds to the temperature T according to steam table
T=40;//Temperature is in deg celsius
mprintf('\n The temperature of water in the second tank is %d deg celsius',T);
//end
```

Scilab code Exa 3.9 To calculate the mass of steam required

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.9
clear;
clc;

//To calculate the mass of steam required
//Given
m2 = 100;//mass of water to be heated
//From diagram,
//m3 = m1+m2;..(a)
//Hs = H1;..(b) since throttling is a constant
   enthalpy process
//m3*H3-(m1*H1+m2*H2)=0;..(c) since delH=0

//From steam tables,
Hs = 681.7//enthalpy of steam at 200 deg cel bleeded
    at the rate of 5Kgf/(cm^2) in Kcal/Kg
H2 = 5.03;//enthalpy of liquid water at 5 deg cel
H3 = 64.98;//enthalpy of liquid water at 65 deg cel
//from equn (a),(b)&(c);(page no 80)
m1 = ((H3-H2)/(Hs-H3))*m2;//mass of steam required
   in Kg  (page no 80)
mprintf('The mass of steam required to heat 100 Kg
   of water is %f Kg',m1);
//end
```

Scilab code Exa 3.10 To calculate the pump work required

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.10
clear;
clc;

//Given
V = 0.3;//Volume of the tank in m^3
P1 = 1;//Initial pressure of the tank in atm
P2 = 0;//Final pressure of the tank in atm
T = 298;//Temperature of the tank in K
t = 10;//evacuation time in min

//delN=(V/(R*T)*delP)..(a) change in moles as V and
    T are constant
//delW=delN*R*T*lnP..(b)pump work required
//From (a)&(b),delW=V*delP*lnP

//To calculate the pump work required
//On doing integration of dW we will get

W = V*(P1-P2);//pump work done in J/sec
W1=(W*(1.033*10^4))/(75*600);
mprintf('The pump work required is %f hp',W1);
//end
```

Scilab code Exa 3.11 To calculate the quality of exit steam

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.11
```

```
clear;
clc;

//Given
H1 = 680.6;//Enthalpy of entering steam at 6Kgf/cm^2 &200 deg cel in Kcal/Kg
u1 = 60;//velocity at which steam entered the nozzle in m/sec
u2 = 600;//velocity at which steam left the nozzle in m/sec
g = 9.8;
Hg = 642.8; Hlq = 110.2;//Enthalpy of saturated vapour & saturated liquid at 1.46 Kgf/cm^2 respectively

//To calculate the quality of exit steam
H2 = H1+((u1^2)-(u2^2))/(2*g*427);//enthalpy of leaving steam in Kcal/Kg
x = (H2-Hlq)/(Hg-Hlq);
mprintf('The quality of exit steam is %f percent',x*100);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.12
clear;
clc;

//Given
```

```
W = 0;//pump work
Mi = 0;//chamber is initially evacuated
M2 = 0;//no exist stream
H1 = 684.2;//enthalpy of steam at 200 deg cel & 3 Kgf/cm^2

//To calculate the internal energy of the steam in the chamber
//Q=150*m1;.. (a) heat lost from the chamber in Kcal/Kg
//m1=mf;..(b) mass of steam added from large pipe is equal to steam in chamber
 //H1*M1-Q=Mf*Ef; using (a)&(b)
 Ef = H1-150;
 mprintf('The internal energy of steam in chamber is %f Kcal',Ef);
 //end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 3
//First Law of Thermodynamics

//Example 3.13
clear;
clc;

//Given
//Q=W=delPE=delKE=0;
//M2=0; no exit stream
Ti = 288;//initial temperature in K
H = 7*Ti;//enthalpy of air in Kcal/Kgmole
Ei = 5*Ti;// initial internal energy of air in Kcal/
```

```
Kgmole
//Ef=5*Tf;Final internal energy of air in Kcal/Kgmole
Pi = 0.3;//initial pressure in atm
V = 0.57;//volume of the tank in m^3
R = 848;//gas constant in mKgf/Kg mole K
Pf = 1;//final prssure in atm

//To calculate the final weight and the final temperature of the air in the tank
Mi = (Pi*V*1.03*10^4)/(R*Ti);//initial quantity of air in tank in Kg mole
//Tf=(Pf*V*1.033*10^4)/(Mf*R)..(a) final temperature ,Mf=final quantity of air in tank in Kg mole
//M1=Mf-Mi..(b) M1 is mass of steam added in Kg mole
//H*M1=(Ef*Mf)-(Ei*Mi)
//H*M1=((5*Pf*V*1.033*10^4)/(Tf*R))*Tf-(Ei*Mi)...(c)
A = [1 -1;0 -H];
B = [Mi;((Ei*Mi)-((5*Pf*V*1.03*10^4)/R))];
x = A\B;
Mf = x(1);
mprintf('The final weight of air in the tank is%f Kg',Mf);

Tf = (Pf*V*1.03*10^4)/(Mf*R);
mprintf('\n The final temperature of air in the tank is %f K',Tf);
//end
```

Scilab code Exa 3.14 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 3
```

```
//First Law of Thermodynamics

//Example 3.14
clear;
clc;

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

Chapter 4

Second Law of Thermodynamics

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

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.1
clear;
clc;

//Given
Q1 = 250;//Heat absorbed in Kcal
T1 = (260+273);//Temperature at which engine absorbs
    heat
T0 = (40+273);//Temperature at which engine discards
    heat
//To Calculate work output, heat rejected, entropy
   change of system,surronding & total change in
   entropy and the efficiency of the heat engine
```

```

//(i)Calculation of work output
W = (Q1*((T1-T0)/T1));//Work done using equations 4.7 & 4.9 given on page no 98
mprintf('(i)The work output of the heat engine is %f Kcal',W);

//(ii)Calculation of heat rejected
Q2 = (Q1*T0)/T1;
mprintf('\n (ii)The heat rejected is %f Kcal',Q2);

//(iii)Calculation of entropy
del_S1 = -(Q1/T1);//Change in the entropy of source in Kcal/Kg K
del_S2 = Q2/T0;//Change in the entropy of sink in Kcal/Kg K
del_St = del_S1+del_S2;//Total change in entropy in Kcal/Kg K
mprintf('\n (iii)Total change in entropy is %d confirming that the process is reversible',del_St);

//(iv)Calculation of efficiency
n = (W/Q1)*100;
mprintf('\n (iv)The efficiency of the heat engine is %f percent',n);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

```

```
//Example 4.2
clear;
clc;

//Given
T1 = 373;//Temperature of the saturated steam in K
T2 = 298;//Temperature of the saturated water in K
//To calculate the total change in entropy and hence
    determine the reversibility of the process

//del_H = del_Q+(V*del_P)
//del_H =del_Q; since it is a constant pressure
   process

//From steam table,
//enthalpy of saturated steam at 373K is
H1 = 6348.5;// in Kcal/Kg
//enthalpy of saturated liquid water at 373K is
H2 = 99.15;//in Kcal/Kg
Q = H2-H1;//heat rejected in Kcal/Kg
del_S1 = Q/T1;//change in entropy of the system in
   Kcal/Kg K
del_S2 = Q/T2;//change in entropy of the surronding
   in Kcal/Kg K
del_St = del_S1+del_S2;//total change in the entropy
    in Kcal/Kg K
if(del_St == 0)
    mprintf('Process is reversible');
else
    mprintf('Process is irreversible');
end
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.3
clear;
clc;

//Given
Cp = 0.09;//specific heat of metal block in Kcal/Kg K
m = 10;//mass of metal block in Kg
T1 = 323;//initial temperature of the block in K
T2 = 298;//final temperature of the block in K
//constant pressure process
//To find out entropy change of block,air and total entropy change

//(i)To calculate the entropy change of block
del_S1 = m*Cp*log(T2/T1);
mprintf('(i)Entropy change of block is %f Kcal/Kg K',del_S1);

//(ii)To calculate the entropy change of air
Q = m*Cp*(T1-T2);//heat absorbed by air = heat rejected by block in Kcal
del_S2 = (Q/T2);
mprintf('\n (ii)Entropy change of air is %f Kcal/Kg K',del_S2);

//(iii)To calculate the total entropy change
del_St = del_S1+del_S2;
mprintf('\n (iii)Total entropy change is %f Kcal/Kg K',del_St);
if(del_St == 0)
   mprintf('\n Process is reversible');
else
   mprintf('\n Process is irreversible');
```

```
end
//end
```

Scilab code Exa 4.4 To calculate the total change in entropy

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.4
clear;
clc;

//Given
m1 = 10;//mass of metal block in Kg
m2 = 50;//mass of water in Kg
Cp1 = 0.09;//Specific heat of metal block in Kcal/Kg
    K
Cp2 = 1;//Specific heat of water in Kcal/Kg K
T1 = 50;//Initial temperature of block in deg
   celsius
T2 = 25;//Final temperature of block in deg celsius

//To calculate the total change in entropy
//Heat lost by block = Heat gained by water
Tf = ((m1*Cp1*T1)+(m2*Cp2*T2))/((m1*Cp1)+(m2*Cp2));
   //final temperature of water in deg celsius
Tf1 = Tf+273.16;//final temperature in K
del_S1 = m1*Cp1*log(Tf1/(T1+273));//change in
   entropy of the block in Kcal/K
del_S2 = m2*Cp2*log(Tf1/(T2+273));//change in
   entropy of the block in Kcal/K
del_St = del_S1+del_S2;
mprintf('The total change entropy is %f Kcal/K',
   del_St);
```

```
//end
```

Scilab code Exa 4.5 To calculate the entropy change

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.5
clear;
clc;

//Given
//Air at 20 deg celsius
//P1 = 250;initial pressure in atm
//P2 = 10;final pressure after throttling in atm

//To calculate the entropy change
//According to the given conditions from figure4.5(
   page no 103)
S1 = -0.38;//initial entropy in Kcal/Kg K
S2 = -0.15;//final entroy in Kcal/Kg K
del_S = S2-S1;
mprintf('Change in entropy for the throttling
   process is %f Kcal/Kg K',del_S);
//From figure 4.6(page no 104), the final
   temperature is -10 deg celsius
//end
```

Scilab code Exa 4.6 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 4
```

```
//Second Law of Thermodynamics

//Example 4.6
clear;
clc;

//Given
//The given problem does not involve any numerical comptation
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.7
clear;
clc;

//Given
//Basis: 1 hour
m = 10;//mass of air in Kg
T = 293;//Constant temperature throughout the process in K
//P1 = 1;//Initial pressure in atm
//P2 = 30;//Final pressure in atm
//According to the given data and using the graph or figure A.2.7 given in page no 105
S1 = 0.02;//Initial entropy in Kcal/Kg
S2 = -0.23;//Final entropy in Kcal/Kg
H1 = 5;//Initial enthalpy in Kcal/Kg
H2 = 3;//Final enthalpy in Kcal/Kg

```

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

Scilab code Exa 4.8 To calculate the effectiveness of the process

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.1
clear;
clc;

//Given
//Basis: 1 Kg of steam
//P1 = 30;Intial pressure in Kgf/cm^2
//P2 = 3;Final pressure in Kgf/cm^2
//T = 300;//Operating temperature
//From figure A.2.8,
H1 = 715;//Initial enthalpy of steam in Kcal/Kg
H2 = 625;//Final enthalpy of steam in Kcal/Kg
S1 = 1.56;//Initial entropy of steam in Kcal/Kg K
S2 = 1.61;//Final entropy of steam in Kcal/Kg K
Q = -1;//heat loss in Kcal/Kg
To = 298;//The lowest surronding temperature in K

//To calculate the effectiveness of the process
W = (-(H2-H1)+Q);//Actual work output by the turbine
    in Kcal
//The maximum or available work can be calculated
   from equation 4.14
del_B = -((H2-H1)-(To*(S2-S1)));// Maximum work that
    can be obtained in Kcal
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.9
clear;
clc;

//Given
m = 1;//mass of liquid water in Kg
T1 = 1350;//initial temperature in deg celsius
T2 = 400;//final temperature in deg celsius
Cp = 1;//Specific heat of water in Kcal/Kg K
Cpg = 0.2;//Specific heat of combustion gases in
   Kcal/Kg K
Hv = 468.35;//Heat of vapourisation at 14 Kgf/cm^2
   and 194.16 deg celsius in Kcak/Kg
To = 298;//Surronding temperature
Tb = 194.16+273;//Boiling point of liquid water

//To Calculate the maximum work obtained and the
   entropy change
//(i)Calculation of maximum work
//Q = del_H = m*Cp*(T2-T1); gas can be assumed to
   cool at constant pressure
//From equation 4.14 (page no 110)
del_B = -((m*Cpg*(T2-T1))-(To*m*Cp*log((T2+273)/(T1
```

```
    +273))));
mprintf('(i)The maximum work that can be obtained is
     %f Kcal/Kg of gas',del_B);

//(ii)To Calculate the change in entropy
del_S =(m*Cp*log(Tb/To))+((m*Hv)/Tb);
mprintf('\n(ii)The entropy change per Kg of water is
     %f',del_S);
//end
```

Scilab code Exa 4.10 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics

//Example 4.10
clear;
clc;

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

Chapter 5

Thermodynamic Potentials and Maxwell Relation

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

```
//Chemical Engineering Thermodynamics
//Chapter 5
//Thermodynamic Potentials and Maxwell's Relation

//Example 5.1
clear;
clc;

//Given
T = 293;//Constant temperature in K
w_NH3 = 20/100;//weight of NH3 in an aqueous
   solution in Kg
w_H2O = 80/100;//weight of H2O in an aqueous
   solution in Kg
V_f = 40;//feed rate in Kg/min
M_NH3 = 17;//Molecular weight of NH3
M_H2O = 18;//Molecular weight of H20
R = 1.98;//gas constant in Kcl/Kg mole K
V_s = 62;//Rate of heating steam in Kg/min
```

```
P1_H2O = 11.6;//Vapour pressure of water in feed in mm Hg
P2_H2O = 17.5;//Vapour pressure of pure water in mm Hg
P1_NH3 = 227;//Vapour pressure of NH3 in feed in mm Hg
P2_NH3 = 6350;//Vapor pressure of pure NH3 in mm Hg
//From steam tables:
Hs = 666.4;//Enthalpy of steam at 160 deg celsius & 2Kgf/cm^2 in Kcal /Kg
Ss = 1.75;//Entropy of steam at 160 deg celsius & 2 Kgf/cm^2V in Kcal/Kg K
Hl = 20.03;//Enthalpy of liquid water at 20 deg celsius in Kcal/Kg
Sl = 0.0612;//Entropy of liquid water at 20 deg celsius in Kcal/Kg K

//To Calculate the efficiency of the separation process
//Material Balance:
n_NH3 = (V*w_NH3)/M_NH3;//Kg moles of NH3 in feed(tops)
n_H2O = (V*w_H2O)/M_H2O;//Kg moles of H2O in feed(bottoms)
//del_F = del_F_NH3 +del_F_H2O;
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
//The available energy of the steam can be calculated from equation 4.14(page no 110)
del_B = -V_s*((Hl-Hs)-T*(Sl-Ss));//Available energy of the steam in Kcal
E = (del_F/del_B)*100;
mprintf('The efficiency of the separation process is %f percent',E);
//end
```

Chapter 6

Thermodynamic Relations

Scilab code Exa 6.0 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Relations

clear;
clc;

//Given
//The chapter does not contain any example which
   involve numerical computation
//end
```

Chapter 7

Ideal Gases

Scilab code Exa 7.1 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 7
//Ideal Gases

//Example 7.1
clear;
clc;

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

Scilab code Exa 7.2 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 7
//Ideal Gases
```

```

//Example 7.2
clear;
clc;

//Given
//The given example is a theoretical problem and it
   does not involve any numerical computation
//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

```
//Chemical Engineering Thermodynamics
//Chapter 7
//Ideal Gases

//Example 7.3
clear;
clc;

//Given
P1 = 15;//initial pressure in Kgf/cm^2
P2 = 1;//final pressure in Kgf/cm^2
V1 = 0.012;//initial volume in m^3
V2 = 0.06;//final volume in m^3
T1 = 420;//initial temperature in K
M = 28;//molecular weight of the gas
Cp = 0.25;//specific heat at constant pressure in
   Kcal/Kg K
R = 1.98;//gas constant in Kcal/Kg mole K
R2 = 848;//gas constant in mKgf/Kgmole K
//Cv = a+0.0005*T1; Specific heat at constant volume

```

```
//To Calculate the final temperature of the ideal gas, work done in an open and closed system, internal energy change for the process
//(a)Calculation of final temperature
//Using ideal gas law:(P*V)/(R*T)
T2 = (P2*V2*T1)/(P1*V1);
mprintf('(a)The final temperature is %d K',T2);

//(b)Calculation of work in an open and closed system
//From equation 7.22(page no 147): P1*(V1^n)=P2*(V2^n)
n = (log(P2/P1))/(log(V1/V2));
//From equation 7.25(page no 149)
W = ((P1*V1)-(P2*V2))/(n-1)*10^4;//work in mKgf
W1 = W/427;//Work in Kcal
mprintf('\n (b)The work in a closed system is %f Kcal',W1);
Ws = n*W1;//from equation 7.28(page no 149)
mprintf('\n    The work in an open system is %f Kcal',Ws);

//(c)Calculation of internal energy change
R1 = R/M;//gas constant in Kcal/Kg
Cv = Cp-R1;//specific heat at constant volume in Kcal/Kg K
a = Cv-(0.0005*T1);
m = (P1*10^4*V1*M)/(R2*T1);//mass of gas in Kg
function y = f(T)
    y = m*(a+(0.0005*T));
endfunction
del_E = intg(T1,T2,f);//internal energy change in Kcal/Kg
del_E1 = M*del_E;//internal energy change in Kcal/Kgmole
mprintf('\n (c)The internal energy change for the process is %f Kcal/Kgmole',del_E1);
```

Scilab code Exa 7.4 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 7
//Ideal Gases

//Example 7.4
clear;
clc;

//Given
//The given example is a theoretical problem and it
   does not involve any numerical computation
//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

```
//Chemical Engineering Thermodynamics
//Chapter 7
//Ideal Gases

//Example 7.5
clear;
clc;

//Given
P1 = 1;//Initial pressure of air in atm
T1 = 15+273;//Initial temperature in K
P2 = 5;//Final pressure of air in atm
```

```
T2 = 15+273;//Final temperature in K
Cv = 5;//specific heat of air at constant volume in Kcal/Kgmole K
Cp = 7;//specific heat of air at constant pressure in Kcal/Kgmole K
R = 0.082;//gas constant in atm-m^3/Kgmole K
R1 = 2;//gas constant in Kcal/Kgmole K
//From the P-V diagram given in page no 155:
//Line 12 represents Isothermal process
//Line b2,c2 & 1a represent Isometric process
//Line a2 & 1c represent Isobaric process
//Line 1b reprsent Adiabatic process

//To find Approx Value
function[A]=approx(V,n)
  A=round(V*10^n)/10^n;//V-Value  n-To what place
  funcprot(0)
endfunction

//To Compute del_H, del_E, Q, W, del_S for the processes given above.
//To indicate the quantities that are state functions
//To verify that the work required in an isothermal process is less than that in an adiabatic process

//Basis:1 Kgmole of air
V1 = (R*T1)/P1;//Initial volume in cubic meter
V2 = (R*T2)/P2;//Final volume in cubic meter

//(i)Isothermal path 12
//Equations 7.7 to 7.9 will be used (page no 145)
del_E_12 = Cv*(T2-T1);
del_H_12 = Cp*(T2-T1);
W_12 = R1*T1*log(P1/P2);
Q_12 = W_12;
del_S_12 = approx((R1*log(P1/P2)),4);
mprintf('\n(i)For isothermal process or path 12
```

```
change in internal energy is %f',del_E_12);
mprintf('\n    For isothermal process or path 12 change in enthalpy is %f',del_H_12);
mprintf('\n    For isothermal process or path 12 heat released is %f Kcal',Q_12);
mprintf('\n    For isothermal process or path 12 work is %f Kcal',W_12);
mprintf('\n    For isothermal process or path 12 change in entropy is %f Kcal/Kgmole K',del_S_12);

//(ii)Path 1a2 = 1a(isometric)+a2(isobaric)
//Equation 7.1 to 7.6 will be used (page no 144 & 145)
Pa = P2;
Ta = (Pa/P1)*T1;//in K
Q_1a = Cv*(Ta-T1);
del_E_1a = Q_1a;
del_H_1a = Cp*(Ta-T1);
W_1a = 0;// Constant volume process
del_E_a2 = Cv*(T2-Ta);
del_H_a2 = Cp*(T2-Ta);
Q_a2 = del_H_a2;
W_a2 = P2*(V2-V1)*((10^4*1.03)/427);
del_H_1a2 = del_H_1a+del_H_a2;
del_E_1a2 = del_E_1a+del_E_a2;
Q_1a2 = Q_1a+Q_a2;
W_1a2 = W_1a+W_a2;
del_S_1a = Cv*log(Ta/T1);
del_S_a2 = Cp*log(T2/Ta);
del_S_1a2 = approx((del_S_1a+del_S_a2),4);
mprintf('\n\n(ii)For path 1a2 change in internal energy is %f',del_E_1a2);
mprintf('\n    For path 1a2 change in enthalpy is %f',del_H_1a2);
mprintf('\n    For path 1a2 heat released is %f Kcal',Q_1a2);
mprintf('\n    For path 1a2 work is %f Kcal',W_1a2);
mprintf('\n    For path 1a2 change in entropy is %f
```

```
   Kcal/Kgmole K',del_S_1a2);

//(iii)Path 1b2 = 1b(adiabatic)+b2(isometric)
//From equation 7.11 (page no 146)
y = Cp/Cv;
Tb = T1*((V1/V2))^(y-1);
//From equation 7.1 to 7.3,7.10 & 7.21,(page no
   144,146,147)
Q_1b = 0;//adiabatic process
del_E_1b = Cv*(Tb-T1);
del_H_1b = Cp*(Tb-T1);
W_1b = -del_E_1b;
Q_b2 = Cv*(T1-Tb);
del_H_b2 = Cp*(T1-Tb);
W_b2 = 0;//constant volume prcess
del_E_b2 = Cv*(T2-Tb);
del_H_1b2 = del_H_1b+del_H_b2;
del_E_1b2 = del_E_1b+del_E_b2;
W_1b2 = W_1b+W_b2;
Q_1b2 = Q_1b+Q_b2;
del_S_1b2 = approx((Cv*log(T1/Tb)),4);
mprintf('\n\n(iii)For path 1b2 change in internal
   energy is %f',del_E_1b2);
mprintf('\n    For path 1b2 change in enthalpy is %f'
   ,del_H_1b2);
mprintf('\n    For path 1b2 heat released is %f Kcal'
   ,Q_1b2);
mprintf('\n    For path 1b2 work is %f Kcal',W_1b2);
mprintf('\n    For path 1b2 change in entropy is %f
   Kcal/Kgmole K',del_S_1b2);

//(iv)Path 1c2 = 1c(isobaric)+c2(isometric);
Pc = P1;
Vc = V2;
Tc = (Pc/P2)*T2;
del_E_1c = Cv*(Tc-T1);
Q_1c = Cp*(Tc-T1);
del_H_1c = Q_1c;
```

```
W_1c = P1*(Vc-V1)*((10^4*1.03)/427);
del_E_c2 = Cv*(T2-Tc);
Q_c2 = del_E_c2;
del_H_c2 = Cp*(T2-Tc);
W_c2 = 0;//constant volume process
del_E_1c2 = del_E_1c+del_E_c2;
del_H_1c2 = del_H_1c+del_H_c2;
Q_1c2 = Q_1c+Q_c2;
W_1c2 = W_1c+W_c2;
del_S_1c = Cp*log(Tc/T1);
del_S_c2 = Cv*log(T2/Tc);
del_S_1c2 = approx((del_S_1c+del_S_c2),4);
mprintf('\n\n(iv)For path 1c2 change in internal energy is %f',del_E_1c2);
mprintf('\n   For path 1c2 change in enthalpy is %f',del_H_1c2);
mprintf('\n   For path 1c2 heat released is %f Kcal',Q_1c2);
mprintf('\n   For path 1c2 work is %f Kcal',W_1c2);
mprintf('\n   For path 1c2 change in entropy is %f Kcal/Kgmole K',del_S_1c2);

//Determination of state & path functions
if((del_E_12 == del_E_1a2)&(del_E_12 == del_E_1b2)&(del_E_12 == del_E_1c2))
    mprintf('\n\n del_E is a state function');
else
    mprintf('\n\n del_E is a path function');
end
if((del_H_12 == del_H_1a2)&(del_H_12 == del_H_1b2)&(del_H_12 == del_H_1c2))
    mprintf('\n\n del_H is a state function');
else
    mprintf('\n\n del_H is a path function');
end
if(del_S_12 == del_S_1a2)&(del_S_12 == del_S_1b2)&(del_S_12 == del_S_1c2)
    mprintf('\n\n del_S is a state function');
```

```
else
    mprintf('\n\n del_S is a path function');
end
if((Q_12 == Q_1a2)&(Q_12 == Q_1b2)&(Q_12 == Q_1c2))
    mprintf('\n\n Q is a state function');
else
    mprintf('\n\n Q is a path function');
end
if((W_12 == W_1a2)&(W_12 == W_1b2)&(W_12 == W_1c2))
    mprintf('\n\n W is a state function');
else
    mprintf('\n\n W is a path function');
end

//Comparison of work required by isothermal &
   adiabatic process
if(-(W_12)<-(W_1b2))
    mprintf('\n\n  Work required by isothermal
       process is less than the work required by an
       adiabatic process');
else
    mprintf('\n\n Statement is incorrect');
end
//end
```

Chapter 8

Third Law of Thermodynamics

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

```
//Chemical Engineering Thermodynamics
//Chapter 8
//Third Law of Thermodynamics

//Example 8.1
clear;
clc;

//Given
C_ps = 0.1;//Molal heat capacity of copper at 20 K
Ti = 0;//Initial temperature in K
Tf = 20;//melting point in K
Tb = 300;//boiling point in K

//To calculate the absolute entropy of copper at 300
    K
//From equation 8.4(page no 164)
a = C_ps/(Tf^3);// a is the charateristic constant
C_p = [0.1 0.80 1.94 3.0 3.9 5.0];
//T1 = log(T);
T1 = [1.301 1.6021 1.7782 1.9031 2.000 2.1761];
```

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

Chapter 9

Fluid Flow in Pipes and Nozzles

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

```
//Chemical Engineering Thermodynamics
//Chapter 9
//Fluid Flow in Pipes and Nozzles
//Example 9.1
clear;
clc;

//Given
R = 848;//gas constant in m Kgf/Kgmole K
M = 29;//molecular weight of air
g = 9.81;
T1 = 90+273;//initial temperature in K
y = 1.4;//gamma = Cp/Cv
W = 800/3600;//Mass rate of air in Kg/sec
P1 = 3.5;//initial pressure in atm
d = 2.5;//diameter of the pipe in cm

//To find out the pressure at the final point
v1 = (R*T1)/(M*P1*1.033*10^4);//specific volume in
```

```
cubic meter/Kg
u1 = (W*v1)/(%pi*(d^2*(10^-4))/4);//inital velocity in m/sec
//Assume final temperature as
T2 = [300 310];
//Assume specific heat capacity in J/KgK corresponding to the above temperature as
Cp = [2987.56 2983.56];
for i = 1:2
    us(i) = (g*y*R*T2(i)/M)^(1/2);//sonic velocity attained in m/sec
    u2(i) = ((u1^2)-((2*g*Cp(i)/M)*(T2(i)-T1)))^(1/2);//From equation 9.18 & 9.19 (page no 170)
end
if us(i)-u2(i) <= 1
    u2 = u2(i);
    T2 = T2(i);
else
end
v2 = u2*(%pi/4)*(d^2/10^4)*(1/W);
P2 = (P1*v1*T2)/(T1*v2);
mprintf('The pressure at the final point is %f atm',P2);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 9
//Fluid Flow in Pipes and Nozzles
//Example 9.2
clear;
clc;

```

```
//Given
A1 = 0.002;//inlet area in sq meter
A2 = 0.0005;//throat area in sq meter
P1 = 1.3*10^4;//inlet pressure in Kgf/sq m
P2 = 0.7*10^4;//throat pressure in Kgf/sq m
g = 9.81;
v = 12*10^-4;//specific volume in cubic m /Kg

//To find out the mass rate of alcohol
u2 = ((v*2*g*(P1-P2))/(1-((A2/A1)^2)))^(1/2);//
   throat velocity in m/sec
W = (u2*A2)/v;
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

```
//Chemical Engineering Thermodynamics
//Chapter 9
//Fluid Flow in Pipes and Nozzles
//Example 9.3
clear;
clc;

//Given
P1 = 50;//initial pressure in Kgf/sq m
T1 = 45+273;//initial temperature in K
g = 9.81;
y = 1.35;//gamma
R = 848;//gas constant in m Kgf/Kgmole K
M = 29;//molecular weight of air
d = 1;//pipe diameter in cm

//(i)To plot velocity,specific volume,mass velocity
```

```
against P2/P1
//(ii)To calculate the critical pressure,critical mass velocity and mass rate of flow
//(i)Plotting of graph
V1 = (R*T1)/(M*P1*1.033*10^4);//initial volume of the gas in cubic m/Kg
//P3 = P2/P1 (say)
//Assume P3 values as
P3 = [1.0 0.8 0.6 0.4 0.2 0.1 0];
G = [0 0 0 0 0 0 0];
for i = 1:7
    u2(i) = (((2*g*y*R*T1)/((y-1)*M))*(1-(P3(i)^((y-1)/y))))^(1/2);//final velocity in m/sec
end
for i = 1:6
     v2(i) = V1/(P3(i)^(1/y));//final specific volume in cubic meter/Kg
end
for i = 1:6
    G(i) = u2(i)/v2(i);//Mass velocity in Kg/sq m sec
end

clf;
xset('window',4);
plot(P3,u2,"o-");
xtitle("Velocity vs P2/P1","P2/P1","Velocity");
xset('window',5);
plot(P3,G,"+-");
xtitle("Mass velocity vs P2/P1","P2/P1","Mass velocity");
xset('window',6);
P_3 = [1.0 0.8 0.6 0.4 0.2 0.1];
plot(P_3,v2,"*-");
xtitle("Sp. volume vs P2/P1","P2/P1","Specific volume");

//(ii)Calculation of critical pressure,critical mass
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 9
//Fluid Flow in Pipes and Nozzles
//Example 9.4
clear;
clc;

//Given
A1 = 0.1;//Inlet area in sq meter
u1 = 60;//inlet velocity in m/sec
v1 = 0.185;//inlet specific volume in cubic meter/Kg
```

```
H1 = 715;//inlet enthalpy in Kcal/Kg
H2 = 660;//exit enthalpy in Kcal/Kg
v2 = 0.495;//exit specific volume in cubic meter/Kg
g = 9.81

//To calculate the area at exit of nozzle and hence decide the type of the nozzle
//From the first law
u2 = ((u1^2)-(2*g*(H2-H1)*427))^(1/2);
W = (u1*A1)/v1;//Mass rate of gas in Kg/sec
A2 = (W*v2)/u2;//Area at exit of nozzle
if(A2 < A1)
    mprintf('The nozzle is convergent');
else
    mprintf('The nozzle is divergent');
end
//end
```

Chapter 10

Compressor

Scilab code Exa 10.1 To calculate the horsepower required

```
//Chemical Engineering Thermodynamics
//Chapter 10
//Compressor
//Example 10.1
clear;
clc;

//Given
V1 = 2.7;//flow rate of CO2 in cubic meter/min
T1 = 273-51;//temperature in K
P1 = 1;//initial pressure in Kgf/sq cm
P2 = 10;//final pressure in Kgf/sq cm
y = 1.3;//gamma
v1 = 0.41;//specific volume in cubic meter/Kg
H1 = 158.7;// initial enthalpy in Kcal/Kg
H2 = 188.7;//final enthalpy in Kcal/Kg

//process is isentropic
//To calculate the horsepower required

//(i)Assuming ideal gas behaviour
```

```
//From equation 10.3 (page no 189)
W = (y/(y-1))*(P1*1.03*10^4*V1)*(1-(P2/P1)^((y-1)/y)
   );//work in m Kgf/min
W1 = W/4500;
mprintf('(i)The horsepower required is %f hp',W1);

//(ii)Using the given data for CO2
//From equation 10.2 (page no 189)
W = -(H2 - H1);//work in Kcal/Kg
M = V1/v1;//Mass rate of gas in Kg/min
W1 = W*M*(427/4500);
mprintf('\n (ii)Compressor work is %f hp',W1);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 10
//Compressor
//Example 10.2
clear;
clc;

//Given
P1 = 1;//Initial pressure in atm
P2 = 29;//Final pressure in atm
C = 0.05;//Clearance
y = 1.4;//gamma of air

//To calculate the volumetric efficiency and the
   maximum possible pressure that can be attained in
    a single stage
//(i)Calulation of volumetric efficiency
//From equation 10.11 (page no 194)
```

```
V_E = 1+C-C*(P2/P1)^(1/y);
mprintf('(i)Volumetric efficiency is %f percent',V_E
   *100);

//(ii)Calculation of maximum pressure
V_E = 0;//Minimum efficiency
P2 = P1*(((1+C-V_E)/C)^y);
mprintf('\n (ii)The maximum  possible pressure
   attained is %f atm',P2);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 10
//Compressor

//Example 10.3
clear;
clc;

//Given
V_d = 5.15;//displacement volume in cubic meter/min
P1 = 1;//initial pressure in Kgf/sq cm
P2 = 8.5;//final pressure in Kgf/sq cm
C = 0.06;//Clearance
M_E = 0.8;//Mechenical efficiency
y = 1.31;//gamma

//To calculate the capacity and the actual horse
   power of the compressor
v1 = V_d*(1+C-(C*((P2/P1)^(1/y))));
```

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

Scilab code Exa 10.4 To Calculate the theoretical horse power required

```
//Chemical Engineering Thermodynamics
//Chapter 10
//Compressor

//Example 10.4
clear;
clc;

//Given
P1 = 1;//Initial pressure in Kgf/sq cm
Pn = 13;//Final pressure in Kgf/sq cm
V1 =27;//flow rate of gas in cubic meter/min
y = 1.6;//gamma of the gas
n = [1 2 3 4 7 10];//number of stages
mprintf('No of stages              Horse power in hp');
//To Calculate the theoretical horse power required
for i = 1:6
    W(i) = n(i)*(y/(y-1))*((P1*10^4)/4500)*V1*(1-(Pn/P1)^((y-1)/(n(i)*y)));
    mprintf('\n  %d',n(i));
    mprintf('                          %f',-W(i))
```

```
end
//end
```

Scilab code Exa 10.5 To find out the presure between stages

```
//Chemical Engineering Thermodynamics
//Chapter 10
//Compressor

//Example 10.5
clear;
clc;

//Given
P1 = 1;//Initial pressure in Kgf/sq cm
P4 = 200;//Final pressure in Kgf/sq cm
n = 4;//no of stages

//To find out the presure between stages
r = (P4/P1)^(1/n);//Compression ratio
P2 = r*P1;
mprintf('The pressure after 1st stage is %f Kgf/sq
   cm',P2);
P3 = r*P2;
mprintf('\n The pressure after 2nd stage is %f Kgf/
   sq cm',P3);
P4 = r*P3;
mprintf('\n The pressure after 3rd stage is %f Kgf/
   sq cm',P4);
//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

```
//Chemical Engineering Thermodynamics
//Chapter 11
//Liquefaction of Gases

//Example 11.1
clear;
clc;

//Given
P1 = 8.74;//Initial pressure in Kgf/sq cm
P2 = 2.41;//Final pressure in Kgf/sq cm
H1 = 327.13;//Enthalpy of inlet stream in Kcal/Kg
H2 = H1;//Enthalpy of exit stream in Kcal/Kg ,since
   throttling is isenthalpic
Hl = 26.8;//Enthalpy of liquid  at the final
   condition in Kcal/Kg
Hg = 340.3;//Enthalpy of gas at the final condition
    in Kcal/Kg
vl = 152*10^-5;//Specific volume of liquid at the
   final condition in cubic meter/Kg
```

```
vg = 0.509;//Specific volume of gas at the final condition in cubic meter/Kg
v1 = 0.1494;//Initial specific volume in cubic meter/Kg

//To Calculate the dryness fraction of exit stream and the ratio of upstream to downstream diameters
//(i)Calculation of the dryness fraction of exit stream
//From equation 3.13(a) (page no 82)
x = (H2- Hl)/(Hg-Hl);
mprintf('(i)The dryness fraction of the exit stream is %f',x);

//(ii)Calculation of the ratio of upstream to downstream pipe diameters
//From equation 3.13(b) (page no 82)
v2 = (v1*(1-x))+(x*vg);//Total specific volume at the final condition in cubic meter/Kg
//u1 = u2; since KE changes are negligible
//From continuity equation: A2/A1 = D2^2/D1^2 = v2/v1 ; let required ratio,r = D2/D1;
r = (v2/v1)^(1/2);
mprintf('\n (ii)The ratio of upstream to downstream diameters  is %f',r);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 11
//Liquefaction of Gases

//Example 11.2
clear;
```

```
clc;

//Given
P1 = 1000*1.033*10^4;//Initial pressure in Kgf/sq m
P2 = 1*1.033*10^4;//Final pressure in Kgf/sq m
T1 = 300;//Inital temperature in K
Cp = 7;//Specific heat of the gas in Kcal/Kgmole K
//Gas obeys the relation: v = (R*T)/P+(b*(T^2))
b = 5.4392*10^-8;//in cubic meter/Kgmole K^2

//To Calculate the temperature of the throttled gas
//From equation (a) (page no 212);which we got after integration
T2 = 1/((1/T1)-((b/Cp)*((P2-P1)/427)));
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

```
//Chemical Engineering Thermodynamics
//Chapter 11
//Liquefaction of Gases

//Example 11.3
clear;
clc;

//Given
//From the figure 11.8 (page no 216) & from figure A.2.7
H3 = 0;
H7 = -47;//in Kcal/Kg
H6 = -93;//in Kcal/Kg
H8 = 7;//in Kcal/Kg

```

```
//To Calculate the fraction of air liquified at steady state and temperature of air before throttling
//(i)Calculation of fraction of air liquified
//From equation 11.3 (page no 215)
x = (H8-H3)/(H8-H6);
mprintf('The fraction of air liquified is %f',x);

//(ii)Calculation of temperature
H4 = H3+(H7*(1-x))-(H8*(1-x));//enthalpy of the gas before throttling
//From figure A.2.7 temperature corresponds to pressure 160 atm and the enthalpy H4 is
T = -112;
mprintf('\n The temperature of air before throttling is %d deg celsius',T);
//end
```

Chapter 12

Refrigeration

Scilab code Exa 12.1 To Calculate the theoretical horse power required

```
//Chemical Engineering Thermodynamics
//Chapter 12
//Refrigeration

//Example 12.1
clear;
clc;

//Given
m = 500;//mass of ice produced per hour  in Kg
T1 = 15;//Initial temperature of water
T2 = -5;//Final temperature of ice
Ci = 0.5;//Specific  heat of ice in Kcal/Kg deg
    celsius
Cw = 1;//Specific heat of water in Kcal/Kg deg
    celsius
L_f = 79.71;//Latent heat of fusion in Kcal/Kg
Tf = 0;//Frezzing point of ice in deg celsius

//To Calculate the theoretical horse power required
Q2 = m*(Cw*(T1-Tf)+L_f+Ci*(Tf-T2));//Heat to be
```

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

Scilab code Exa 12.2 To Calculate the compressor load

```
//Chemical Engineering Thermodynamics
//Chapter 12
//Refrigeration

//Example 12.2
clear;
clc;

//Given
Ta = 298;//Initial temperature in K
Tb = 203;//Final temperature in k
T1 = 298;//Water temperature in K
n = 1;//Kgmole of CO2
//Cp = 5.89+0.0112T ; Specific heat of CO2 in Kcal/Kgmole K

//To Calculate the compressor load
//From equation 12.2a and b (page no 221)
function y = f(T)
    y = ((T1-T)/T)*n*(5.89+0.0112*T);
endfunction
W = intg(Ta,Tb,f);
mprintf('The compressor load is %f Kcal/Kgmole',W);
//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

```
//Chemical Engineering Thermodynamics
//Chapter 12
//Refrigeration

//Example 12.3
clear;
clc;

//Given
//Consider the figure 12.4 (page no 226)
m = 5;//tonnes of refrigeration
T1 = 273-10;//temperature of the saturated vapour in
    K
T2 = 273+35;//temperature of the super heated vapour
    in K
T3 = 273+25;//temperature of the saturated liquid in
    K
T4 = 273+25;//temperature of the wet vapour in K
H1 = 341.8;//enthalpy of the saturated vapour in
    Kcal/Kg
H2 = 409.0;//enthalpy of the super heated vapour in
    Kcal/Kg
H3 = 350.0;//enthalpy of the saturated liquid in
    Kcal/Kg
H4 = 71.3;//enthalpy of the wet vapour in Kcal/Kg

//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
//(i)Calculation of the C.O.P of the compression
    cycle
//From equation 12.6 (page no 226)
C.O.P = (H1-H4)/(H2-H1);
mprintf('(i)C.O.P of the compression cycle is %f',C.
    O.P);

//(ii)Calculation of mass of refrigerant required
//From equation 12.7 (page no 226)
M = (m*50.4)/(H1-H4);
mprintf('\n (ii)The mass of refrigerant required is
    %f Kg/mt',M);

//(iii)Calculation of the compressor horse power
//From equation 12.5 (page no 226)
C_hp = (H2-H1)*M*(427/4500);
mprintf('\n (iii)The compressor horse power is %f hp
    ',C_hp);

//(iv)Calculation for reversed Carnot cycle
//From equation 12.1 (page no 220)
C.O.P = T1/(T3-T1);
mprintf('\n\n (iv)C.O.P for the reversed Carnot
    cycle is %f',C.O.P);
Q2 = m*50.4*(427/4500);//in hp
C_hp = Q2/C.O.P;
mprintf('\n    Compressor horse power for the
    reversed Carnot cycle is %f hp',C_hp);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 12
//Refrigeration

//Example 12.4
clear;
clc;

//Given
//Water at 20 deg cel is chilled to 10 deg cel by flash evaporation
Pv = 0.012;//Vapour pressure of water at 10 deg celsius in Kgf/sq.cm
H1 = 20.03;//Enthalpy of liquid water at 20 deg cel in Kcal/Kg
H2 = 10.4;//Enthalpy of liquid water at 10 deg cel in Kcal/Kg
Hv = 601.6;//Enthalpy of saturated vapour at 10 deg cel in Kcal/kg

//To calculate the pressure in the tank and the amount of make up water required
P = Pv;//pressure in the tank = vapour pressure of water
mprintf('The pressure in the tank is %f Kgf/sq.cm',P);
//From equation 12.8 (page no 234)
x = (H1-H2)/(Hv-H2);
mprintf('\n The amount of make up water required is %f Kg',x);
//end
```

Chapter 13

Thermodynamics in Phase Equilibria

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.1
clear;
clc;

//Given
//N2 obeys the relation : Z = 1+(2.11*10^-4*P)
Tc = 126;//Critical temperature in K
Pc = 33.5;//Critical pressure in atm
T = 373;//in K
P = 100;//in atm

//To Calculate the fugacity of N2 at 373K and 100 atm
//(i)Using the Z relation given above
```

```
//From equation 13.12 (page no 239)
phi = %e^(2.11*10^-4*(P-0));//fugacity coefficient
f = phi*P;
mprintf('(i)The fugacity of N2 using the given Z relation is %f atm',f);

//(ii)Using the fugacity chart given in figure A.2.9
Pr = P/Pc;//Reduced pressure in atm
Tr = T/Tc;//Reduced temperature in K
//From figure A.2.9,
phi = 1.04
f = phi*P;
mprintf('\n (ii)The fugacity of N2 using the fugacity chart is %f atm',f);
//end
```

Scilab code Exa 13.2 To Calculate the fugacity of liquid water

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.2
clear;
clc;

//Given
P1 = 50*1.03*10^4;//Initial pressure in Kgf/sq m
T = 373;//Temperature in K
P2 = 1.03*10^4;//Final pressure in Kgf/sq m
V = 0.001*18;//Volume in cubic meter
R = 848;//gas constant in m Kgf/Kgmole K

//To Calculate the fugacity of liquid water
//From equation 13.13(page no 240)
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.3
clear;
clc;

//Given
x1 = 0.1;//mole fraction of methane
x2 = 0.9;//mole fraction of propane
P = [28.1 31.6 35.1];//Pressure in Kgf/sq cm are
K1 = [5.8 5.10 4.36];//Vapourisation constants of methane at the corresponding presssures
K2 = [0.61 0.58 0.56];//Vapourisation constants of propane at the correspondig pressures

//To Calculate the bubble point pressure of the solution
//From equation 13.27 (page no 245)
for i = 1:3
    y1(i) = K1(i)*x1;//mole fraction of methane in the vapour phase
    y2(i)= K2(i)*x2;//mole fraction of propane in
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.4
clear;
clc;

//Given
T = [80.6 79.0 77.3 61.4];//Various temperature in deg cel
x1 = [0.0 15.0 29.0 100.0];//mole fraction of CHCl3 in liquid phase
y1 = [0.0 20.0 40.0 100.0];//mole fraction of CHCl3 in vapour phase
P1 = [1370 1310 1230 700];//Vapour pressure of CHCl3 in mm Hg
P = 760;//Total pressure in mm Hg

//To Calculate the equilibrium data i.e y/x and compare with the experimental values
```

```
//From equation 13.27 (page no 245);K = y1/x1 = Pi/P
mprintf('Temperature    Experimental   Calculated');

for i = 1:4
    mprintf('\n %f',T(i));
    if x1(i) == 0
        mprintf('     Not defined');
        else
 K_ex(i) = y1(i)/x1(i);
mprintf('        %f',K_ex(i));
 end
K_c(i) = P1(i)/P;
mprintf('      %f',K_c(i));
end

if K_ex(i) == K_c(i)
    then mprintf('\n\n The liquid solution is perfect');
else
    mprintf('\n\n The liquid solution is imperfect');
end
//end
```

Scilab code Exa 13.5 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.5
clear;
clc;

//Given
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.6
clear;
clc;

//Given
x1 = 0.1;//Mole fraction of dichloromethane (CCl2H2)
x2 = 0.9;//Mole fraction of methyl acetate (C3H6O2)
M1 = 85;//Molecular weight of CCl2H2
M2 = 74;//Molecular weight of C3H602
D1 = 1.3163;//Density of CCl2H2 in gm/cc
D2 = 0.9279;//Density of C3H6O2 in gm/cc

//To Calculate the volume of 10% dichloromethane
   solution
V1 = M1/D1;//Specific volume of pure CCL2H2 in cc/
   gmole
V2 = M2/D2;//Specific volume of C3H6O2 in cc/gmole
//From equation 13.62(page no 256)& 13.78 (page no
   257)
V_e = x1*x2*(1.2672-0.771*x1);//excess volume in cc/
   gmole
V = V1*x1+V2*x2+V_e;
mprintf('The volume of 10 percent dichloromethane is
    %f cc/gmole',V);
```

```
//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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.7
clear;
clc;

//Given
x_T = 0.957;//mole fraction of Toluene
x_D = 0.043;//mole fraction of 1,2-dichloroethane
t = [90; 100; 110];//temperature in deg cel
R = 1.98;//gas constant in Kcal/Kgmole K

//To Calculate the vapour pressure of the solution, bubble point at 686 mm Hg and the vapour composition at equilibrium,
//compare the experimental value of 91.2% toluene in vapour with the calculated value & calculate the free energy of mixing
//(1) Calculation of vapour pressure
mprintf('(1)Temp(deg cel)      P_T(mmHg)             P_D(mmHg)             P_s(mmHg)');
for i = 1:3
    P_T(i) = 10^(6.95464-(1344.8/(219.482+t(i))));//Given as equation(a)(page no 260)
    P_D(i) = 10^(7.03993-(1274.079/(223+t(i))));//Given as equation(b)(page no 260)
    P_s(i) = x_T*P_T(i)+x_D*P_D(i);//pressure of the solution in mm Hg
```

```
    mprintf('\n    %f',t(i));
    mprintf('           %f',P_T(i));
    mprintf('         %f',P_D(i));
    mprintf('          %f',P_s(i));
end

//(2)Calculation of bubble point and comparison of values
clf;
plot(t,P_s);
xtitle("t vs P_s","t","P_s");
T = interpln([P_s';t'],686);
P = 686;//pressure of solution in mm Hg
y_T_e = 0.912;//experimental value of mole fraction of toluene
//From the graph we found that the temperature at P = 686 mm Hg is
//t = 105.3;//in deg cel
mprintf('\n\n(2)The bubble point is %f deg cel',T);
//From equation (a)(page no 260)
P_T = 10^(6.95464-(1344.8/(219.482+T)));//vapour pressure of Toluene in mmHg
//From equation 13.27 (page no 245)
y_T_c = (x_T*P_T)/P;
y_D_c = 1-y_T_c;
mprintf('\n  The vapour composition of toluene is %f',y_T_c);
mprintf('\n  The vapour composition of 1,2-dichloroethane is %f',y_D_c);
e = ((y_T_e-y_T_c)/y_T_e)*100;
mprintf('\n The percentage error is %f percent',e);

//(3)Calculation of free energy
del_F = R*(T+273)*((x_T*log(x_T))+(x_D*log(x_D)));
mprintf('\n\n(3)The free energy of mixing is %f Kcal/Kgmole',del_F);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.8
clear;
clc;

//Given
//Consider the diagram shown in page no 263
w1 = 100;//weight of LiBr entered as feed in the evaporator per hour in Kg
x1 = 0.45;//weight  fraction of LiBr entered as feed
x2 = 0;//weight fraction of steam in the LiBr soln
x3 = 0.65;//weight fraction of LiBr formed as product
H1 = -39;//Enthalpy of 45% solution at 25 deg cel in Kcal/Kg
H3 = -4.15;//Enthalpy of 65% solution at 114.4 deg cel in Kcal/Kg
H2 = 649;//Enthalpy of superheated steam at 100 mmHg and 114.4 deg cel in Kcal/Kg

//To Calculate the heating load required for the process
//According to material balance
w3 = (w1*x1)/x3;//weight of LiBr solution formed after evaporation per hour in Kg
w2 = w1-w3;// weight of steam formed in Kg/hr
//According to energy balance
Q = (w2*H2)+(w3*H3)-(w1*H1);
```

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

Scilab code Exa 13.9 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.9
clear;
clc;

//Given
// 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
//end
```

Scilab code Exa 13.10 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.10
clear;
clc;

//Given
//The given example is a theoretical problem and does not involve any numerical computation
```

```
//end
```

Scilab code Exa 13.11 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.11
clear;
clc;

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.12
clear;
clc;

//Given
x_A = [0 0.0435 0.0942 0.1711 0.2403 0.3380 0.5981];
   //mole fraction of acetic acid
p_A = [0 17.2 30.5 46.5 57.8 69.3 95.7];//partial
   pressure of acetic acid in mmHg
```

```
P_T1 = 202;//vapour pressure of toulene in mmHg
P_T2_ex = 167.3;//experimental partial pressure in mmmHg

//To Calculate the partial pressure of toulene in the solution and check with the experimental value
//From the equation 13.95,
//ln(P_T2/P_T1) = -intg(x_A/((1-x_A)*p_A))
for i = 1:7
    if (p_A(i) ~= 0)
    x(i) = (x_A(i)/((1-x_A(i))*p_A(i)))*10^4
    end
end
plot(x,p_A);
xtitle(" ","(x_A/((1-x_A)*p_A))*10^4", "p_A");
//Area of the graph drawn is
A = -0.138;
P_T2 = (%e^A)*P_T1;
e = ((P_T2-P_T2_ex)*100)/P_T2_ex;
mprintf('The partial pressure of toulene is %f mmHg',P_T2);
mprintf('\n This deviates %i percent from the reported value',e);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.13
clear;
```

```
clc;

//Given
P = 760;//pressure at maximum boiling azeotrope of A and B in mmHg
x_A = 0.6;//mole fraction of A in liquid phase
x_B = 0.4;//mole fraction of B in liquid phase
p_A = 600;//vapour pressure of A at 90 deg cel
p_B = 300;//vapour pressure of B at 90 deg cel

//To Check whether the activity coefficient of the solution can be represented by the Margules equation
y_A = P/p_A;//Activity coefficient of A
y_B = P/p_B;//Activity coefficient of B
//From the Margules equation or equation (a) & (b)
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))];
V = [log(y_A); log(y_B)];
W = U\V;
//Now the value of constants A and B in equations(a)&(b) are given as
A = W(1);
B = W(2);
//let us assume
x_A = [0.0 0.2 0.4 0.6 0.8 1.0];
x_B = [1.0 0.8 0.6 0.4 0.2 0.0];
//C = lny_A; D = lny_B; E = ln(y_A/y_B)
for i = 1:6
    C(i) = (x_B(i)^2)*(2*(B-A)*x_A(i)+A);
    D(i) = (x_A(i)^2)*(2*(A-B)*x_B(i)+B);
    E(i) = C(i)-D(i);
end
clf;
plot(x_A,E);
xtitle(” ”,”x_A”,”ln(y_A/y_B)”);
a = get(”current_axes”);
set(a,”x_location”,”origin”);
```

```
//Since the graph drawn is approximately symmetrical .Thus it satisfies the Redlich-Kister Test
mprintf('The actvity coefficients of the system can be represented by Margules equation');
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.14
clear;
clc;

//Given
P = 760;//Total pressure of the mixture in mmHg
T = [80 90 95 100];//Temperature in deg celsius
P1 = [87.4 129.0 162.0 187.0];//vapour pressure of 1,1,2,2-tetrachloroethane in mmHg
P2 = [356 526 648 760];//Vapour pressure of water in mmHg

//To Calculate the composition of the vapour evolved
clf;
plot2d(T,P1,style=3);
plot2d(T,P2,style=5);
xtitle(" ","Temp in deg cel","Vapour pressure in mmHg");
legend("1,1,2,2-tetrachloroethane","Water");
//From the graph we conclude that at 93.8 deg cel
P1 = 155;//in mm Hg
P2 = 605;//in mm Hg
y_1 = P1/P;
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.15
clear;
clc;

//Given
T = [146.2 142.3 126.1 115.9 95.0 98.0 100];//Temperature in deg cel
P1 = [760.0 685.0 450.3 313.0];//Vapour pressure of 1,1,2,2-tetrachloroethane at the coressponding temperature in mm Hg
P2_5 = 648.0;//Vapour pressure of water at 95 deg cel in mm Hg
P2_6 = 711.0;//Vapour pressure of water at 98 deg cel in mm Hg
P = 760;//Total pressure of mixture in mm Hg

x1 = [0 0 0 0 0 0 0];
//To plot a graph between temperature and vapour phase composition
for i = 1:4
    x1(i) = P1(i)/P;//mole fraction of 1,1,2,2-
```

```
tetrachloroethane
end
x2_5 = P2_5/P;//mole fraction of water at 95 deg cel
x2_6 = P2_6/P;//mole fraction of water at 98 deg cel
x1(5) = 1-x2_5;
x1(6) = 1-x2_6;

clf;
plot(x1,T);
xtitle("","mole fraction of 1,1,2,2-tetrachloroethane","Temperature in deg cel");
mprintf('The required graph has been ploted in the graphic window');
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.16
clear;
clc;

//Given
//B = -(1.203*10^10)*(T^2.7); second virial coefficient, T is in K
//log P = 6.95464-(1344.8/(219.482+t))...(a);Vapour pressure of toulene
t = 107.2;//Temperature in deg cel
T = t+273.16;//in K
H_ex = 7964;//experimental value of heat of
```

```
vapourisation in Kcal/Kgmole
d = 800;//density of liquid toulene in Kg/cubic meter
R = 1.98;//gas constant in Kcal/Kgmole K
M = 92.14;//molecular weight of toulene

//To Calculate the heat of vapourization of toulene by using ideal gas law, second virial coefficient but neglecting vl and including vl
//From equation (a), let K = dlogP/dT
K = 1344.8/(219.482+t)^2;
//(i)Using ideal gas behaviour
//From equation 13.112(page no 286)
H_c = (2.303*R*(T^2))*K;
mprintf('(i)The heat of vapourization  using ideal gas behaviour is %f Kcal/Kgmole',H_c);
D = ((H_c-H_ex)/H_c)*100;
mprintf('\n    The deviation is %f percent',D);

//(ii)Using second virial coeff but neglecting vl
//From equation(a)
P = 10^(6.95464-1344.8/(219.482+t));//in mm Hg
P1 = P*1.033*10^4/760;//in Kgf/sq m
B = -((1.203*10^10)/(T^2.7))*10^-3;//in cubic meter/Kgmole
//From equation 13.111 (page no 286) neglecting vl,
l = (R*T)+((B*P1)/427);//in Kcal/Kgmole
H_c = K*2.303*T*l;
mprintf('\n\n(ii)The heat of vapourisation using second virial coefficient but neglecting vl is %f Kcal/Kgmole',H_c);
D = ((H_c-H_ex)/H_c)*100;
mprintf('\n    The deviation in this case is %f percent',D);

//(iii)Using second virial coeff including vl
vl = M/d;//Liquid specific volume in cubic meter/Kgmole
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.17
clear;
clc;

//Given
H_ex = 539;//Heat of vapoization of water in Kcal/Kg
Tc = 647;//Critical temperature in K
Pc = 218;//Critical pressure in atm
Tb = 373;//Boiling point of water in K
t = 100;//temperature in deg cel
M = 18;//Molecular weight of water
P = 1;//pressure at boiling point in atm
P1 = 1.033*10^4;//pressure in Kgf/sq m

//To Calculate the heat of vapourisation of water by Vishwanath and Kuloor method and by Riedel's method and compare with the experimental value
```

```
//(i) Using Vishwanath and Kuloor method
H_c = (4.7*Tc*((1-(P/Pc))^0.69)*log(P/Pc))/((1-(Tc/Tb))*18);
mprintf('(i)The heat of vapourisation of water using Vishwanath and Kuloor method is %f Kcal/Kg',H_c);
D = (H_c-H_ex)*100/H_c;
mprintf('\n    The deviation occurs using this method is %f percent',D);

//(ii)Using Riedel's method
H_c = (Tb*2.17*(log(218)-1))/((0.93-(Tb/Tc))*18);
mprintf('\n\n(ii)The heat of vapourisation of water using Riedel method is %f Kcal/Kg',H_c);
D = (H_c-H_ex)*100/H_c;
mprintf('\n    The deviation occurs using this method is %f percent',D);

//(iii)By using given vapour equation; logP = 8.2157-(2218.8537/(273.16+t)), t is in deg cel
//From steam table,
Vv = 1.673;//in cubic meter/Kg
Vl = 0.001;//in cubic meter/Kg
H_c = (2218.8/(273.16+t)^2)*(2.3*Tb*P1*(Vv-Vl)/427);
mprintf('\n\n(iii)The heat of vapourisation using the given vapour equation is %f Kcal/Kg',H_c);
D = (H_c-H_ex)*100/H_c;
mprintf('\n    The deviation occurs using this method is %f percent',D);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.18
clear;
clc;

//Given
T1 = 273-87;//temp in K
T2 = 273;//temp in K
H1 = 115;//Latent heat of saturated ethane at 1 atm and -87 deg cel in Kcal/Kg
H2_ex = 72.44;//Experimental value of latent heat at 0 deg cel in Kcal/Kg
Tc = 306;//Critical temperature in K
M = 30;//Molecular weight of ethane

//To Calculate the latent heat of saturated ethane at 0 deg cel
Tr1 = T1/Tc;//reduced temp in K
Tr2 = T2/Tc;//reduced temp in K
//(i)Using Waton's method:
H2_c = H1*((1-Tr2)/(1-Tr1))^0.38;
mprintf('(i)The latent heat of saturated ethane at 0 deg cel using Waton method is %f Kcal/Kg',H2_c);
D = (H2_ex-H2_c)*100/H2_ex;
mprintf('\n   The deviation occurs using this method is %f percent',D);

//(ii)Using Vishwanath and Kuloor method
//From equation 13.117 (page no 289)
n = (0.00133*(H1*M/T1)+0.8794)^(1/0.1);
H2_c = H1*((1-Tr2)/(1-Tr1))^n;
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);
D = (H2_ex-H2_c)*100/H2_ex;
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 13
//Thermodynamics in Phase Equilibria

//Example 13.19
clear;
clc;

//Given
H_s_ex = 32.7;//experimental value of latent heat of the solution in KJ/mole
x1 = 0.536;//mole percent of toulene in the solution
x2 = 1-0.536;//mole percent of 1,1,1-trichloroethane in the solution
H1 = 33.34;//Latent heat of toulene in KJ/gmole
H2 = 29.72;//Latent heat of 1,1,1-trichloroethane in KJ/gmole
He = 0;//excess enthalpy is neglected
Cp1 = 39.55;//Specific heat of toulene in cal/gmole deg cel
Cp2 = 24.62;//Specific heat of 1,1,1-trichloroethane in cal/gmole deg cel
T_D = 100;//dew point temperature in deg cel
T_B = 92.6;//bubble point temperature in deg cel

//To calculate the latent heat of the solution and compare it with the one which calculated from the
```

```
    given vapour pressure equation
//(i)Calculation of latent heat of the solution
//From equation 13.118 (page no 291)
H_s = H1*x1+H2*x2+He+(Cp1*x1+Cp2*x2)*10^-3*4.17*(T_D
   -T_B);
mprintf('(i)The latent heat of the solution is %f KJ
   /gmole',H_s);
D = ((H_s_ex-H_s)*100)/H_s_ex;
mprintf('\n    The deviation occurs using this
   method is %f percent',D);

//(ii)Calculation of latent heat from the vapour
   pressure equation
//From equation (a) (page no 291)
K = 1657.599/((273.16+5)^2);
H_s = (K*2.303*8.314*(273.16+5)^2)*10^-3;
mprintf('\n\n(ii)The latent heat of the solution is
   %f KJ/gmole',H_s);
D = ((H_s_ex-H_s)*100)/H_s_ex;
mprintf('\n    The deviation occurs using this
   method is %f percent',D);
//end
```

Chapter 14

Thermodynamics of Chemical Reactions

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.1
clear;
clc;

//Given
H_f_C2H4 = 12500;//Standard heat of formation of ethylene at 25 deg cel in Kcal/Kgmole
H_f_C2H4O = -11667;//Standard heat of formation of ethylene oxide at 25 deg cel in Kcal/Kgmole

//To Calculate the standard heats of reaction at 25 deg celsius
//The reaction is: C2H4 + (1/2)O2 - C2H4O
del_H_rxn = H_f_C2H4O-H_f_C2H4;//Since, Standard
```

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

Scilab code Exa 14.2 To Calculate the sensible heat required

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.2
clear;
clc;

//Given
T1 = 25+273;//Initial temperature in K
T2 = 450+273;//Final temperature in K
//Specific heat of sulphur dioxide is given by the relation:
//Cp = 7.116+9.512*10^-3*T+(3.511*10^-6)*T^2

//To Calculate the sensible heat required
//Basis: 1 Kgmole of sulphur dioxide
Q = 7.116*(T2-T1)+(9.512*10^-3*(T2^2-T1^2)/2)+((3.51*10^-6)*(T2^3-T1^3)/3);
mprintf('Sensible heat required is %d Kcal/Kgmole',Q);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.3
clear;
clc;

//Given
H_C2H4 = 12500;//Standard heat of formation  of ethylene at 25 de cel
H_C2H4O = -12190;//Standard heat of formation of ethylene oxide at 25 deg cel
H_CO2 = -94052;//Standard heat of formation of CO2 at 25 deg cel
H_H2O = -57798;//Standard heat of formation of H2O at 25 deg cel
T1 = 200;//temperature at which mixture entered in deg cel
Ti = 25;//intermediate temperature in deg cel
T2 = 260;//product temperature in deg cel
Cp_air_a = 7;//Mean specific heat for 25 to 200 deg cel in Kcal/Kgmole
Cp_C2H4_a = 18;//Mean specific heat for 25 to 200 deg cel in Kcal/Kgmole
//Mean specific heat for 25 to 260 deg cel in Kcal/Kgmole are given as:
Cp_C2H4_b = 19;
Cp_C2H4O_b = 21;
Cp_O2_b = 7.30;
Cp_N2_b = 7.00;
Cp_CO2_b = 10.00;
Cp_H2O_b = 8.25;
//Basis: 1 Kgmole of ethylene as feed
n_air = 9;//Kgmoles
n_C2H4 =1;//Kgmoles
n_C2H4_1 = 0.6//ethylene consumed while converting in C2H4O in Kgmoles (Rxn 1)
```

```
n_C2H4_2 = 0.3;//ethylene burnt completely to CO2 in Kgmoles (Rxn 2)

//To Calculate the heat must be removed if the product temperature should not exceed 260 deg cel
n_O2 = n_air*0.21;//Kgmoles of O2 fed
n_N2 = n_air-n_O2;//Kgmoles of N2 fed
//Rxn 1: (0.6)C2H4 + (0.3)O2 - (0.6)C2H4O;...(i) 60% of C2H4 is converted to C2H4O
n_O2_1 = n_C2H4_1/2;//Kgmoles of oxygen consumed
n_C2H4O_1 = n_C2H4_1;//C2H4O formed in Kgmoles
//Rxn 2: (0.3)C2H4 + (0.9)O2 - (0.6)CO2+ (0.6)H20;...(ii) 30%conversion
n_O2_2 = 3*n_C2H4_2;//Kgmoles of O2 reacted
n_CO2_2 = 2*n_C2H4_2;//Kgmoles of CO2 formed
n_H2O_2 = 2*n_C2H4_2;//Kgmoles of H2O formed
n_C2H4_r = n_C2H4 - n_C2H4_1 - n_C2H4_2;//unreacted ethylene in Kgmoles
n_O2_r = n_O2 - n_O2_1-n_O2_2;//unreacted O2 in Kgmoles
//The overall rxn is given by (i)&(ii),
//(0.9)C2H4 + (1.2)O2 - (0.6)C2H4O + (0.6)CO2 + (0.6)H2O...(iii)
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
Q1 = (n_C2H4*Cp_C2H4_a + n_air*Cp_air_a)*(Ti-T1);//Sensible heat in feed in Kcal
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
Q = Q1+Q2+del_H;
mprintf('The heat to be removed is %f Kcal so that the product temperature is 260 deg celsius',-Q);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.4
clear;
clc;

//Given
//Basis: 1Kgmole of C0
//CO + (1/2)O2 - CO2
//Whem mixture entered,their compositions are given as:
n_CO = 1;//Kgmole
del_H = -67636;//Standard heat of reaction in Kcal/Kgmole at 25 deg cel
T1 = 95;//Temperature at which mixture entered in deg celsius
T2 = 25;//Intermediate temperature in deg celsius
//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)
Cpm_CO = 6.95;
Cpm_O2 = 7.1;
Cpm_N2 = 6.95;

//To Calculate the theoretical flame temperature when both air and CO2 enter at 95 deg celsius
n_O2 = 1;//Kgmole, as 100% excess air is given
n_N2 = n_O2*(0.79/0.21);//Kgmole
//After the rxn:
```

```
n_CO2 = n_CO;//Kgmole
n_O2_r = n_O2-(n_CO/2);//remaining Kgmole of O2
//In equation 14.18 (page no 307) say: H_2-H_R = Ha, H_P-H_3 = Hb, Hc = del_H+Ha & Ht = Hc+Hb
Ha = (n_CO*Cpm_CO + n_O2*Cpm_O2 + n_N2*Cpm_N2)*(T2-T1);//in Kcal/Kgmole
Hc = del_H+Ha;//in Kcal/Kgmole
//For calculating Hb let us assume the temperature as
T = [530 1000 1650];//in deg celsius
Cpm_CO2 = [10.85 12 12.75];//Mean specific heat of CO2 at the coresspondig temperature (from figure 14.4)
Cpm_O2 = [7.55 7.8 8.3];//Mean specific heat of O2 at the coresspondig temperature (from figure 14.4)
Cpm_N2 = [7.15 7.5 7.85];//Mean specific heat of N2 at the coresspondig temperature (from figure 14.4)
for i = 1:3
    Hb(i) = (n_CO2*Cpm_CO2(i)+n_O2_r*Cpm_O2(i)+n_N2*Cpm_N2(i))*(T(i)-T2);//in Kcal/Kgmole
    Ht(i) = Hc+Hb(i);//in Kcal/Kgmole
end
clf;
plot(T,Ht);
xtitle(" ","Temperature, deg celsius","Ht in Kcal/Kgmole");
a = get("current_axes");
set(a,"x_location","origin");
Tf = interpln([Ht';T],0);
mprintf('The adiabatic temperature is read as %d degree celsius',Tf);
//end
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.5
clear;
clc;

//Given
T = 298;//Temperature in Kelvin
//Standard enthalpy in Kcal/Kgmole of the following components at 298 K are given as
H_SO2 = -70960;
H_SO3 = -94450;
H_O2 = 0;
//Standard entropy in Kcal/Kgmole K of the following components at 298 K are given as
S_SO2 = 2.48;
S_SO3 = -19.7
S_O2 = 0;
//Basis: 1 Kgmole of SO2
//SO2 +(1/2)O2 - SO3

//To Calculate the standard free energy for the reaction
n_SO2 = 1;//Kgmole of SO2 fed
n_O2 = (1/2)*2;//Kgmole of O2  fed as 100% excess O2 is given
n_SO3 = n_SO2;//Kgmole of SO3 formed
```

```
//From equation 14.38 (page no 312)
del_F = (H_SO3-(T*S_SO3))-(H_SO2-(T*S_SO2))-(H_O2-(T*S_O2));
mprintf('The standard free energy for the reaction at 25 degree celsius is %f Kcal/Kgmole',del_F);
//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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.6
clear;
clc;

//Given
//SO2 + (1/2)O2 - SO3
//Basis: 1 Kgmole of SO2
n_SO2 = 1;// SO2 fed in Kgmole
//From table 14.1 (page no 301)
//alpha values for the following components are given as
a_SO2 = 7.116;
a_O2 = 6.148;
a_SO3 = 6.077;
//beta values for the following components are given as
b_SO2 = 9.512*10^-3;
b_O2 = 3.102*10^-3;
b_SO3 = 25.537*10^-3;
//Standard enthalpy of the following components at
```

```
25 deg cel in Kcal/Kgmole are given as
H_SO2 -70960;
H_O2 = 0;
H_SO3 = -94450;
//Standard free energy of the following components at 25 deg cel in Kcal/Kgmole K are given as
F_SO2 = -71680;
F_O2 = 0;
F_SO3 = -88590;
n_O2 = n_SO2;//O2 fed in Kgmole; since 50 mole percent mixture of SO2 & O2 is fed
n_SO3 = n_SO2;//SO3 formed in Kgmole
n_O2_e = n_O2-(n_O2/2);//Kgmoles of O2 in exit gas
n_O2_r = n_O2/2;//Kgmoles of O2 reacted
R = 1.98;//gas constant in Kcal/Kgmole K

//To show  the variation of the standard heats of reaction with temperature and the equilibrium constant with temperature graphically in the given temperature range
//(i)Variation of the standard heats of reaction with temperature
del_H = (n_SO3*H_SO3)-(n_O2_r*H_O2)-(n_SO2*H_SO2);// in Kcal/Kgmole
del_F = (n_SO3*F_SO3)-(n_O2_r*F_O2)-(n_SO2*F_SO2);// in Kcal/Kgmole
//From equation 14.10 (page no 301)
del_a = (n_SO3*a_SO3)-(n_O2_r*a_O2)-(n_SO2*a_SO2);
del_b = (n_SO3*b_SO3)-(n_O2_r*b_O2)-(n_SO2*b_SO2);
//In equation 14.11 (page no 302), substituting del_H at
T = 298;//in deg cel
I = del_H - del_a*T - (del_b*(T^2)/2);// integrating constant
mprintf('(i)The standard heat of reaction at any tempperature can be calculated by the relation:');
mprintf('\n     del_Ht = %fT + %fT^2 %f',del_a,del_b
```

```
/2,I);

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.7
clear;
clc;

```

```
//Given
//SO2 + (1/2)O2 - SO3
//Basis: 1 Kgmole of SO2
n_SO2 = 1;// SO2 fed in Kgmole
n_O2 = n_SO2;//O2 fed in kgmole

//To Calculate the conversion of SO2 to SO3 at 1atm and at various temperature
//(1)Calculate the conversion of SO2 to SO3
P = 1;//Pressure in atm
T = 850;//Temperature in K
m = 1-1-(1/2);
//From example 14.6
Ta = [700 800 825 850 900 1000 1100 1300 1500];
Ka = [395.40 52.51 34.60 23.44 11.59 3.527 1.48 0.398 0.0016];
clf;
xset('window',2);
plot2d(Ta,Ka,style=3);
xtitle("Equilibrium constant vs Temperature","Temperature in K","Ka");
Ka1 = interpln([Ta;Ka],850);
//Let Nc be the moles of SO3 at equilibrium
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];
//From equation 14.49 (page no 320) and using the given data ,we got equation (b) (page no 323)
for i = 1:17
    Ka(i) = (((n_SO2+n_O2-0.5*Nc(i))/(n_O2-0.5*Nc(i)))^(1/2))*(Nc(i)/(n_SO2-Nc(i)));
end
xset('window',1);
plot2d(Nc,Ka,style=2);
xtitle("Equilibrium constant vs Kgmoles of SO3","Kg moles of SO3","Ka");
Nc1 = interpln([Ka;Nc],Ka1);
C = Nc1*100/n_SO2;
mprintf('(1)The conversion of SO2 to SO3 at 1atm and
```

```
850K is %f percent',C);

//(2)Calculation of conversion at 1 atm and 850 K under the following conditions
//(i) Given:
n_N2 = 3.75;//Kgmoles of N2 fed
//Let Nc be the moles of SO3 at equilibrium
Nc = [0.85 0.87 0.90];
//From equation 14.49 (page no 320) and using the given data ,we got equation (c) (page no 324)
for i = 1:3
    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)));
end
xset('window',1);
plot2d(Nc,Ka2,style=5);
Nc2 = interpln([Ka2';Nc],Ka1);
C2 = Nc2*100/n_SO2;
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);

//(ii)SO3 is also sent along the original feed
n_SO3 = 1;//Kgmoles of SO3 fed
//Let Nc be the moles of SO3 at equilibrium
Nc = [0.80 0.86 0.92];
//From equation 14.49 (page no 320) and using the given data ,we got equation (d) (page no 326)
for i = 1:3
    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)));
end
xset('window',1);
plot2d(Nc,Ka3,style=6);
Nc3 = interpln([Ka3';Nc],Ka1);
C3 = Nc3*100/n_SO2;
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);

//(iii)Variation of SO2 to O2 ratio:
//(a)SO2:O2 = 1:1 ; This has been worked out in part 1
mprintf('\n    (iii)(a)The conversion of SO2 to SO3 at 1atm and 850K when SO2:O2 = 1:1 is %f percent',C);
Xc = Nc1/(n_SO2+n_O2-0.5*Nc1);

//(b)SO2:O2 = 1.1:0.5 ,Now
n_SO2 = 1.1;//Kgmoles of SO2 fed
n_O2 = 0.5;//Kgmoles of O2 fed
//Let Nc be the moles of SO3 at equilibrium
Nc = [0.9 0.91 0.92];
//From equation 14.49 (page no 320) and using the given data ,we got equation (e) (page no 327)
for i = 1:3
        Ka4(i) = (((n_SO2+n_O2-0.5*Nc(i))/(n_O2-0.5*Nc(i)))^(1/2))*(Nc(i)/(n_SO2-Nc(i)));
end
xset('window',1);
plot2d(Nc,Ka4,style=1);
Nc4 = interpln([Ka4';Nc],Ka1);
C4 = Nc4*100/n_SO2;
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);
Xc1 = Nc4/(n_SO2+n_O2-0.5*Nc4);

//(c)SO2:O2 = 1:0.5
n_SO2 = 1;//Kgmoles of SO2 fed
n_O2 = 0.5;//Kgmoles of O2 fed
//Let Nc be the moles of SO3 at equilibrium
Nc = [0.8 0.85 0.86 0.87];
//From equation (a)
for i = 1:4
```

```
    Ka5(i) = (((n_SO2+n_O2-0.5*Nc(i))/(n_O2-0.5*Nc(i)))^(1/2))*(Nc(i)/(n_SO2-Nc(i)));
end
xset('window',1);
plot2d(Nc,Ka5,style=4);
Nc5 = interpln([Ka5';Nc],Ka1);
C5 = Nc5*100/n_SO2;
mprintf('\n   (iii)(c)The conversion of SO2 to SO3 at 1atm and 850K when SO2:O2 = 1:0.5 is %f percent',C5);
Xc2 = Nc5/(n_SO2+n_O2-0.5*Nc5);

if(Xc2>Xc) and (Xc2>Xc1)
    mprintf('\n         SO2:O2 = 1:0.5 gives the maximum concentration of SO3 at equilibrium.');
else
    if(Xc1>Xc) and (Xc1>Xc2)
        mprintf('\n         SO2:O2 = 1.1:0.5 gives the maximum concentration of SO3 at equilibrium');
    else
        if(Xc>Xc1) and (Xc>Xc2)
            mprintf('\n         SO2:O2 = 1:1 gives the maximum concentration of SO3 at equilibrium');
        end
    end
end

//(3)Conversion of SO2 to SO3 at 50 atm and 850 K when SO2:O2 = 1:1
n_SO2 = 1;//Kgmole of SO2 fed
n_O2 = 1;//Kgmoles of O2 fed
P = 50;//Pressure in atm
//From figure A.2.9
phi_SO2 = 0.99;
phi_SO3 = 0.972;
```

```
phi_O2 = 1;
//From equation 14.48 (page no320), Ka = Ky*(P^m)*K_phi
K_phi = phi_SO3/(phi_SO2*(phi_O2^2));
//Let Nc be the moles of SO3 at equilibrium
Nc = [0.99 0.985 0.97 0.96];
for i = 1:4
    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))));
end
xset('window',1);
plot2d(Nc,Ka6,style=3);
Nc6 = interpln([Ka6';Nc],Ka1);
C = Nc6*100/n_SO2;
mprintf('\n\n (3)The conversion of SO2 to SO3 at 50 atm and 850K  when SO2:O2 = 1:1 is %f percent',C);
legend("1 part","2.(i) part","2.(ii)part","2.(iii).(b)part","2.(iii).(c)part","3 part");
//end
```

Scilab code Exa 14.8 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.8
clear;
clc;

//Given
//The given example is a theoretical problem and it does not involve any numerical computation.
```

```
//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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.9
clear;
clc;

//Given
//2A(g) - B(g)+C(g)
T = 400;//Temperature in Kelvin
P = 1;//Pressure in atm
R = 1.98;//gas constant in Kcal/Kgmole K
del_Fo = 3000;//Standard free energy of the reaction in Kcal/Kgmole
n_A = 1;//Kgmoles of A
n_B = 0.1;//Kgmoles of B
n_C = 0.1;//Kgmoles of C

//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)To find out the equilibrium has been attained or not. If not then calculate the equilibrium composition
//P_B/P_C = 1 (Given)
```

```
n_T = n_A+n_B+n_C;//Total Kgmoles of the component
p_A = (n_A/n_T)*P;//Partial pressure of A
p_B = (n_B/n_T)*P;//Partial pressure of B
p_C = (n_C/n_T)*P;//Partial pressure of C
//Using the relation 14.36 (page no 312)
del_F = del_Fo + (R*T)*log((p_B*p_C)/(p_A^2));
if del_F == 0;
    then mprintf('1.Equilibrium has been attained.');
else
    mprintf('1.Equilibrium has not been attained.');
end
//Equilibrium composition
//At equilibrium del_F = 0
//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
//ln(p_C^2/(P-(2*p_C^2)))= -del_Fo/(R*T);
Kp = %e^(-del_Fo/(R*T))//equilibrium constant in terms of pressure
p_C = (Kp^(1/2))/(1+2*(Kp^(1/2)));//Partial pressure of C at equilibrium in atm
p_B = p_C;//as p_B/p_C = 1
p_A = P-(2*p_C);//Partial pressure of A at equilibrium in atm
N_A = p_A*P*100;
N_B = p_B*P*100;
N_C = p_C*P*100;
mprintf('\n    Equilibrium composition of A,B and C are %f,%f and %f mole percent respectively.',N_A,N_B,N_C);

//2.Calculation of composition at 400 K and 3 atm and vapour pressure of C at 400 K is 0.3 atm
P = 3;//Pressure in atm
P_C = 0.3;//Vapour pressure of C in atm
//Since m=0,pressure will not have an effect on equilibrium compositions.
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.10
clear;
clc;

//Given
//SO2(A) + (1/2)O2 (B) - SO3(C)
//Basis: 1 Kgmole SO2
n_A = 1;//Kgmole of SO2 fed
n_B = n_A;//Kgmole of O2 fed
T1 = 273+400;//Temperature in K at which reactants enter
To = 298;//room temperature in K
del_H = -23490;//Standar heat of reaction at 25 deg cel from example 14.6 in Kcal/Kgmole
```

```

//At T1,
C_A_T1 = 11.0; C_B_T1 = 7.4;//in Kcal/Kgmole
//Assume the various temperature be
T = [913 1073 1373 1573];//in K
//Mean specific heats of the components A,B & C at various temperature are given below in Kcal/Kgmole K
C_A = [11.6 11.8 12.3 12.5];
C_B = [7.7 7.8 8.0 8.2];
C_C = [  16.6 17.2 18.2 18.6];

//To Calculate the final temperature for various conversions and the maximum conversion that can be attained in a single reactor operating adiabatically
//In equation 14.18 (page no 307), H2-Hr = K  & (Hp-H3)= L(say)
K = ((n_A*C_A_T1)+(n_B*C_B_T1))*(To-T1);//in Kcal/Kgmole
mprintf('Adiabatic reaction temp in K          pecentage conversion of SO2');
for i = 1:4
    n_C(i) = (-K-(C_A(i)*(T(i)-To))-(C_B(i)*(T(i)-To)))/((T(i)-To)*(C_C(i)-C_A(i)-0.5*C_B(i))+del_H);
mprintf('\n   %d',T(i));
mprintf('                                                        %f',n_C(i)*100);
end

clf;
//plot(T,n_C*100);
plot2d(T,n_C*100,style =2);
//Now equilibrium conversion at various temperature taken from figure 14.7 (page no 325) are given as
Ta = [850 900 1000 1100 1200 1300 1400];
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.11
clear;
clc;

//Given
//Basis: 1 Kgmole of benzene
//C6H6 (A) + HNO3 (B) - C6H5NO2 (C) + H2O (D)
T = 298;//Temperature in K
R = 1.98;//gas constant in Kcal/Kgmole K
//Standard enthalpy in Kcal/Kgmole at 25 deg celsius of the above components are given as
H_A = 11718;
H_B = -41404;
H_C = -68371;
H_D = 3800;
//Standard entropy in Kcal/Kgmole K at 25 deg
```

```
celsius of the above components are given as
S_A = 41.30;
S_B = 37.19;
S_C = 16.72;
S_D = 53.60;

//To Calculate the conversion of benzene at 25 degree celsius and 1 atm
del_F = (H_C+H_D-(T*(S_C+S_D)))-(H_A+H_B-(T*(S_A+S_B)));
Ka = %e^(-del_F/(R*T));//Equilibrium constant
x = (Ka^(1/2)/(1+(Ka^(1/2))));
mprintf('The conversion is almost %f percent for this reaction.',x*100);
//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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.12
clear;
clc;

//Given
//C + 2H2 - CH4
//Basis: 1 Kgmole of C fed
T = 1000;//Temperature in K
P1 = 2;//Pressure in atm
del_F = 4580;//Standard free energy in Kcal/Kgmole

```

```

//To Calculate the maximum CH4 concentration under the condition of 2 atm and the  quantity of methane obtained if pressure is 1 atm
Ka = %e^(-del_F/(R*T));//Equilibrium constant
//In relation (d) (page no 339) p_H2 = p (say)
p = poly(0,'p');
q = Ka*(p^2)+p-P1;
r = roots(q);
p_H2 = r(2);//partial pressure of H2
p_CH4 = P1-p_H2;//partial pressure of CH4
X_H2 = p_H2*100/P1;//mole percent of H2
X_CH4 = p_CH4*100/P1;//mole percent of CH4
mprintf('Under the conditions of 2 atm and 1000 K, the maximum CH4 concentration is %f percent and further increase is not pssible',X_CH4);
//Now. pressure has become
P2 = 1;//in atm
q = Ka*(p^2)+p-P2;
r = roots(q);
p_H2 = r(2);//partial pressure of H2
p_CH4 = P2-p_H2;//partial pressure of CH4
X_H2 = p_H2*100/P2;//mole percent of H2
X_CH4 = p_CH4*100/P2;//mole percent of CH4
mprintf('\n\n Under the conditions of 1 atm and 1000 K,Methane = %f percent and Hydrogen = %f percent ',X_CH4,X_H2);
//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

```
//Chemical Engineering Thermodynamics
//Chapter 14
```

```
//Thermodynamics of Chemical Reactions

//Example 14.13
clear;
clc;

//Given
T1 = 273+110;//Temperature in K
T = 298;//Room temperature in K
P = 1;//Pressure in atm
R = 1.98;//gas constant in Kcal/Kgmole
//Ag2CO3(s) (A) = Ag2O(s) (B) + CO2(g) (C)
a = 1;//Stoichiometry coefficient of A
b = 1;//Stoichiometry coefficient of B
c = 1;//Stoichiometry coefficient of C
//Standard entropy of the above components in Kcal/Kgmole K at 25 deg cel are given as
S_A = 40.17;
S_B = 29.09;
S_C = 51.08;
//Standard enthalpy of the above components in Kcal/Kgmole at 25 deg cel are given as
H_A = -119900;
H_B = -6950;
H_C = -94036;
//Specific heat (assumed constant) of the above components in Kcal/Kgmole K are given as
C_A = 26.1;
C_B = 16.5;
C_C = 9.6;

//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
del_H = H_C+H_B-H_A;//Standard heat of reaction  at 25 deg cel in Kcal/Kgmole
del_C = b*C_B+c*C_C-a*C_A;
```

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

Scilab code Exa 14.14 Theoretical problem

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.14
clear;
clc;

//Given
```

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

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

```
//Chemical Engineering Thermodynamics
//Chapter 14
//Thermodynamics of Chemical Reactions

//Example 14.15
clear;
clc;

//Given
//C3H8 = C3H6 + H2... (i)
//C3H8 = C2H4 +CH4...(ii)
Kp1 = 7.88;//Equilibrium constant of equation (i)
Kp2 = 775;//Equilibrium constant of equation (ii)
T = 760+273;//Temperature in K

//To Calculate the equilibrium composition of the mixture
//Basis: 1 mole of C3H8 in feed
//From the equations (a) &(b) (page no 343); y/x = z (say)
z = (Kp2/Kp1)^(1/2);
//Substituting y = z*x in equation(a), we got the equation p:
x = poly(0,'x')
p = (1+Kp1+Kp1*(z^2)+2*Kp1)*x^2 - Kp1;
q = roots(p);
x = q(1);
y = z*x;
```

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

```
//Chemical Engineering Thermodynamics
//Chapter 15
//Fuel Cells

//Example 15.1
clear;
clc;

//Given
del_F = -56.29;//Standard free energy change in Kcal
   /Kgmole
del_H = -68.317;//Standard heat of reaction in Kcal/
   kgmole
F = 23.06;//Electro-chemical equivalent in Kcal/volt
J = 2;//Valance for H2

//To Calculate the emf of the cell, cell efficiency
   and heat to be removed to maintain isothermal
   conditions
//Basis: 1 Kgmole of H2
```

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