# Scilab Textbook Companion for Introduction To Chemical Engineering Thermodynamics by J. M. Smith, H. C. Van Ness And M. M. Abbott[1]

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# Book Description

**Title:** Introduction To Chemical Engineering Thermodynamics

**Author:** J. M. Smith, H. C. Van Ness And M. M. Abbott

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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

# List of Figures

# Chapter 1

# Introduction

**Scilab code Exa 1.1** Find the Astronaut Mass and Weight on moon

```
clear;
clc;

//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

//Example 1.1
//Caption : Program To find the Astronaut's Mass and Weight on moon.

//Given values

F=730;//Force(N)
g_texas=9.792;//Acceleration of gravity in Houston, Texas(m/s^2).
g_moon=1.67;//Acceleration of gravity at moon(m/s^2)
```

```
    .

//Solution

m=approx(F/g_texas,2);//Mass of Astronaut(Kg)
F_moon=approx(m*g_moon,2);//Force on Moon(N)
disp('Kg',m,'Mass of Astronaut');
disp('N',F_moon,'Force on Moon');

//End
```

**Scilab code Exa 1.2** Find Gauge Pressure and absolute Pressure

```
clear;
clc;

//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

//Example 1.2
//Caption : Program To Find Gauge Pressure and
    absolute Pressure

//Given values

d=0.01;//Diameter(m)
m=6.14;//Mass(Kg)
g=9.82;//Acceleration of gravity
Pb=748;//Barometric Pressure(Torr)

```

```
//Solution

F=approx(m*g,3);//Force(N)
A=(%pi/4)*d*d;//Area(m^2)
Pg=approx(F/A,-2);//Gauge Pressure(N/m^2)
Pa=approx(Pg+(Pb*0.013332*(10^4)),-2);//Absolute
   Pressure(Pa)
disp('N',F,'Force ');
disp('(X 10^4) N/m^2',Pg/10^4,'Gauge Pressure ');
disp('KPa',Pa/1000,'Absolute Pressure');

//End
```

**Scilab code Exa 1.3** Find Pressure in a Manometer

```
clear;
clc;

//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

//Example 1.3
//Caption : Program To Find Pressure in a Manometer

//Given Values

T=300.15;//Temp=300.15K(27‘C)
h=60.5*(10^-2);//Height=60.5cm
rho=13530;//Density(Kg/m^3)
g=9.784;//Acceleration of gravity(m/s^2)
```

```

//Solution

P=approx(h*rho*g,0);
disp('KPa',P/1000,'Pressure in KPa');
disp('bar',P/100000,'Pressure in bar');

//End
```

**Scilab code Exa 1.4** Find the velocity and Energy

```
clear;
clc;

//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

//Example 1.4
//Caption : Program to find the velocity and Energy

//Given values

M=2500;//Mass=2500Kg
h1=10;//height1=10m
h2=100;//height2=100m
g=9.8;//Acceleration of gravity(m/s^2)

//Solution
//(a)
PE1=M*h1*g;//(J)
```

```
disp('J',PE1,'(a)Potential energy of the elevator in its Initial Position')

//(b)
W=M*g*integrate('1','l',h1,h2);//(J)
disp('J',W,'(b)Work Done in Raising the Elevator')

//(c)
PE2=M*g*h2;//(J)
disp('J',PE2,'(c)Potential energy of the elevator in its Highest Position')

//(d)
KE2=0;
PE3=0;
KE3=PE2;//(J)   //Conservation Of Mechanical Energy
u=approx((2*KE3/M)^(1/2),2);//(m/s)
disp('m/s',u,'(d)Velocity of the Elevator')
disp('J',KE3,'(d)Kinetic Energy of the Elevator')

//(e)
PE_Spring=KE3;//(J)
disp('J',PE_Spring,'(e)Potential energy of compressed spring ')

//(f)
TE=PE1+W;
disp('J',TE,'(f)Total Energy of the System')

//End
```

# Chapter 2

# The First Law And Other Basic Concepts

**Scilab code Exa 2.1** Find Energy in a Waterfall

```
clear;
clc;

//Example 2.1
//Caption : Program to find Energy in a Waterfall


//Given values
H=100;//height=100m
M=1;//Mass of water=1Kg
g=9.8066;//Acceleration due to gravity(m/s^2)

//Solution

//Del(Energy of the system)=0
//hence,del(U)+del(KE)+del(PE)=0

```

```
//(a)
PE1=M*H*g;//(J)
disp('J',PE1,'(a)Potential energy of Water at the Top');

//(b)
del_U=0;
KE1=0;
PE2=0;
KE2=PE1;//(J)
disp('J',KE2,'(b)Kinetic energy of Water');

//(c)
del_U=KE2;
disp('J',del_U,'(c)Change in Internal energy when 1 kg Water added');

//End
```

**Scilab code Exa 2.3** Find the energy change in a System

```
clear;
clc;

//Example 2.3
//Caption : Program to find the energy change in a System

//Given values

P_atm=101.3;//Atm Pressure=101.3KPa
V1=0.1;//Volume1=0.1m^3
V2=0.2;//Volume2=0.2m^3
```

```

//Solution

del_V=V2-V1;
W_by=P_atm*del_V;
W_on=-W_by;
Q=0;
del_Energy=Q+W_on;//KJ
disp('KJ',del_Energy,'Energy Change')

//End
```

**Scilab code Exa 2.4** Find the Heat flow in the Path

```
clear;
clc;

//Example 2.4
//Caption : Program to find the Heat flow in the Path

//Given values
W_acb=40;//J
Q_acb=100;//J
W_aeb=20;//J
W_bda=30;//J

//Solution

del_U_ab=Q_acb-W_acb;

//(a)
Q_aeb=del_U_ab-W_aeb;//J
```

```
disp('J',Q_aeb,'(a)Heat Flow in acb')

//(b)
del_U_ba=-del_U_ab;//J
Q_bda=del_U_ba-W_bda;
disp('J',Q_bda,'(b)Heat Flow in bda')

//End
```

**Scilab code Exa 2.5** Find The degree of freedom for the various systems

```
clear;
clc;

//Example 2.5
//Caption : Program To Find The degree of freedom for the various systems

//Formula To be Used  F=2-#+N (Where,#(pi)-no of phases,N-number of chemical species)

//(a)-Liquid Water in equllibrium with its vapour.
N=1;
pi=2;
F=2-pi+N;
disp(F,'(a)Degree Of freedom is');

//(b)-Liquid Water in equllibrium with a mixture of vapour and nitrogen.
N=2;
pi=2;
F=2-pi+N;
disp(F,'(b)Degree Of freedom is');
```

```

//(c)-A liquid Soln of alcohol in water in equillibrium with its vapour
N=2;
pi=2;
F=2-pi+N;
disp(F,'(c)Degree Of freedom is');

//End
```

**Scilab code Exa 2.6** Find the work done by gas

```
clear;
clc;

//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

//Example 2.6
//Caption : Program to find the work done by gas

//Given values
P=14;//Pressure=14bar
V1=0.03;//Initial volume=0.03m^3
V2=0.06;//Final Volume
//Process is isothermal
//(a)-To find the work done by gas in moving the External force
//(b)-To find the work done by gas if external force is suddenly reduced to half its initial value
```

```

//Solution
//(a)
K=P*V1*(10^5);//J
W1=approx(-K*integrate('1/V','V',0.03,0.06),0);//J
P2=K/V2;//Final Pressure(Pa)
P2=P2/(10^5);//bar
disp('J',W1,'(a)The work done by gas in moving the External Force is')

//(b)
W2=-P2*(10^5)*integrate('1','V',0.03,0.06)
n=approx((W2/W1)*100,1);//Efficiency
disp('J',W2,'(b)The work done by gas if external force is reduced to half is')
disp('%',n,'Hence the efficiency is')

//End
```

**Scilab code Exa 2.7** Find the Enegy Changes in the Process

```
clear;
clc;

//Example 2.7
//Caption : Program to find the Enegy Changes in the Process

//Given values
P=7;//pressure=7bar
m=45;//Mass of cube
mt=23;//mass of piston,piston rod,pan
x=0.5;//Distance moved=0.5m
```

```
g=9.8;//Acceleration Due to gravity(m/s^2)

//Solution

//Acc to Eqn del_U_sys+del_U_surr+del_PE_surr=0
del_PE_surr=(m+mt)*g*x;
//ans=del_U_sys+del_U_surr
disp('J',-del_PE_surr,'Energy Changes in the Process')

//End
```

**Scilab code Exa 2.8** Find Change in Enthalpy and Internal Energy

```
clear;
clc;

//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

//Example 2.8
//Caption : Program to find Change in Enthalpy and Internal Energy

//Given values
m=1;//1kg of water
T=373.15;//Temp=373.15K(100‘C)
P=101.325;//Pressure=101.325KPa
V2=1.673;//Final Volume[m^3]
V1=0.00104;//Initial Volume[m^3]
```

```
Sv_liqiud=0.00104;//Specific Volume of Liqiud
Sv_vapour=1.673;//Specific Volume of Vapour
del_H=2256.9;//Heat Added(KJ)

//Solution
Q=del_H;
del_V=V2-V1;
W=P*del_V;//KJ
del_U=approx(del_H-(P*del_V),1);
disp('KJ',del_H,'Change in Enthalpy');
disp('KJ',del_U,'Change in Internal energy');
//End
```

**Scilab code Exa 2.9** Find Work Heat del U and del H

```
clear;
clc;

//Example 2.9
//Caption : Program To Find Work,Heat,del U and del H

//Given values
//Initial
P1=1;//Pressure=1bar
T1=298.15;//Temp=298.15K(25‘C)
V1=0.02479;//Molar Volume=0.02479m^3/mol
//Final
P2=5;//Pressure=5bar
Cv=20.78;//J/mol/K
Cp=29.10;//J/mol/K

//to Find del_U,del_H by two processes
```

```
V2=V1*(P1/P2);//m^3(1 mol)
disp('m^3',V2,'Final Volume')

//Solution

//(a)-Cooling at const pressure followed by heating at const Volume
T2=T1*(V2/V1);//K
disp('K',T2,'Final Temperature')
del_H=round(Cp*(T2-T1));//J
Q1=del_H;//J
del_U1=round(del_H-(P1*(10^5)*(V2-V1)));//J
//Second Step
del_U2=round(Cv*(T1-T2));//J
Q2=del_U2;
Q=Q1+Q2;
del_U=0;
W=del_U-Q;//J
del_H=0;//const Temperature

disp('(a) Cooling at const Pressure Followed by Heating at const Volume')
disp('J',Q,'Heat Required')
disp('J',W,'Work Required')
disp('J',del_H,'Change in enthalpy')
disp('J',del_U,'Change in Energy')
//(b)-heating at Const Volume Followed by cooling at const Pressure
T2=T1*(P2/P1);//K
del_U1=round(Cv*(T2-T1));//J
Q1=del_U1;
del_H=round(Cp*(T1-T2));//J
Q2=del_H;
del_U2=round(del_H-(P2*(10^5)*(V2-V1)));//J
Q=Q1+Q2;
del_U=0;
W=del_U-Q;//J
del_H=0;//const Temperature
```

```
disp('(b) Heating at const Volume Followed by Cooling at const Pressure')
disp('J',Q,'Heat Required')
disp('J',W,'Work Required')
disp('J',del_H,'Change in enthalpy')
disp('J',del_U,'Change in Energy')


//Note
disp('Note : The Answer varies From That in the book because in Book 4956.44 has been rounded to 4958 which is absurd')
//End
```

**Scilab code Exa 2.10** Find change in Internal Energy and Enthalpy

```
clear;
clc;

//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

//Example 2.10
//Caption : Program to Find change in Internal Energy and Enthalpy

//Given values

//Initial values
T1=277;//Temp=277K
```

```
P1=10;//Pressure=10bar
V1=2.28;//molar Volume=2.28m^3/Kmol

//Final value
T2=333;//Temp=333K
P2=1;//Pressure=1atm

Cv=21;//KJ/Kmol/K
Cp=29.3;//KJ/Kmol/K

//Solution
//(a)-Cooled at const Vol to the final pressure
//(b)-Heated at const Pressure to final temperature
T_=T1*(1/10);//Intermediate temperature
del_Ta=T_-T1;
del_Tb=T2-T_;
del_Ua=Cv*del_Ta;//KJ/Kmol
del_Ha=del_Ua+(V1*(P2-P1)*(10^5)/(10^3));//KJ/Kmol
V2=(V1*P1*T2)/(P2*T1);//m^3/kmol
del_Hb=Cp*del_Tb;
del_Ub=del_Hb-(P2*(V2-V1)*(10^5)/(10^3));//KJ/Kmol

del_U=approx(del_Ua+del_Ub,0);
del_H=approx(del_Ha+del_Hb,0);
disp('KJ/Kmol',del_U,'Change In Internal Energy')
disp('KJ/Kmol',del_H,'Change In Enthalpy')

//End
```

**Scilab code Exa 2.13** Find the time for a certain Temperature Drop

```
clear;
clc;
```

```

//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

//Example 2.13
//Caption : Program to Find the time for a certain Temperature Drop

//Given values
M=190;//Mass=190Kg
T0=333.15;//Temperature=333.15K(60‘C)
m=0.2;//Steady rate of mass(Kg/s)
T=308.15;//Temperature=308.15K(35‘C)
T1=283.15;//Temperature=283.15K(10‘C)

//Solution
//Using the Eqn (2.29)
t=approx(-(M/m)*log((T-T1)/(T0-T1)),1);//s
disp('s',t,'Time Taken for temperature of water to drop from 333.15K to 308.15K')
t=round(t/60);//min
disp('min',t,'Time Taken for temperature of water to drop from 333.15K to 308.15K')

//End
```

**Scilab code Exa 2.14** Find the Enthalpy of Steam

```
clear;
clc;
```

```

//Example 2.14
//Caption : Program to find the Enthalpy of Steam

//Given values

rQ=4.15;//[g/s]  flow rate
rQ2=12740;//Rate of Heat addition from resistance heater

//Solution
//del_z and del_u*2 are negligible  if Ws and H1=0.. then H2=Q
H2=round(rQ2/rQ);//[J/g]
disp('J/g',H2,'Enthalpy of Steam')

//End
```

**Scilab code Exa 2.15** Find the Heat to be Removed during Compression

```
clear;
clc;

//Example 2.15
//Caption : Program To find the Heat to be Removed during Compression

//Given values

V=600;//[m/s]
W_compression=240;//[KJ/Kg]

//Solution
```

```
//Using Eqn(2.32a)
Q=(1/2*(V*V)/1000)-W_compression;

disp('KJ/kg',-Q,'Thus Heat Removed from each KG of air compressed is')

//End
```

**Scilab code Exa 2.16** Find the Heat to be Removed during Compression

```
clear;
clc;

//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

//Example 2.15
//Caption : Program to Find the Temperature in the second Tank

//Given values

R=3.15*10^-3;//[m^3/s]  Rate of pumping
rH=-700;//[KW]  Rate of Heat lost
h=15;//[m]  Height
rW=1.5;//[KW]
rho=958;//[Kg/m^3]  at 366.65K
g=9.805;
gc=1000;
del_z=h;
```

```

//Solution

rm=approx(R*rho,3);//[Kg/s]  Mass flow rate
Q=approx(rH/rm,1);//[KJ/Kg]
W=approx(rW/rm,3);//[KJ/Kg]  Shaft Work
K=approx(g/gc*del_z,3);

//using Eqn(2.32b)
del_H=Q+W-K;

//From Steam tables for water at 366.65K
H1=391.6;//[KJ/Kg]
H2=del_H+H1;
disp('KJ/Kg',H2,'Enthalpy')
//From Steam Tables temp at this enthalpy is
T=311.35;//[K]
disp('K',T,'Temperature in the Second tank')

//End
```

# Chapter 3

# Volumetric Properties Of Pure Fluids

**Scilab code Exa 3.1** Find Volume Change and Pressure generated

```
clear;
clc;

//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

//Example 3.1
//Caption : Program to Find Volume Change and Pressure generated for Acetone

//Given Values for Acetone
P1=1;//Pressure=1Bar
T1=20;//Temp=293.15K(20'C)
Beta=1.487*10^(-3);//vol expansivity(K^-1)
```

```
k=62*10^(-6);//isothermal compressibility(bar^-1)
V1=1.287*10^(-3);//Volume(m^3 kg^-1)

//Solution
//(a)
//Find (dP/dT)v??
//Using eq.(3.4),V constant hence dV=0
ans_a=round(Beta/k);
disp('K^-1',ans_a,'(a)The value of (dp/dT)v is ')

//(b)
//Find Pressure when acetone heated at const. Vol from T1(1bar) to T2.
T2_b=30;//Temp2=303.15K(30‘C)
del_P=ans_a*(T2_b-T1);
ans_b=P1+del_P;
disp('bar',ans_b,'(b)The pressure is ')

//(c)
//Find vol. change when acetone changed from T1(P1) to T2(P2)
T2_c=0;//Temp2=273.15K(0‘C)
P2=10;//pressure=10bar
//solve using Eq. (3.5)
ln_value=(Beta*(T2_c-T1))-(k*(P2-P1));//ln(V2/V1)
ratio=exp(ln_value);//taking antilog,V2/V1
V2=ratio*V1;
del_V=approx(V2-V1,6)
disp('(X 10^-3) m^3 kg^-1',del_V*1000,'(c)The change in Volume is ')

//End
```

**Scilab code Exa 3.2** Find Work Heat del H del H

```
clear;
clc;

//Example 3.2
//Caption : Program to Find Work,Heat,del H,del H

//Given Values for the Gas

//Figure
P=[1 5];
V=[25 25];
plot2d(V,P,style=1)

V=5:0.5:25;
P=25*V^-1;
plot2d(V,P,style=2)
P=P^1.4;
plot2d(V,P,style=3)
P=[5 9.52];
V=[5 5];
plot2d(V,P,style=3,rect=[0,0,30,10])
xtitle("Diagram for Ex.3.2","V x 10^3(m^3)","P(bar)"
   )
legend("(a)","(b)","(c)")
P=[5 5];
V=[5 25];
plot2d(V,P,style=1)

clear;
//Initial Stage
P1=1;//Pressure=1bar
T1=298.15;//Temp1=298.15K(25'C)

//Final Stage
P2=5;//Pressure=1bar
//Temp same as Temp1(Isothermal)
```

```

R=8.314;//J/Mol/K
Cv=(5/2)*R;//J/Mol/K
Cp=(7/2)*R;//J/Mol/K

//(a)
//Const Vol follwd by const Pressure
T2=T1*(P2/P1);
//By Eq 2.23
del_T=T2-T1;
Q1=Cv*(T2-T1);//Heat at const Vol
Q2=Cp*(T1-T2);//Heat at const pressure

Q_a=round(Q1+Q2);
W_a=-Q_a;//W=del_U-Q, here del_U=0
disp('       (a) Heating at constant volume Followed by cooling at constant Pressure')
disp('J',W_a,'work done by heating at const vol followed by const Pressure ')

disp('J',Q_a,'Heat Transferred Q ')

disp('change in Internal Energy and enthalpy = 0')

//(b)
//Isothermal Compression
//By Eq. (3.26)
Q_b=round(R*T1*log(P1/P2));
W_b=-Q_b;
disp('       (b) Isothermal compression')

disp('J',W_b,'work done by Isothermal compression ')
disp('J',Q_b,'Heat Transferred Q')
disp('change in Internal Energy and enthalpy = 0')

//(c)
//Adiabatic compression
gama=Cp/Cv;
```

```
V1=(R*T1)/(P1^(10^5));
V2=V1*(P1/P2);
T2_c=T1*((V1/V2)^(gama-1));//Kelvin(K)
P2_c=P1*((V1/V2)^gama);//bar
//Using Eq. (3.31)
W_c=round(Cv*(T2_c-T1));//W=Cv*del_T(Joules)
Q_c=-W_c;

disp('        (c) Adiabatic compression followed by cooling at constant Volume')

disp('J',W_c,'work done by Adiabatic compression Followed by Cooling at const Vol ')

disp('J',Q_c,'Heat Transferred Q')
disp('change in Internal Energy and enthalpy = 0')

//End
```

**Scilab code Exa 3.3** Find W Q del U and del H for the Figure

```
clear;
clc;

//Example 3.3
//Caption : Program to Find W,Q,del U and del H for the Figure

//Figure
V=2083:0.5:2853;
P=2853*V^-1;
```

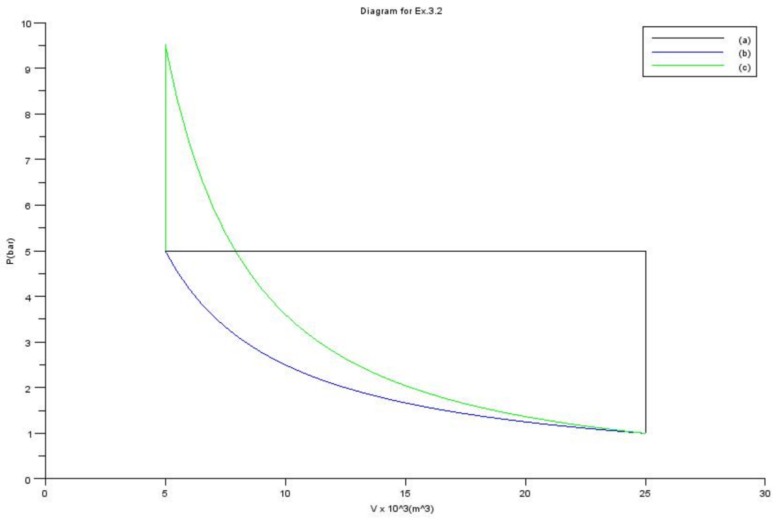

Figure 3.1: Find Work Heat del H del H

```
P=P^1.67;
plot2d(V,P,style=1)
P=[1.698 1.698];
V=[1690 2083];
plot2d(V,P,style=2)
V=1690:0.5:2853;
P=2853*V^-1;
plot2d(V,P,style=3,rect=[1500,0.8,3000,2])
xtitle("Diagram for Ex.3.3","V","P")
legend("(a)","(b)","(c)")
clear;


//Given Values for the Ideal Gas
R=8.314;//J/Mol/K
Cv=(3/2)*R;//J/Mol/K
Cp=(5/2)*R;//J/Mol/K
gama=Cp/Cv;

```

```
//Solution

//(a)
//Adiabatic Compression
P1=1;//Pressure=1bar
T1=343.15;//Temp1=343.15K(70‘C)
T2=423.15;//Temp2=423.15K(150‘C)
Q_a=0;//Adiabatic Compression
del_U_a=round(Cv*(T2-T1));
W_a=del_U_a;
del_H_a=round(Cp*(T2-T1));
//Using Eq. (3.29b)
P2=P1*((T2/T1)^(gama/(gama-1)));//bar

//(b)
//cooled form 150‘C to 70‘C at Const pressure
//Using Eq.(3.27)
Q_b=round(Cp*(T1-T2));
del_H_b=Q_b;
//for Ideal Gas
del_U_b=round(Cv*(T1-T2));
//by First law
W_b=del_U_b-Q_b;//Joules

//(c)
//Expanded Isothermally to original state
del_U_c=0;//isothermal
del_H_c=0;//isothermal
Q_c=round(R*T1*log(P2/P1));
W_c=-Q_c;

//Entire process
Qt = Q_a+Q_b+Q_c;
Wt = W_a+W_b+W_c;
del_Ut=del_U_a+del_U_b+del_U_c;
del_Ht=del_H_a+del_H_b+del_H_c;
```

```
//PartII(Irreversible)
eta=.80;//Efficiency=80%

//(a)
Wm_a=round(W_a/eta);
Qm_a=del_U_a-Wm_a;//del_U remains same (by First Law)

//(b)
Wm_b=round(W_b/eta);
Qm_b=del_U_b-Wm_b;//del_U remains same (by First Law)

//(c)
Wm_c=round(W_c*eta);
Qm_c=del_U_c-Wm_c;//del_U remains same (by First Law)

//Entire Process
Qmt = Qm_a+Qm_b+Qm_c;
Wmt = Wm_a+Wm_b+Wm_c;


del_U_rev=[del_U_a,del_U_b,del_U_c];
del_H_rev=[del_H_a,del_H_b,del_H_c];
Qrev=[Q_a,Q_b,Q_c];
Wrev=[W_a,W_b,W_c];
Sumr=[del_Ut,del_Ht,Qt,Wt];

del_U_irev=del_U_rev;
del_H_irev=del_H_rev;
Qirev=[Qm_a,Qm_b,Qm_c];
Wirev=[Wm_a,Wm_b,Wm_c];
Sumi=[del_Ut,del_Ht,Qmt,Wmt];


disp('      (a)Adiabatic Compression')
disp('      (b)Cooled form 150‘C to 70‘C at Const
pressure')
disp('     (c)Expanded Isothermally to original state')

disp('   Mechanically reversible');

Ans_rev=[del_U_rev',del_H_rev',Qrev',Wrev'];

disp(Sumr,'Sum',Ans_rev,'    del U    del H      Q      W')

disp('          Irreversible');

Ans_irev=[del_U_irev',del_H_irev',Qirev',Wirev'];

disp(Sumi,'Sum',Ans_irev,'    del U    del H      Q      W')

//End
```

**Scilab code Exa 3.4** Find Q W del U and del H in a PV Diagram

```
clear;
clc;

//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

```

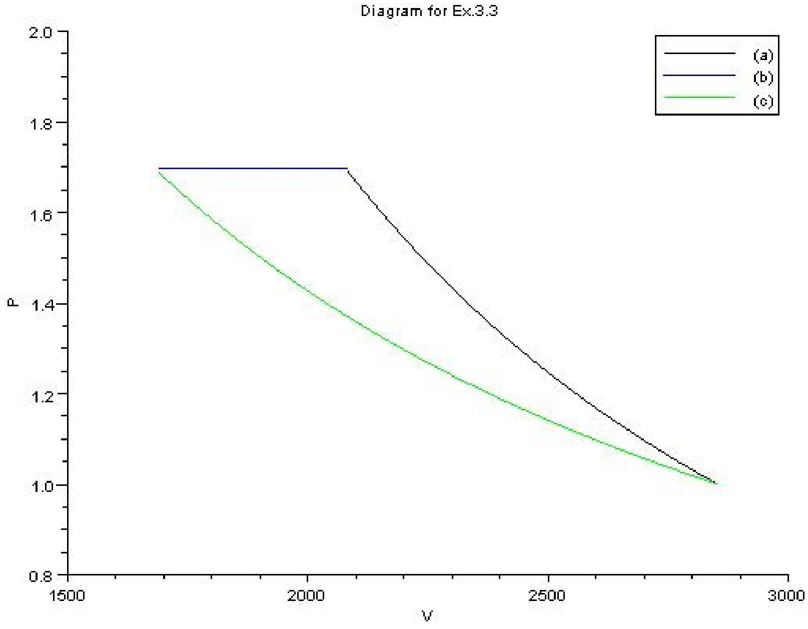

Figure 3.2: Find W Q del U and del H for the Figure

```
//Example 3.4
//Caption : Program To find Q,W,del_U and del_H in a PV Diagram

//Figure
P=[1.35 1.35];
V=[0.24 0.264];
plot2d(V,P,style=2)
V=0.12:0.001:0.24;
P=0.324*V^-1;
plot2d(V,P,style=5)
P=[2.7 2.97];
V=[0.12 0.12];
plot2d(V,P,style=9,rect=[0.1,0.5,0.3,3])
xtitle("Diagram for Ex.3.4","V(m^3)","P(bar)")
legend("(a)","(b)","(c)")
P=[2.97 2.97];
V=[0 0.12];
plot2d(V,P,style=4)
P=[2.7 2.7];
V=[0 0.12];
plot2d(V,P,style=4)
P=[1.35 1.35];
V=[0 0.24];
plot2d(V,P,style=4)
P=[0 2.7];
V=[0.12 0.12];
plot2d(V,P,style=4)
P=[0 1.35];
V=[0.24 0.24];
plot2d(V,P,style=4)
P=[0 1.35];
V=[0.264 0.264];
plot2d(V,P,style=4)

clear;

//Given Values for Nitrogen Gas
```

```
m=0.4;//Kg
M=28;//Molecular Mass Of Nitrogen
T1=300.15;//Temp=300.15K(27'C)
Pn=0.35;//Pressure of nitrogen = 0.35bar
Pa=1;//Atm Pressure = 1bar
R=8.314;//J/Mol/K
Cv=(5/2)*R;//J/Mol/K
Cp=(7/2)*R;//J/Mol/K
gama=Cp/Cv;

n=(m/M)*1000;//moles

//Solution

//(a)
//Immersed In ice/water bath
T2=273.15;//Temp=273.15K(0'C)
W_a=-round(n*R*(T2-T1));//Joules
del_H_a=approx(Cp*(T2-T1),0);
Q_a=round(n*del_H_a);
del_U_a=approx((Q_a+W_a)/n,0);
disp('(a)Immersed In ice/water bath')
disp('J',W_a,'work done ')
disp('J',Q_a,'Heat Transferred Q = ')
disp('J',del_U_a,'change in Internal Energy ')
disp('J',del_H_a,'change in enthalpy ')


//(b)
//Isothermal Compression
del_U_b=0;//Isothermal
del_H_b=0;//Isothermal
W_b=-round(n*R*T2*log(1/2));//W=nRTln(V3/V2),here V3/V2=0.5(Given)
Q_b=-W_b;
disp('(b)Isothermal Compression')
disp('J',W_b,'work done by Isothermal Compression ')
disp('J',Q_b,'Heat Transferred Q = ')
disp('J',del_U_b,'change in Internal Energy ')
disp('J',del_H_b,'change in enthalpy ')


//(c)
//constant Vol Process
W_c=0;//const Vol
del_H_c=approx((Cp*(T1-T2))/n,0);
del_U_c=approx(Cv*(T1-T2),0);
Q_c=round(n*del_U_c);
disp('(c)Constant Vol Process')
disp('J',W_c,'work done by Const Vol Process ')
disp('J',Q_c,'Heat Transferred Q = ')
disp('J',del_U_c,'change in Internal Energy ')
disp('J',del_H_c,'change in enthalpy ')


//End
```

**Scilab code Exa 3.6** Find Change in KE and Temperature

```
clear;
clc;

//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


```

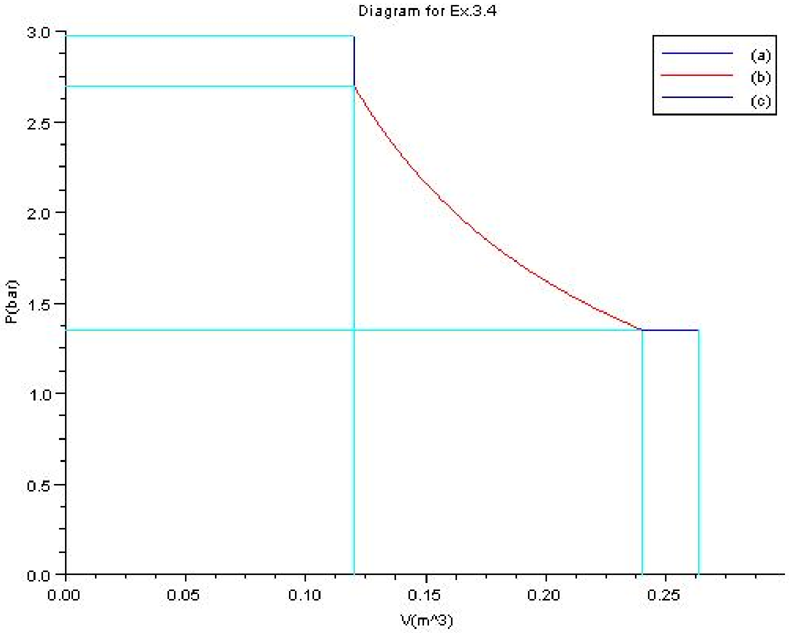

Figure 3.3: Find Q W del U and del H in a PV Diagram

```
//Example 3.6
//Caption : Program To find (a)Kinetic energy Change (b)change in temperature

//Given values
n=1;//Molar Rate(mol/s)
D=5;//inner Diameter(cm)
R=83.14;
Cp=(7/2)*R;
M=29*10^-3;//Molar mass(g/mol)
T=293.15;//temperature=293.15K(20‘C)
P1=6;//Upstream Pressure
P2=3;//Downstream Pressure

//Solution
//from Eq.(2.24b)
A=(%pi/4)*((D*10^-2)^2);//Area(m^2)
//upstream molar Volume
V1=(R*T/P1)*10^-6;//m^3/mol
u1=n*V1/A;//velocity(m/s)
V2=2*V1;
u2=2*u1;
del_KE=approx(n*M*((u2^2)-(u1^2))/2,3);//J/s(W)
del_T=approx(-del_KE/(Cp*0.1),4);//K
disp('W or J/s',del_KE,'Change in KE ')
disp('K',del_T,'Change in Temperature ')

//End
```

**Scilab code Exa 3.7** Find V and Z for isopropyl vapor

```
clear;
clc;
```

```

//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

//Example 3.7
//Caption : Program to Find V and Z for isopropyl vapor

//Given Values
T=473.15;//Temp=473.15k(200'C)
P=10;//Pressure=10bar
B=-0.388;//Viral Coefficient(m^3/Kmol)
C=-26*(10^(-3));//Viral Coefficient(m^6/(kmol)^2)
//Calculate V and Z for isopropyl vapor

//Solution

R=83.14*(10^(-3));//m^3bar/Kmol/K

//(a)
//Ideal Gas equation
V_a=approx((R*T)/P,3);
Z_a=1;//Ideal Gas
disp('(a) By Ideal gas Equation')
disp('m^3/kmol',V_a,'V = ')
disp(Z_a,'Z = ')

//(b)
//Using Eqution 3.37 -> Z=PV/RT=1+BP/RT
V_b=approx((R*T/P)+B,3);
Z_b=approx(P*V_b/(R*T),4);
disp('(b) Using Eqution 3.37 -> Z=PV/RT=1+BP/RT')
disp('m^3/kmol',V_b,'V = ')
disp(Z_b,'Z = ')

```

```
//(c)
//Using Equation 3.39 -> Z=PV/RT=1+(B/V)+(C/(V^2))
//Iterations
a=V_a;//Initial
i=-1;
while(i==-1)
   b=((R*T/P)*(1+(B/a)+(C/(a^2))));
   c=abs(b-a)
   if(c<=0.0001)
     i=1;
     break;
   end
   a=b;
end

V_c=approx(b,3);
Z_c=approx(P*V_c/(R*T),4);
//Ans
disp('(c) Using Equation 3.39 -> Z=PV/RT=1+(B/V)+(C
   /(V^2))')
disp('m^3/kmol',V_c,'V = ')
disp(Z_c,'Z = ')

//End
```

**Scilab code Exa 3.8** Find Molar Volume of nButane

```
clear;
clc;

//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

//Example 3.8
//Caption : Program to Find Molar Volume of n-Butane

//Given Values
T=350;//Temp=350K(76.85‘C)
P=9.4573;//Pressure=9.4573bar
R=83.14;

Tc=425.1;//App B
Pc=37.96;//App B
Tr=T/Tc;
Pr=P/Pc;
//Parameters for RK
si=0.42748;
omega=0.08664;
epsilon=0;
sigma=1;
a=Tr^-0.5;

//Solution

//Using Eq(3.51)
q=si*a/(omega*Tr);
Beta=omega*Pr/Tr;

disp('The Following Results given By Redlich/Kwong Equation')
//(a)
Z=1;//initial
a=Z;
for i=0:10
  b=1+Beta-((q*Beta)*(a-Beta)/(a*(a+Beta)));
   if((b-a)==0.0001)
     break;
   end
   a=b;
   i=i+1;
end
Z=approx(b,4)
V=round(Z*R*T/P);
disp('cm^3/mol',V,'Molar Volume of saturated Vapor is ');

//(b)
Z=Beta;//initial
a=Z;
for i=0:20
  b=Beta+(a*(a+Beta)*(1+Beta-a)/(q*Beta));
   if((b-a)==0.0001)
     break;
   end
   a=b;
   i=i+1;
end
Z=approx(b,5)
V=approx(Z*R*T/P,1);
disp('cm^3/mol',V,'Molar Volume of Saturated Liquid is ');

//Given Values
T=350;//Temp=350K(76.85 'C)
P=9.4573;//Pressure=9.4573bar
R=83.14;

Tc=425.1;//App B
Pc=37.96;//App B
Tr=T/Tc;
Pr=P/Pc;
//Parameters for eqns[vdW,RK,SRK,PR]
si=[27/64,0.42748,0.42748,0.45724];
omega=[1/8,0.08664,0.08664,0.07779];
epsilon=[0,0,0,(1-sqrt(2))];
sigma=[0,1,1,(1+sqrt(2))];
```

```
w=0.2;//App B
aSRK=(1+((0.480+(1.574*w)-(0.1768*w^2))*(1-Tr^0.5)))^2;
aPR=(1+((0.37464+(1.54226*w)-(0.26992*w^2))*(1-Tr^0.5)))^2;
a=[1,Tr^-0.5,aSRK,aPR];

//Solution

disp('      By All Equations')
//Using Eq(3.51)
q=si.*a./(omega.*Tr);
Beta=omega.*Pr./Tr;

//disp('The Following Results given By Redlich/Kwong Equation')
//(a)
for j=1:4

    Z=1;//initial
    A=Z;
    for i=0:10
      b=1+Beta(j)-((q(j)*Beta(j))*(A-Beta(j))/((A+(epsilon(j)*Beta(j)))*(A+(sigma(j)*Beta(j)))));
       if((b-A)==0.0001)
         break;
       end
       A=b;
       i=i+1;
    end
    z(j)=approx(b,4);
end
V=round(z.*R*T/P);
disp('Molar Volume(Vv) of Saturated Vapor');
disp(V','    vdW       RK       SRK       PR')

//(b)
```

```
for j=1:4
    Z=Beta(j);//initial
    A=Z;
    for i=0:20
      b=Beta(j)+((A+(epsilon(j)*Beta(j)))*(A+(sigma(j)*Beta(j)))*(1+Beta(j)-A)/(q(j)*Beta(j)));
       if((b-A)==0.0001)
         break;
       end
       A=b;
       i=i+1;
    end
    z(j)=approx(b,5);
end
V=approx(z*R*T/P,1);
disp('Molar Volume(Vl) of Saturated Liquid');
disp(V','     vdW        RK        SRK         PR')

disp('Note : Exp Value is Vv = 2482 cm^3/mol and Vl = 115 cm^3/mol')

//End
```

**Scilab code Exa 3.9** Find Molar Volume of n Butane by Various Eqn

```
clear;
clc;

//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
```

```

//Example 3.9
//Caption : Program to Find Molar Volume of n-Butane by Various Eqn
//Given Values
T=510;//Temp=510K
P=25;//Pressure=25bar
R=0.08314;

//(a)
//By the Ideal-gas Equation

V=approx(R*T/P,4);//m^3/kmol
disp('(a)By the Ideal-gas Equation')
disp('m^3/kmol',V,'The Molar Volume is ')

//(b)
//The Generalized compressibility-factor Correlation
Tc=425.1;//From App.B
Pc=37.96;//From App.B
Tr=approx(T/Tc,1);
Pr=approx(P/Pc,3)
//Interpolation in Tables E.1 and E.2 then provides
Z0=0.865;
Z1=0.038;
w=0.200;
Z=Z0+(w*Z1);
V=approx(Z*R*T/P,2);//m^3/kmol
disp('(b)The Generalized compressibility-factor Correlation')
disp('m^3/kmol',V,'The Molar Volume is ')

//(c)
//The Generalized Virial-coefficient Correlation
B0=0.083-(0.422/(Tr^1.6));//Eqn (3.61)
B1=0.139-(0.172/(Tr^4.2));//Eqn (3.62)
K=approx(B0+(w*B1),3)//K=BPc/RTc By Eqn (3.59)
//By Eqn(3.58)
```

```
Z=approx(1+(K*Pr/Tr),3)
V=approx(Z*R*T/P,4);//m^3/kmol
disp('(c)The Generalized Virial-coefficient
    Correlation')
disp('m^3/kmol',V,'The Molar Volume is ')

//End
```

**Scilab code Exa 3.10** Find Pressure generated for methane

```
clear;
clc;

//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

//Example 3.10
//Caption : Program To Find Pressure generated for
    methane

//Given Values
T=323.15;//Temp=323.15K(50'C)
V=0.125;//Volume=0.125m^3
R=0.08314;

//(a)
//By Ideal-gas equation,
P=approx(R*T/V,1);//in bar
disp('(a)By Ideal-gas equation')
disp('bar',P,'Pressure is ')
```

```

//(b)
//for Redlich/Kwong equation
Tc=190.6;//App B
Tr=T/Tc;
si=0.42748;
omega=0.08664;
Pc=45.99;//App B
a=approx(si*((Tr^(-0.5))*(R^2)*(Tc^2))/Pc,3)//Eqn
    (3.42)Units of a(T) bar m^6
b=approx(omega*R*Tc/Pc,5)//Eqn (3.43)Units of b m^3
//Using eqn (3.41)
//P=RT/(V-b)-a(T)/(V+Eb)(V+~b),E->epsilon,~->sigma
epsilon=0;
sigma=1;
P=approx(((R*T/(V-b))-(a/((V+(epsilon*b))*(V+(sigma*
    b))))),2);
disp('(b)for Redlich/Kwong equation')
disp('bar',P,'Pressure is ')

//(c)
//A generalized Correlation
Z0=0.887;//from Table E.3 and E.4
Z1=0.258;//from Table E.3 and E.4
w=0.012;
Z=Z0+(w*Z1);
P=approx(Z*R*T/V,1);//bar
disp('(c)A generalized Correlation')
disp('bar',P,'Pressure is ')

//End
```

**Scilab code Exa 3.11** Find Pressure generated for ammonia

```
clear;
clc;

//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

//Example 3.11
//Caption : Program to Find Pressure generated for ammonia

//Given Values
T=338.15;//Temp=338.15K(65‘C)
Vt=0.03;//Volume=0.03m^3
R=0.08314;
m=0.5;//mass in Kg
M=17.02;//Molecular Mass
V=Vt/(m/M);// n=m/M(moles)

//(a)
//By Ideal-gas equation,
P=approx(R*T/V,2);//in bar
disp('(a)By Ideal-gas equation')
disp('bar',P,'Pressure is ')

//(b)
//A generalized correlation
Tc=405.7;//App B
Tr=T/Tc;
Pc=112.8;//App B
B0=0.083-(0.422/(Tr^1.6));//Eqn (3.61)
B1=0.139-(0.172/(Tr^4.2));//Eqn (3.62)
//Substituting in eq(3.59)
w=0.253;
K=B0+(w*B1);//K=BPc/RTc
B=K*R*Tc/Pc;//m^3 kmol^-1
```

```
//solving eq.(3.37)
P=approx(R*T/(V-B),2);
disp('(b)A generalized Correlation')
disp('bar',P,'Pressure is ')

//End
```

**Scilab code Exa 3.12** Find density for ammonia

```
clear;
clc;

//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

//Example 3.12
//Caption : Program to Find density for ammonia

//Given Values
T=310;//Temp=310K(36.85'C)
M=17.02;

//Solution

//(a)
//saturated liquid
Tc=405.7;//App B
Vc=0.07247;//App B
Zc=0.242;//App B
Vsat=approx(Vc*(Zc^((1-Tr)^0.2857)),5);//m^3kmol^-1
```

```
rho=approx(M/Vsat,2);
disp('(a)Saturated liquid')
disp('m^3/kmol',Vsat,'Volume is ')
disp('kmol/m^3',rho,'Density is ')

//(b)
//Liquid at 100bar
P=100;//Pressure=100bar
Pc=112.8;//App B
Pr=P/Pc;
rho_r=2.38;//From Graph
V=Vc/rho_r;
//but this Gives large error
rho_r1=2.34;
V_new=approx(V*rho_r1/rho_r,5);
//In exceptance with Experimental Value

rho=approx(M/V_new,2);
disp('(b)For Liquid at 100bar')
disp('m^3/kmol',V_new,'Volume is ')
disp('kmol/m^3',rho,'Density is ')

//End
```

# Chapter 4

# Heat Effects

**Scilab code Exa 4.2** Find Heat Required to Heat Methane gas

```
clear;
clc;

//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

function[Q]=ICPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D
     /(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction


//Example 4.2
//Caption : Program to find Heat Required to Heat
```

```
   Methane gas

//Given values for methane
R=8.314;
T0=533.15;
T=873.15;
A=1.702;
B=9.081*(10^-3);
C=-2.164*(10^-6);
D=0;



//Solution
Q=approx(R*ICPH(T0,T,A,B,C,D),0);
disp('J',Q,'Heat Required')

//End
```

**Scilab code Exa 4.3** Find the Final Temperature with Heat Given

```
clear;
clc;

//Example 4.3
//Caption : Program To Find the Final Temperature with Heat Given

function[Q]=MCPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))
  funcprot(0);
endfunction
```

```


//Given values for Ammonia
R=8.314;
T0=533.15;
A=3.578;
B=3.020*(10^-3);
C=0;
D=-0.186*(10^5);
Q=422*(10^3);
n=11.3;
del_H=Q/n;

//Solution
i=-1;
a=round(T0);//Initial
while (i==-1)
  b=R*MCPH(T0,a,A,B,C,D);
  c=b*(a-T0);
  flag=del_H-c;
  if(flag<=100) then
    T=a-1;
    i=1;
  else
    a=a+1;
    i=-1;
  end
end


disp('K',T,'Temperature Required(Approx)')

//End
```

**Scilab code Exa 4.4** Find the Latent Heat

```
clear;
clc;

//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

//Example 4.4
//Caption : Program to find the Latent Heat

del_H1=2257;//latent Heat of Vapourisation of water at 373.15K(100'C)[KJ/Kg]
Tr1=373.15/647.1;
Tr2=573.15/647.1;

del_H2=approx(del_H1*((1-Tr2)/(1-Tr1))^0.38,0);//KJ/Kg
disp('KJ/Kg',del_H2,'latent Heat at 573.15K')

disp('Note: The Value as given in steam tables at 573.15K is 1406 KJ/Kg')

//End
```

**Scilab code Exa 4.5** Find the Standard Heat at 298K

```
clc;
clear;

```

```
//Example 4.5
//Caption : Program to Find the Standard Heat at 298.15K

//4HCL + O2 −−> 2H2O + 2Cl2
del_H_HCL=-92.307;//KJ Heat Of Formation
del_H_H2O=-241.818;//KJ

//4HCL −−> 2H2 + 2Cl2
del_H_298_HCL=4*(-1)*del_H_HCL;
//2H2 + O2 −−> 2H2O
del_H_298_H2O=2*del_H_H2O;
//Final
del_H_298=del_H_298_HCL+del_H_298_H2O;

disp('KJ',del_H_298,'Standard Heat')

//End
```

**Scilab code Exa 4.6** Find the Standard Heat of Methanol Synthesis

```
clear;
clc;

//Example 4.6
//Caption : Program to Find the Standard Heat of Methanol Synthesis

//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
```

```

function[Q]=IDCPH(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=(dA+((dB/2)*T0*(t+1))+((dC/3)*T0*T0*((t^2)+t+1))+(dD/(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction


//Methanol Synthesis @ 1073.15K(800`C)
//CO + 2H2 --> CH3OH
del_H_CO=-110.525//@298K from Table C.4
del_H_CH3OH_g=-200.660;//@298K from Table C.4
del_H_298=((1)*del_H_CH3OH_g)-((1)*del_H_CO);//KJ/mol
T0=298.15;
T=1073.15;
R=8.314;
//Moles (CH3OH,CO,H2)
n=[1;-1;-2];
//A..from Table C.1
A=[2.211;3.376;3.249];
//B..from Table C.1
B=(10^-3)*[12.216;0.557;0.422];
//C..from Table C.1
C=(10^-6)*[-3.450;0;0];
//D..From table C.1
D=(10^5)*[0;-0.031;0.083];

del_A=0;
del_B=0;
del_C=0;
del_D=0;
for(i=1:3)
  del_A=del_A+n(i,1)*A(i,1);
  del_B=del_B+n(i,1)*B(i,1);
  del_C=del_C+n(i,1)*C(i,1);
  del_D=del_D+n(i,1)*D(i,1);
```

```
end

I=IDCPH(T0,T,del_A,del_B,del_C,del_D);
del_H=approx(del_H_298+(R*I/10^3),3);

disp('KJ',del_H,'Standard Heat Of Enthalpy');

//End
```

**Scilab code Exa 4.7** Find Max Temperature reached in Combustion of CH4

```
clear;
clc;

//Example 4.7
//Caption : Program To Find Max Temperature reached in Combustion of Methane

function[Q]=MCPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))
  funcprot(0);
endfunction


//Combustion Of methane
//CH4 + 2O2 --> CO2 + 2H2O
R=8.314;
del_H_CO2=-393509;//from table C.4
del_H_O2=-241818;//from table C.4
del_H_CH4=-74520;//from table C.4
```

```
del_H_298=del_H_CO2+(2*del_H_O2)-del_H_CH4;
del_Hp=-del_H_298;
//moles of reactants
n_CH4=1;
n_O2=2+(0.2*2);//20% Excess
n_N2=n_O2*(79/21);
//Moles Of Products..(CO2,H2O,O2,N2)
np=[1;2;0.4;9.03];
//A..from Table C.1
A=[5.457;3.470;3.639;3.280];
//B..from Table C.1
B=(10^-3)*[1.045;1.450;0.506;0.593];
//C..from Table C.1
C=(10^-6)*[0;0;0;0];
//D..From table C.1
D=(10^5)*[-1.157;0.121;-0.227;0.040];

E_A=0;
E_B=0;
E_C=0;
E_D=0;
for(i=1:4)
  E_A=E_A+np(i,1)*A(i,1);
  E_B=E_B+np(i,1)*B(i,1);
  E_C=E_C+np(i,1)*C(i,1);
  E_D=E_D+np(i,1)*D(i,1);
end

T0=298.15;
a=round(T0);//Initial
i=-1
while (i==-1)
  b=R*MCPH(T0,a,E_A,E_B,E_C,E_D);
  c=b*(a-T0);
  flag=del_Hp-c;
  if(flag<=100) then
    T=a-1;
    i=1;
  else
    a=a+1;
    i=-1;
  end
end
disp('K',T,'Temperature Required(Approx)')
//End
```

**Scilab code Exa 4.8** Find the Heat Requirement for the Reactor

```
clc;
clear;

//Example 4.8
//Caption : Program to Find the Heat Requirement for the Reactor

//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

function[Q]=MCPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))
  funcprot(0);
endfunction


//CH4 + H2O --> CO + 3H2 (A)
//CH4 + 2H2O --> CO2 + 4H2  (B)
```

```
del_H_A=205813;//J
del_H_B=164647;//J
//0.87 mol of CH4 for (A) (1-0.87)mol of CH4 for (B)
del_H_298=(0.87*del_H_A)+(0.13*del_H_B);
R=8.314;
T0=298.15;
T_A=600;//Cooled
T_B=1300;//Heated
//Moles of reactants (CH4,H2O)
nr=[1;2];
//Moles of Products (CO,H2,CO2,H2O)
np=[0.87;3.13;0.13;0.87];
//For Reactants
//for CH4
I1=MCPH(T0,T_A,1.702,9.081*(10^-3),-2.164*(10^-6),0);
//For H2O
I2=MCPH(T0,T_A,3.470,1.450*(10^-3),0,0.121*(10^5));
del_Hr=R*((nr(1,1)*I1)+(nr(2,1)*I2))*(T0-T_A);//J
//For Products
//for CO
I1=MCPH(T0,T_B,3.376,0.557*(10^-3),0,-0.031*(10^5));
//For H2
I2=MCPH(T0,T_B,3.249,0.422*(10^-3),0,0.083*(10^5));
//for CO2
I3=MCPH(T0,T_B,5.457,1.045*(10^-3),0,-1.157*(10^5));
//For H2O
I4=MCPH(T0,T_B,3.470,1.450*(10^-3),0,0.121*(10^5));
del_Hp=R*((np(1,1)*I1)+(np(2,1)*I2)+(np(3,1)*I3)+(np(4,1)*I4))*(T_B-T0);//J
//del_H
del_H=del_H_298+del_Hr+del_Hp;
Q=approx(del_H,-1);
disp('J',Q,'Heat Required');

//End
```

# Chapter 5

# The Second Law Of Thermodynamics

**Scilab code Exa 5.1** Find the Heat discarded to the River

```
clear;
clc;

//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

//Example 5.1
//Caption : Program To Find the Heat discarded to the River

//Given Values
Tc=295;//K
Th=585;//K
W=800000;//KW
```

```
n_max=1-(Tc/Th);
n=approx(0.7*n_max,3)
Qc=approx(((1-n)/n)*W,-2);
disp('KW',Qc,'Heat required');

//End
```

**Scilab code Exa 5.3** Find the Final Temperature

```
clear;
clc;

//Example 5.3
//Caption : Program to Find the Final Temperature in Reversible Adiabatic Expansion

function[Q]=MCPS(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A)+(((B*T0)+(((C*T0*T0)+(D/(t*t*T0*T0)))*(t+1)/2))*((t-1)/log(t)))
  funcprot(0);
endfunction


//Given values
P2=1;//bar
P1=5;//bar
T0=550;//K
A=1.702;
B=9.081*(10^-3);
C=-2.164*(10^-6);
D=0;

```

```
//Equation to be used
//(<Cp>s/R)ln(T2/T1)=ln(P2/P1) since del_S=0
//let I=(<Cp>s/R)

//T2=exp(log(1/5)/I);
a=T0-1;//Initial
i=-1;
while (i==-1)
  b=MCPS(T0,a,A,B,C,D);
  c=(log(1/5))/(log(a/T0));
  flag=c-b;
  if(flag<=0.0001) then
    T=a;
    i=1;
  else
    a=a-.01;
    i=-1;
  end
end

disp('K',T,'Final Temperature')

//End
```

**Scilab code Exa 5.4** Find the change in entropy in a steel Casing

```
clear;
clc;

//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

//Example 5.4
//Caption : Program To Find the change in entropy in a steel Casing

//Given Values

//For Casting
Cp_Casting=0.5;//[KJ/Kg/K]
T1=723.15;//[K]
T0=298.15;//[K]
M_Casting=40;//[Kg]
//For Oil
Cp_Oil=2.5;//[KJ/Kg/K]
M_Oil=150;//[Kg]

//Formula  M1Cp1dT`=M2Cp2dT
//40*0.5*(T-723.15)=150*2.5*(298.15-T)
//Whence
T=((T1*M_Casting*Cp_Casting)+(T0*M_Oil*Cp_Oil))/((M_Casting*Cp_Casting)+(M_Oil*Cp_Oil));

//(a)-change in entropy For casting
del_S_Casting=approx(M_Casting*Cp_Casting*integrate('1/T','T',T1,T),2);

disp('KJ/K',del_S_Casting,'(a)Change In Entropy of Casting')

//(b)-change in entropy For Oil
del_S_Oil=approx(M_Oil*Cp_Oil*integrate('1/T','T',T0,T),2);

disp('KJ/K',del_S_Oil,'(b)Change In Entropy of Oil')

//(c)-Total
del_S_total=del_S_Casting+del_S_Oil;
```

```
disp('KJ/K',del_S_total,'(c)Total entropy change')

//End
```

**Scilab code Exa 5.5** Find the Rate of Heat Transfer and Entropy

```
clear;
clc;

//Example 5.5
//Caption : Program to Find the Rate of Heat
   Transfer and Entropy

//Given Values

//Gas A
rn_A=1;//rate[mol/s]
T_A=600;//[K]

//Gas B
rn_B=2;//rate[mol/s]
T_B=450;//[K]

//product
rn=rn_A+rn_B;//[mol/s]
T=400;//[K]
R=8.314;
Cp=(7/2)*R;
T_s=300;//Temperature[K]

//By equation (2.30) rQ=rn*H−rn_A*H_A−rn_B*H_B=rn_A(
   H−H_A)+rn_B*(H−H_B)  Rate of heat transfer
rQ=(rn_A*Cp*(T-T_A))+(rn_B*Cp*(T-T_B));//[J/s] or  [
W]
//By eqn (5.22) rSg=rn*S-(rn_A*S_A)-(rn_B*S_B)-(rQ/T_s)  rate of entropy generation for the process
rSg=approx((rn_A*Cp*log(T/T_A))+(rn_B*Cp*log(T/T_B))-(rQ/T_s),3);//[J/K/s]

disp('J/s or W',rQ,'Rate of heat transfer')
disp('J/K/s',rSg,'Rate of entropy generation')

//End
```

**Scilab code Exa 5.6** Find the Feasibility of a Process

```
clear;
clc;

//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

//Example 5.6
//Caption : Program to Find the Feasibility of a Process

//Given Values
//Saturated Steam
//At T=373.15K
H1=2676;//[KJ/Kg] from Steam table(App F)
S1=7.3554;//[KJ/Kg/K] from steam table(App F)
//At T=273.15K  Liquid water
H2=0;
```

```
S2=0;

T_sigma=273.15;//[K]
T_r=473.15;//[K]
Q_r=-2000;//[KJ]

del_H=H2-H1;
Q=del_H;
Q_sigma=Q-Q_r;

del_S=S2-S1;
//For Heat Reservoir at 473.15K
del_St_T_r=(-Q_r/T_r);//[KJ/K]
//For Heat reservoir provided by cooling water at 273.15K
del_St_T_sigma=-Q_sigma/T_sigma;
del_S_total=del_S+del_St_T_r+del_St_T_sigma;
disp('Since del_S_total<0 Process not feasible')

//Actual
Q_r=approx((T_r/(T_r-T_sigma))*(del_H-(T_sigma*del_S)),1);
disp('KJ/Kg',Q_r,'Actual Heat transfer')

//End
```

**Scilab code Exa 5.7** Find the Maximum Work obtained

```
clear;
clc;


//Example 5.7
```

```
//Caption : Program to Find the Maximum Work obtained in a Steady state Flow



//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

function[Q]=ICPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction

function[Q]=ICPS(T0,T,A,B,C,D)
  t=T/T0;
  Q=((A)*log(t))+(((B*T0)+(((C*T0*T0)+(D/(t*t*T0*T0)))*(t+1)/2))*(t-1))
  funcprot(0);
endfunction


//Given Values
P1=50;//bar
P2=1.013;//bar
T1=800;//[K]
T2=300;//[K]
R=8.314;

//del_H=intergral(CpdT) in the limits T1 and T2
A=3.280;
B=0.593*(10^-3);
C=0;
D=0.040*(10^5);
del_H=R*ICPH(T1,T2,A,B,C,D);//[J/mol]
```

```

//del_S=integral[Cp(dT/T)] -Rln(P2/P1)  btw the limits T1,T2
del_S=(R*ICPS(T1,T2,A,B,C,D))-(R*log(P2/P1));//[J/mol/K]
W_ideal=approx(del_H-(T2*del_S),0);//[J/mol]
disp('J/mol',W_ideal,'Maximum Work')

//End
```

**Scilab code Exa 5.8** Find the Maximum Possible Work for Ideal Condition

```
clear;
clc;

//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

//Example 5.8
//Caption : Program To Find the Maximum Possible Work for Ideal Condition

//Given Values
//Saturated Steam
//At T=373.15K
H1=2676;//[KJ/Kg] from Steam table(App F)
S1=7.3554;//[KJ/Kg/K] from steam table(App F)
//At T=273.15K  Liquid water
H2=0;
```

```
S2=0;

T_sigma=273.15;//[K]
T_r=473.15;//[K]

del_H=H2-H1;
del_S=S2-S1;
W_ideal=del_H-(T_sigma*del_S);//[KJ/Kg]
Q=approx(abs(W_ideal*(T_r/(T_sigma-T_r))),1);//[KJ]
disp('KJ',Q,'Maximum Possible Work')

//End
```

**Scilab code Exa 5.9** Find the Lost Work in Heat Exchangers

```
clear;
clc;

//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

//Example 5.9
//Caption : Program to find the Lost Work in Heat Exchangers

//Given Values

T_H1=400;//[K]
T_H2=350;//[K]
T_C1=300;//[K]
```

```
T_sigma=300;//[K]
rn_H=1;//[mol/s]
R=8.314;
Cp=(7/2)*R;

T_C2_a=T_H2-10;
T_C2_b=T_H1-10;

//Figure
mtlb_axis('auto');
subplot(1,2,1);
X=[0,1];
Y=[T_C1,T_C2_a];
plot2d(X,Y);
Y=[T_H1,T_H2];
plot2d(X,Y,style=3,rect=[0,290,1,410]);
legend('Tc','Th')
X=[1,1];
Y=[290,410];
plot2d(X,Y);
X=[0,0.25];
Y=[T_C1,T_C1];
plot(X,Y,'--');
Y=[T_H1,T_H1];
plot(X,Y,'--');
X=[0.75,1];
Y=[T_C2_a,T_C2_a];
plot(X,Y,'--');
Y=[T_H2,T_H2];
plot(X,Y,'--');
xtitle("(a)Case 1,Cocurrent","Qc","T");

subplot(1,2,2);
X=[0,1];
Y=[T_C1,T_C2_b];
plot2d(X,Y);
Y=[T_H2,T_H1];
plot2d(X,Y,style=3,rect=[0,290,1,410]);
```

```
legend('Tc','Th')
X=[1,1];
Y=[290,410];
plot2d(X,Y);
X=[0,0.25];
Y=[T_C1,T_C1];
plot(X,Y,'--');
Y=[T_H2,T_H2];
plot(X,Y,'--');
X=[0.75,1];
Y=[T_C2_b,T_C2_b];
plot(X,Y,'--');
Y=[T_H1,T_H1];
plot(X,Y,'--');
xtitle("(b)Case 2,Countercurrent","Qc","T");

//Solution
//Equation to be used
//(rn_H*Cp(T_H2-T_H1))+(rn_C*Cp(T_C2-T_C1))=0   Eq(A)
//del_rS=rn_H*Cp*(ln(T_H2/T_H1)+kln(T_C2/T_C1))   k=rn_C/rn_H   r-->Rate   Eqn(B)
//rW_lost=T_sigma*del_rS   Eqn(C)

//(a)-Cocurrent
//by Eqn(A)
T_C2_a=T_H2-10;
k=(T_H1-T_H2)/(T_C2_a-T_C1);//k=rn_C/rn_H
//By Eqn(B)
del_rS=approx(rn_H*Cp*(log(T_H2/T_H1)+(k*log(T_C2_a/T_C1))),3);//[J/K/s]
//By Eqn(C)
rW_lost=approx(T_sigma*del_rS,1);//[J/s] or [W]
disp('(a)-Cocurrent')
disp('J/K/s',del_rS,'Rate Of change of entropy')
disp('J/s or W',rW_lost,'Lost Work')

//(b)-Countercurrent
T_C2_b=T_H1-10;
```

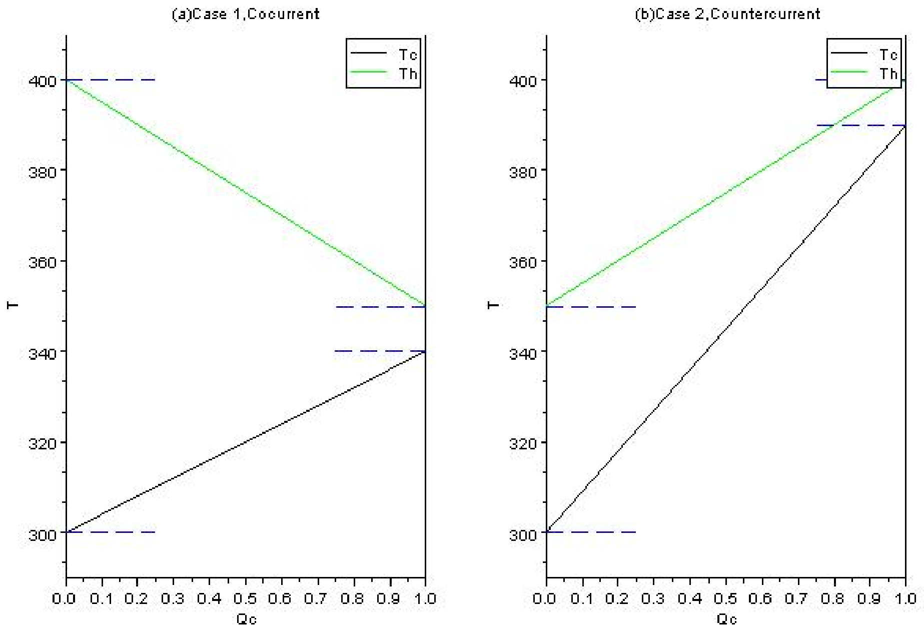

Figure 5.1: Find the Lost Work in Heat Exchangers

```
k=(T_H1-T_H2)/(T_C2_b-T_C1);//k=rn_C/rn_H
//By Eqn(B)
del_rS=approx(rn_H*Cp*(log(T_H2/T_H1)+(k*log(T_C2_b/
   T_C1))),3);//[J/K/s]
//By Eqn(C)
rW_lost=approx(T_sigma*del_rS,1);//[J/s] or [W]
disp('(b)-Countercurrent')
disp('J/K/s',del_rS,'Rate Of change of entropy')
disp('J/s or W',rW_lost,'Lost Work')

//End
```

# Chapter 6

# Thermodynamic Properties Of Fluids

**Scilab code Exa 6.1** Find the Changes in enthalpy and entropy

```
clear;
clc;

//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

//Example 6.1
//Caption : Program To find the Changes in enthalpy
   and entropy

//Given Values

//At Temp T1=298.15K
T1=298.15;//[K]
```

```
P1=1;//[bar]
P2=1000;//[bar]
Cp_T1=75.305;//[KJ Kmol/K]
V1_T1=18.071*10^-3;//[m^3/Kmol]
V2_T1=18.012*10^-3;//[m^3/Kmol]
beta1_T1=256*10^-6;//[1/K]
beta2_T1=366*10^-6;//[1/K]

//At Temp T2=323.15K
T2=323.15;//[K]
P1=1;//[bar]
P2=1000;//[bar]
Cp_T2=75.314;//[KJ Kmol/K]
V1_T2=18.234*10^-3;//[m^3/Kmol]
V2_T2=18.174*10^-3;//[m^3/Kmol]
beta1_T2=458*10^-6;//[1/K]
beta2_T2=568*10^-6;//[1/K]

//Solution

//Formula to be used
//Eqn (6.28) del_H=((Cp)(T2-T1))-((V)(1-(beta)(T2)(
   P2-P1))
//Eqn (6.29) del_S=((Cp)ln(T2/T1)-((beta)(V)(P2-P1))

//For P=1
Cp=(Cp_T1+Cp_T2)/2;
//For T=323.15K
V=(V1_T2+V2_T2)/2;
beta_T=(beta1_T2+beta2_T2)/2;

del_H=approx((Cp*(T2-T1))+(V*(1-(beta_T*T2))*(P2-P1)
   *10^5*10^-3),0);
del_S=approx((Cp*(log(T2/T1)))-(beta_T*V*(P2-P1)
   *10^5*10^-3),2);

disp('KJ/Kmol',del_H,'Change In Enthalpy')
disp('KJ/Kmol/K',del_S,'Change In Entropy')
```

```

//End
```

**Scilab code Exa 6.3** find Entropy and Enthalpy of Saturated isobutane

```
clear;
clc;

//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

function[Q]=ICPS(T0,T,A,B,C,D)
  t=T/T0;
  Q=((A)*log(t))+(((B*T0)+(((C*T0*T0)+(D/(t*t*T0*T0)))*(t+1)/2))*(t-1))
  funcprot(0);
endfunction

function[Q]=ICPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0))))*(T-T0)
  funcprot(0);
endfunction

//Example 6.3
//Caption : Program to find Entropy and Enthalpy of Saturated isobutane Vapor

//Given Values
```

```

T0=300;//[K]
T=360;//[K]
R=8.314;
P=15.14;//[bar]
A=1.7765;
B=33.037*10^-3;
C=0;
D=0;
H0=18115;   //J/mol
S0=295.976;//J/mol/K

//Graph
X=[0,0.10,0.50,2,4,6,8,10,12,14,15.41];
Y1
   =[1.780,1.700,1.514,1.293,1.290,1.395,1.560,1.777,2.073,2.432,2.7
   //[(dZ/dT)p/P]
Y2
   =[2.590,2.470,2.186,1.759,1.591,1.544,1.552,1.592,1.658,1.750,1.8
   //[-(Z-1)/P]
subplot(1,2,1);
plot2d(Y1,X);
xgrid();
xtitle("(a)","P(bar)","[(dZ/dT)p/P]X10^4(K^-1 bar
   ^-1)");
subplot(1,2,2);
plot2d(Y2,X);
xgrid();
xtitle("(b)","P(bar)","[-(Z-1)/P]X10^2(bar^-1)");


//Area Under the Curve (a)
Y1=Y1*10^-4;
A1=0;
for i=2:11;
  A1=A1+((X(i-1)-X(i))*Y1(i));
end
disp('(X 10^-4) K^-1',A1*10000,'Area under the graph
(a)')
//Area Under the Curve (b)
Y2=Y2*10^-2;
A2=0;
for i=2:11;
  A2=A2+((X(i-1)-X(i))*Y2(i));
end
disp(approx(A2,4),'Area under the graph(b)')


K=A1*T;//Hr/RT
//From Eqn(6.47)
Hr=R*T*(K);//[J/mol]
//From Eqn(6.48)
Sr=R*(K-(A2));//[J/mol/K]

//From Eqn(6.49) and Eqn(6.50)
H1=R*ICPH(T0,T,A,B,C,D);
S1=R*ICPS(T0,T,A,B,C,D);

H=H0+H1+Hr;
S=approx(S0+S1+Sr-(R*log(P)),3);

disp('J/mol',H,'Enthalpy')
disp('J/mol/K',S,'Entropy')
disp('Note: The Answer is different with that of the Book because the Method Used to find the Area under the Graph is done by finding the area of small       Rectangles')

//End
```

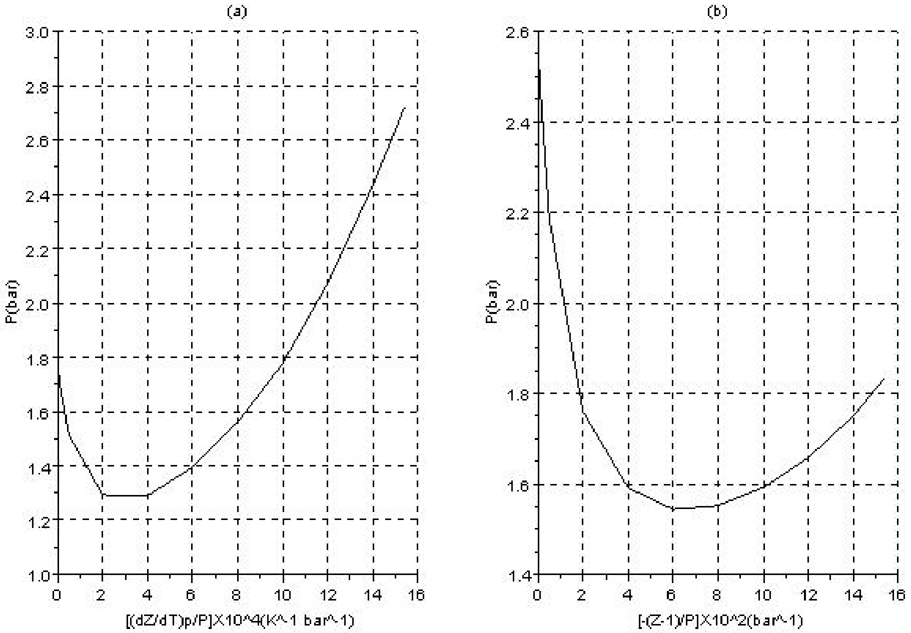

Figure 6.1: find Entropy and Enthalpy of Saturated isobutane

**Scilab code Exa 6.4** Find the Residual Enthalpy and Residual Entropy

```
clear;
clc;

//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

//Example 6.4
//Caption : Program to Find the Residual Enthalpy and Residual Entropy

//Given Values and values from Table(3.1)
T=500;//[K]
R=8.314;
Tc=425.1;//[K]
P=50;//[bar]
Pc=37.96;//[bar]
omega=0.08664;
si=0.4636;
Tr=T/Tc;
Pr=P/Pc;
alpha_Tr=Tr^(-0.5);//a(Tr)
//Using Eqn(3.50)
Beta=omega*(Pr/Tr);
//Using Eqn(3.51)
q=si*alpha_Tr/(omega*(Tr^1.5));

//using eqn(3.49)
//Z=1+beta-q*beta*((Z-beta)/((Z+(epsilon*beta))*(Z+(sigma*beta)))

//calculation of Z
Z=1;//Initial
a=Z;
for i=0:10
  b=1+Beta-(q*Beta*((a-Beta)/(a*(a+Beta))));
  if((b-a)==0.0001)
     break;
   end
   a=b;
   i=i+1;
end
Z=approx(b,3)

//Using Eqn(6.64) and eqn(6.65)
//(Hr/RT)=Z-1+[(d ln(alpha_Tr)/d ln Tr)-1]qI   I=ln((Z+beta)/Z)  d ln(alpha_Tr)/d ln Tr=-0.5
//Sr/R)=ln(Z-beta)+[d ln(alpha_Tr)/d ln Tr]qI  I=ln((Z+beta)/Z)  d ln(alpha_Tr)/d ln Tr=-0.5
I=log((Z+Beta)/Z);
Hr=approx(R*T*(Z-1+((-0.5-1)*q*I)),0);
Sr=approx(R*(log(Z-Beta)+(-0.5*q*I)),3);

disp('Using Redlich/Kwong Equation')
disp('J/mol',Hr,'Residual Enthalpy')
disp('J/mol/K',Sr,'Residual Entropy')

//End
```

**Scilab code Exa 6.6** Find the State of Steam at the Exit Nozzle

```
clear;
clc;

//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

//Example 6.6
//Caption : Program to Find the State of Steam at the Exit Nozzle

//Given values
P1=1000;//[KPa]
T=533.15;//[K]
P2=200;//[KPa]
H1=2965.2;//[KJ/kg]  from Steam tables
S1=6.9680;//[KJ/Kg/K] From steam tables
S2=S1;
S_l=1.5301;//[KJ/Kg/K]  Entropy Of Saturated Liquid @ 200KPa
S_v=7.1268;//[KJ/Kg/K]  Entropy Of Saturated vapor @ 200KPa
H_l=504.7;//[KJ/Kg]     Enthalpy Of saturated liquid  @ 200KPa
H_v=2706.7;//[KJ/Kg]    Enthalpy Of saturated vapor @ 200KPa


//Solution
//find x_v from the eqn S=(1-x_v)S_l+x_c*S_v
x_v=approx((S1-S_l)/(S_v-S_l),4);

//From Eqn(6.73a)
H2=((1-x_v)*H_l)+(x_v*H_v);
del_H=approx(H2-H1,0);//[KJ/Kg]

disp('%',x_v*100,'Percent vapor')
disp('%',(1-x_v)*100,'Percent Liquid')
disp('KJ/Kg',del_H,'Change In Enthalpy')

//End
```

**Scilab code Exa 6.7** Find how much Energy must be Transferred

```
clear;
clc;

//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

//Example 6.7
//Caption : Program to Find how much Energy must be Transferred to the Tank

//Given values(from steam tables)
H=293;//[KJ/Kg]  at 343.15K
H_liquid=419.1;//[KJ/Kg]  at 373.15K
H_vapor=2676;//[KJ/Kg]    at 373.15K
V_vapor=1.5;//[m^3]
m1_liquid=500;//[Kg]
rho_liquid=0.001044;//[m^3/Kg]
rho_vapor=1.673;//[m^3/Kg]
del_m=750;//[Kg]

//using the eqn Q=(m2H2)tank-(m1H1)tank-(H*del_m)tank
m1_vapor=(V_vapor-(m1_liquid*rho_liquid))/rho_vapor;
//Term2=((m1H1)tank
Term2=(m1_liquid*H_liquid)+(m1_vapor*H_vapor);
mT=m1_liquid+del_m+m1_vapor;
//Solving Eqn By matrix Method
```

```
//m_vapor+m_liquid=mT and  (rho_vapor*m_vapor)+(rho_liquid*rho_vapor)=V_vapor
A=[1,1;rho_vapor,rho_liquid];
B=[mT;V_vapor];
X=inv(A)*B;
m2_vapor=X(1,1);
m2_liquid=X(2,1);

Term1=(m2_liquid*H_liquid)+(m2_vapor*H_vapor);
Q=approx(Term1-Term2-del_m*H,0);

disp('KJ',Q,'Heat Required')
disp('Note: The Answer Varies With That of The Book because the calculations as in Book do not give the Answer the Book results')
//End
```

**Scilab code Exa 6.8** Find V U S and H fo 1 butene

```
clear;
clc;

//Example 6.8
//Caption : Program to Find V U S and H fo 1-butene

//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

function[Q]=SRB(Tr,Pr,omega)
  B0=0.083-(0.422/(Tr^1.6));
  diffr_B0=0.675/(Tr^2.6);//dB0/dTr
  B1=0.139-(0.172/(Tr^4.2));
  diffr_B1=0.722/(Tr^5.2);//dB0/dTr
  Q=-Pr*(diffr_B0+(omega*diffr_B1));
  funcprot(0);
endfunction

function[H]=HRB(Tr,Pr,omega)
  B0=0.083-(0.422/(Tr^1.6));
  diffr_B0=0.675/(Tr^2.6);//dB0/dTr
  B1=0.139-(0.172/(Tr^4.2));
  diffr_B1=0.722/(Tr^5.2);//dB0/dTr
  H=Pr*(B0-(Tr*diffr_B0)+(omega*(B1-(Tr*diffr_B1))));
  funcprot(0);
endfunction

function[Q]=ICPS(T0,T,A,B,C,D)
  t=T/T0;
  Q=((A)*log(t))+(((B*T0)+(((C*T0*T0)+(D/(t*t*T0*T0)))*(t+1)/2))*(t-1))
  funcprot(0);
endfunction

function[Q]=ICPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction

//Example 6.8
//Caption : Program to Find V U S and H fo 1-butene

//Given values(from steam tables)
Tc=420;//[K]
Pc=40.43;//[bar]
omega=0.191;
```

```
Tn=266.9;//[K]
A0=1.967;
B0=31.630*10^-3;
C0=-9.837*10^-6;
D0=0;
T1=473.15;//[K]
P=70;//[bar]
R=8.314;
//From Table(E.3) And Table(E.4)
Z0=0.485;
Z1=0.142;

Tr=T1/Tc;
Pr=P/Pc;
Z=Z0+(omega*Z1);
V=approx((Z*R*T1*10^-2)/P,4);//[m^3/Kmol]

//step(a) vaporization at T1 and P1=P_saturated
//using eqn(6.70)  lnP_sat=A-(B/T)
//Solving eqn ln(1.0133)=A-(B/266.9) and ln(40.43)=A-(B/420)
a=[1,(-1/266.9);1,(-1/420)];
b=[log(1.0133);log(40.43)];
x=(a^-1*b);
A=x(1,1);
B=x(2,1);
//using eqn(4.12)  del_Hn/RTn=1.092*(ln Pc-1.013)/(0.930-Tr_n)
Tr_n=Tn/Tc;
del_Hn=R*Tn*(1.092*(log(Pc)-1.013)/(0.93-Tr_n));//[J/mol]
T2=273.15;//[K]
Tr=T2/Tc;
//Using Eqn(4.13)  del_H/del_Hn=((1-Tr)/(1-Tr_n))^0.38
del_H_a=del_Hn*((1-Tr)/(1-Tr_n))^0.38;
del_S_a=approx(del_H_a/T2,2);

```

```
//Step(b)transition to ideal gas State at(T1,P1)
P_sat=exp(A-(B/273.15));
Pr=P_sat/Pc;
Tr=T2/Tc;
Hr_b=approx(R*Tc*HRB(Tr,Pr,omega),0)//[J/mol]
Sr_b=approx(R*SRB(Tr,Pr,omega),2)//[J/mol/K]

//Step(c) Change to (T2,P2) in ideal-gas state

H_c=approx(R*ICPH(T2,T1,A0,B0,C0,D0),0);//[J/mol]
S=R*ICPS(T2,T1,A0,B0,C0,D0);//[J/mol/K]
del_S_c=approx(S-(R*log(P/P_sat)),2);//[J/mol/K]

//Step(d) Transition to actual final state at(T2,P2)
//Using eqn(6.76) and eqn(6.77)
//Hr/RTc=Hr0/RTc+(omega*Hr1/RTc)
//Sr/R=Sr0/R+(omega*Sr1/R)  Sr0,Sr1 from Tables(E.5)
Tr=T1/Tc;
Pr=P/Pc;
Hr_d=R*Tc*(-2.294+(omega*-0.713));
Sr_d=R*(-1.566+(omega*-0.726));

H=approx(del_H_a-Hr_b+H_c+Hr_d,0);
S=approx(del_S_a-Sr_b+del_S_c+Sr_d,2);
U=approx(H-(P*V*10^2),0);

disp('m^3/Kmol',V,'Volume(V)=')
disp('J/mol',U,'Internal energy(U)=')
disp('J/mol',H,'Enthalpy(H)=')
disp('J/mol/K',S,'Entropy(S)=')

disp('Note: The Answer here Slightly Varies with
   That of Book because of the different
   approximation')

//End
```

**Scilab code Exa 6.9** Find Residual Enthalpy and Entropy and V

```
clear;
clc;

//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


//Example 6.9
//Caption : Program to Find Residual Enthalpy and Entropy and V by Lee/Kesler


//Given Values
T=450;//[K]
P=140;//[bar]

//pseudo parameters
Tc1=304.2;//[K]
Tc2=369.8;//[K]
Pc1=73.83;//[bar]
Pc2=42.48;//[bar]
Tpc=(0.5*Tc1)+(0.5*Tc2);
Ppc=(0.5*Pc1)+(0.5*Pc2);

Tpr=T/Tpc;
Ppr=P/Ppc;

```

```
Z0=0.697;
Z1=0.205;

omega1=0.224;
omega2=0.152;
omega=(0.5*omega1)+(0.5*omega2);

Z=Z0+(omega*Z1);

V=approx(Z*R*T*10/P,1);//[cm^3/mol]

//(H/RT)0=-1.73  (H/RT)1=-0.169
H=approx(R*Tpc*(-1.73+(omega*-0.169)),0);//[J/mol]
S=approx(R*(-0.967+(omega*-0.330)),2);//[J/mol/K]

disp('cm^3/mol',V,'Volume(V)=')
disp('J/mol',H,'Residual Enthaply(H)=')
disp('J/mol/K',S,'Residual Entropy(S)=')

//End
```

# Chapter 7

# Applications Of Thermodynamics To Flow Process

**Scilab code Exa 7.2** Find the Ratio of Area in a Nozzle

```
clear;
clc;

//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


//Example 7.2
//Caption : program to find the Ratio of Area's in a Nozzle for Diff Pressures

//Given Values
```

```
T=573.15;//[K]
P=[700,600,500,400,300,200];//[KPa]
//values for H,V,S for various P from steam tables
H=[3059.8,3020.4,2975.71,2923.5,2859.9,2777.35];//[KJ/Kg]
V=[371.39,418.25,481.26,571.23,711.93,970.04];//[cm^3/g]
S=7.29997*ones(1,6);//[KJ/Kg/K]  Isentropic
u0=30;//[m/s]
u=zeros(1,6);

//Using Eq(7.3)
//u^2=u1^2-2(H-H1)
u=approx(sqrt((u0^2-2*(H-H(1))*10.^3)),1);

//Using Eq(2.27)
//A/A1=u1*V/V1*u;
c=u(1)./V(1);
K=approx((c*V./u),3);//K=A/A1  c=u1/V1

Ans=[P',V',u',K'];
disp(Ans,' P/[KPa] V/[cm^3/g]  u/[m/s]  A/A1')

//End
```

**Scilab code Exa 7.3** Find Critical Pressure and Discharge Pressure

```
clear;
clc;

//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


//Example 7.3
//Caption : Program to Find the Critical Pressure and the Discharge Pressure

//Given Values
T1=573.15;//[K]
R=8314;
P1=700;//[KPa]
M=18.015;
Gamma=1.3;
u0=30;//[m/s]

//(a)
//Using Eqn(7.12)
//K=P2/P1=(2/(Gamma+1))^(Gamma/(Gamma−1))
K=approx((2/(Gamma+1))^(Gamma/(Gamma-1)),2);//rounding to 2 decimal places

P1V1=round(R*T1/M);//m^2/s^2
//Using Eqn(7.11)
//u_throat^2=u^2+2(Gamma)(P1V1)/(Gamma−1)[1−(P2/P1)^((Gamma−1)/Gamma))]
u_throat=approx(sqrt(u0^2+((2*Gamma*P1V1/(Gamma-1))*(1-(K^((Gamma-1)/Gamma))))),2);

disp(K,'(a)Critical Pressure ratio(P2/P1)')
disp('  m/s',u_throat,'  Velocity at the throat')

//(b)Mach No 2.0
u=2*u_throat;
K=(1-((u^2-u0^2)*(Gamma-1)/(2*Gamma*P1V1)))^(Gamma/(Gamma-1));//K=P2/P1
P2=round(K*P1);

```

```
disp('KPa',P2,'(b)Discharge Pressure for Mach Number of 2.0')

//End
```

**Scilab code Exa 7.4** Find the final Temperature and its Entropy change

```
clear;
clc;

//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

function[H]=HRB(Tr,Pr,omega)
  B0=0.083-(0.422/(Tr^1.6));
  diffr_B0=0.675/(Tr^2.6);//dB0/dTr
  B1=0.139-(0.172/(Tr^4.2));
  diffr_B1=0.722/(Tr^5.2);//dB0/dTr
  H=Pr*(B0-(Tr*diffr_B0)+(omega*(B1-(Tr*diffr_B1))));
  funcprot(0);
endfunction

function[Q]=SRB(Tr,Pr,omega)
  B0=0.083-(0.422/(Tr^1.6));
  diffr_B0=0.675/(Tr^2.6);//dB0/dTr
  B1=0.139-(0.172/(Tr^4.2));
  diffr_B1=0.722/(Tr^5.2);//dB0/dTr
  Q=-Pr*(diffr_B0+(omega*diffr_B1));
  funcprot(0);
```

```
endfunction

//Example 7.4
//Caption : Program to Find the final Temperature and its Entropy change

//Given Values
P1=20;//[bar]
T=400;//[K]
P2=1;//[bar]
R=8.314;

//Solution

//using Eq(6.84)
//del_H=Cp(T2-T1)+Hr2-Hr1=0  but Hr2=0
//T2=Hr1/Cp + T1
Tc=369.8;//[K]
Pc=42.48;//[bar]
omega=0.152;
a=T;//Initial
for i=1:2
  Tr=a/Tc
  Pr=P1/Pc;
  Hr1=R*Tc*HRB(Tr,Pr,omega);//[J/mol]
  Cp=R*(1.213+(28.785*10^-3*a)-(8.824*10^-6*a*a));//[J/mol/K]
  T2=(Hr1/Cp)+a;
  Tm=(a+T2)/2;
  i=i+1;
  a=Tm;
end
Tm=a;
T2=round(Tm)//[K]
Tr=T/Tc;
Sr=R*SRB(Tr,Pr,omega);

del_S=approx((Cp*log(T2/T))-(R*log(P2/P1))-Sr,2);
```

```

disp('J/mol/K',del_S,'Entropy')
disp('Positive Entropy represents the irreversibility of Throttling Process')
disp('K',T2,'Final Temperature')

//End
```

**Scilab code Exa 7.6** Find the state of Steam at Discharge and Mass Rate

```
clear;
clc;

//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

//Example 7.6
//Caption : Program to Find the state of Steam at Discharge & Mass Rate of Flow

//Given Values
P1=8600;//[KPa]
T1=773.15;//[K]
//values of Enthalpy and Entropy from Steam tables
H1=3391.6;//[KJ/Kg]
S1=6.6858;//[KJ/Kg/K]
eta=0.75;
P2=10000;//[KPa]
rW=56400;//[KW] or [KJ/s]
S2i=S1;//Isentropic
```

```

S2_liquid=0.6493;
S2_vapor=8.1511;
H2_liquid=191.8;
H2_vapor=2584.8;

x2=(S2i-S2_liquid)/(S2_vapor-S2_liquid);

H2i=H2_liquid+(x2*(H2_vapor-H2_liquid));
del_Hs=H2i-H1;//[KJ/Kg]
del_H=eta*del_Hs;

H2=approx(H1+del_H,0);//[KJ/Kg]
x2=(H2-H2_liquid)/(H2_vapor-H2_liquid);
S2=approx(S2_liquid+(x2*(S2_vapor-S2_liquid)),4);

rm=approx(-rW/(H2-H1),2);//[Kg/s]
disp('KJ/Kg',H2,'Enthalpy')
disp('KJ/Kg/K',S2,'Entropy')
disp('Kg/s',rm,'Rate of mass change')

//End
```

**Scilab code Exa 7.7** Find the isentropic Work Produced

```
clear;
clc;

//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
```

```

function[Q]=MCPS(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A)+(((B*T0)+(((C*T0*T0)+(D/(t*t*T0*T0)))*(t+1)/2))*((t-1)/log(t)))
  funcprot(0);
endfunction

function[Q]=MCPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))
  funcprot(0);
endfunction

function[H]=HRB(Tr,Pr,omega)
  B0=0.083-(0.422/(Tr^1.6));
  diffr_B0=0.675/(Tr^2.6);//dB0/dTr
  B1=0.139-(0.172/(Tr^4.2));
  diffr_B1=0.722/(Tr^5.2);//dB0/dTr
  H=Pr*(B0-(Tr*diffr_B0)+(omega*(B1-(Tr*diffr_B1))));
  funcprot(0);
endfunction

function[Q]=SRB(Tr,Pr,omega)
  B0=0.083-(0.422/(Tr^1.6));
  diffr_B0=0.675/(Tr^2.6);//dB0/dTr
  B1=0.139-(0.172/(Tr^4.2));
  diffr_B1=0.722/(Tr^5.2);//dB0/dTr
  Q=-Pr*(diffr_B0+(omega*diffr_B1));
  funcprot(0);
endfunction

//Example 7.7
//Caption : Program to Find the isentropic Work Produced

```

```
//Given Values

T1=573.15;//[K]
P1=45;//[bar]
P2=2;//[bar]
Tc=282.3;//[K]
Pc=50.4;//[bar]
omega=0.087;
A=1.424;
B=14.394*10^-3;
C=-4.392*10^-6;
D=0;
R=8.314;

//Using Eqn(6.84)
//del_H=<Cp>h (T2-T1)+Hr2-Hr1
//Using Eqn(6.85))
//del_S=<Cp>s ln(T2/T1) - R*ln(P2/P1)+Sr2-Sr1

//(a) equations for Ideal gas
//No residuals terms, whence

//del_H=<Cp>h(T2-T1)
//del_S=<Cp>s ln(T2/T1) - R*ln(P2/P1)

del_S=0//isentropic
//Whence K = <Cp>s/R ln(T2/T1) = ln(P2/P1)
K=log(P2/P1);
//let c = <Cp>s/R
//T2=exp(K/c+ln(T1))
i=-1;
a=round(T1);//Initial
while (i==-1)
  b=MCPS(T1,a,A,B,C,D);
  temp=exp((K/b)+log(T1));
  flag=a-temp;
  if(flag<=0.1) then
    T2=a;
    i=1;
  else
    a=temp-0.1;
    i=-1;
  end
end
disp('(a)by Equations for an Ideal gas')
disp('K',approx(T2,1),'Temp = ')
Cp_h=R*MCPH(T1,T2,A,B,C,D);
del_Hs=Cp_h*(T2-T1);
Ws_a=approx(del_Hs,0);
disp('J/mol',Ws_a,'Work')

//(b)-Appropriate Generalized correlations

Tr1=T1/Tc;
Pr1=P1/Pc;

Hr1=R*Tc*HRB(Tr1,Pr1,omega);//[J/mol]
Sr1=R*SRB(Tr1,Pr1,omega);//[J/mol/K]

Tr2=T2/Tc;
Pr2=P2/Pc;

Sr2=R*SRB(Tr2,Pr2,omega);

//Using Eqn(6.85))
//del_S=<Cp>s ln(T2/T1) - R*ln(P2/P1)+Sr2-Sr1
//del_S=0 isentropic
//K=<Cp>s ln(T2/T1)=Rln(P2/P1)-Sr2+Sr1
K=R*log(P2/P1)-Sr2+Sr1;
//T2=exp((K/<Cp>s)+ln T1)
i=-1;
a=round(T1);//Initial
while (i==-1)
  b=R*MCPS(T1,a,A,B,C,D);
  temp=exp((K/b)+log(T1));
  flag=a-temp;
  if(flag<=0.1) then
    T2=a;
    i=1;
  else
    a=temp-0.1;
    i=-1;
  end
end

disp('(b)by Appropriate generalized correlations')
disp('K',approx(T2,1),'Temp = ')
Tr2=T2/Tc;

Sr2=R*SRB(Tr2,Pr2,omega);//[J/mol/K]
Hr2=R*Tc*HRB(Tr2,Pr2,omega);//[J/mol]
Cp_h=R*MCPH(T1,T2,A,B,C,D);
del_Hs=Cp_h*(T2-T1)+Hr2-Hr1;
Ws_b=approx(del_Hs,-1);
disp('J/mol',Ws_b,'Work')

//End
```

**Scilab code Exa 7.8** Find the Work Required and Properties of Steam

```
clear;
clc;

//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

```

```
//Example 7.8
//Caption : Program to Find the Work Required and Properties of Discharge Steam

//Given Values

P1=100;//[KPa]  (Tsat/tsat)=327.78K/99.63‘C)

//From Steam Tables @ 100KPa
S1=7.3598;//[KJ/Kg/K]
H1=2675.4;//[KJ/Kg]

P2=300;//[KPa]
//From Steam Tables @ 300KPa
S2=S1;//Isentropic
H2i=2888.8;//[KJ/Kg]

eta=0.75;//Efficiency

del_H=H2i-H1;
del_H=del_H/eta;
H2=approx(H1+del_H,1);//[KJ/Kg]

//From Steam Tables w.r.t H2
T2=519.25;//[K]
S2=7.5019;//[KJ/Kg/K]

Ws=approx(del_H,1);//[KJ/Kg]  Work Reqd

disp('KJ/Kg',H2,'Enthalpy')
disp('KJ/Kg/K',S2,'Entropy')
disp('K',T2,'Temperature')
disp('KJ/Kg',Ws,'Work Done')

//End
```

**Scilab code Exa 7.9** Find Work Reqiured and Discharge Temperature

```
clear;
clc;

//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

function[Q]=MCPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))
  funcprot(0);
endfunction

function[Q]=MCPS(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A)+(((B*T0)+(((C*T0*T0)+(D/(t*t*T0*T0)))*(t+1)/2))*((t-1)/log(t)))
  funcprot(0);
endfunction

//Example 7.9
//Caption : Program to Find Work Reqiured and Discharge Temperature of Methane

//Given Values

R=8.314;
```

```
T1=293.15;//[K]

P1=140;//[KPa]
P2=560;//[KPa]

eta=0.75;//[Efficiency]
A=1.702;
B=9.081*10^-3;
C=-2.164*10^-6;
D=0;

i=-1;
a=round(T1);//Initial
while (i==-1)
  b=MCPS(T1,a,A,B,C,D);
  b=b^-1;
  c=T1*((P2/P1)^b);
  flag=c-a;
  if(flag<=0.0001) then
    T2i=a;
    i=1;
  else
    a=a+0.01;
    i=-1;
  end
end

Cps=R*MCPS(T1,T2i,A,B,C,D);
Cph=approx(R*MCPH(T1,T2i,A,B,C,D),3);

//from Eqn(7.19)
Ws=approx(Cph*(T2i-T1),0)//[J/mol]
Ws=approx(Ws/eta,0)//Actual work
del_H=Ws;

//From eqn(7.21)  Actual discharge Temperature
//T2=T1+(del_H/Cph)
i=-1;
```

```
a=round(T2i);//Initial
chk=1;
while (i==-1)
  b=R*MCPH(T2i,a,A,B,C,D);
  c=del_H/(a-T1);
  flag=c-b;
  if(flag<=0.001) then
      T2=a;
      i=1;
  else
      a=a+0.001;
      i=-1;
  end
end
Cph_T2=approx(R*MCPH(T2i,T2,A,B,C,D),2);
disp('K',T2,'Temperature')
disp('J/mol/K',Cph_T2,'Enthalpy')
disp('J/mol',Ws,'Actual Work')

disp('Note: The answer in the Book varies with that of this code because the Calculation in the Book does not leads to the answer given')

//End
```

**Scilab code Exa 7.10** Find Work Temperature Change and Entropy Change

```
clear;
clc;

//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

//Example 7.10
//Caption : Program to Find Work,Temperature Change and Entropy Change in Pump

//Given Values
T1=318.15;//[K]
P1=10;//[KPa]
P2=8600;//[KPa]
eta=0.75;//Efficiency

//Properties of saturated liquid water @ 318.15K
V=1010;//[cm^3/Kg]
V=1010*10^-6;//[m^3/Kg]
Beta=425*10^-6;//[K^-1]
Cp=4.178;//[KJ/Kg/K]

//From Eqn(7.24)
Ws=V*(P2-P1);//[KPa m^3/Kg]
del_H=Ws;
//From Eqn(7.17)
del_H=del_H/eta;
Ws=approx(del_H,2);

//From Eqn(7.25)
del_T=approx((del_H-(V*(1-(Beta*T1))*(P2-P1)))/Cp,2);

//From Eqn(7.26)
T2=T1+del_T;
del_S=approx(Cp*log(T2/T1)-(Beta*V*(P2-P1)),3);

disp('KJ/Kg',Ws,'Work Done')
disp('K',del_T,'Change in Temperature')
disp('KJ/Kg/K',del_S,'Change in Entropy')

```

```
//End
```

# Chapter 8

# Production Of Power From Heat

**Scilab code Exa 8.1** Find the Thermal efficiency in a Steam Turbine

```
clear;
clc;

//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

//Example 8.1
//Caption : Program to Find the Thermal efficiency in a Steam Turbine

//Given Values
//(a)-As in Example(7.6)
P1=8600;//[KPa]
T1=773.15;//[K]
```

```
//values of Enthalpy and Entropy from Steam tables
H1=3391.6;//[KJ/Kg]
S1=6.6858;//[KJ/Kg/K]

P2=10;//[KPa]
S2i=S1;//Isentropic

S2_liquid=0.6493;
S2_vapor=8.1511;
H2_liquid=191.8;
H2_vapor=2584.8;

x2=(S2i-S2_liquid)/(S2_vapor-S2_liquid);

H2i=H2_liquid+(x2*(H2_vapor-H2_liquid));
del_Hs_1=approx((H2i-H1),1);//[KJ/Kg]
Ws=del_Hs_1;
H3i=H2i;
H4=H2_liquid;
//Applying Eqn(8.2)
Q_condenser=approx((H4-H3i),1);//heat Of condenser [KJ/Kg]
//From Example(7.10)
//Properties of saturated liquid water @ 318.15K
V=1010;//[cm^3/Kg]
V=1010*10^-6;//[m^3/Kg]
Beta=425*10^-6;//[K^-1]
Cp=4.178;//[KJ/Kg/K]

//From Eqn(7.24)
Ws_2=approx((V*(P1-P2)),1)//[KPa m^3/Kg]
del_Hs_2=Ws_2;
H1=H4+del_Hs_2;
//Enthalpy Of saturated steam at 8600KPa and 773.15K
H2=3391.6;//[KJ/Kg]
//Applying Eqn(8.2)
Q_boiler=H2-H1;

```

```
Ws_Rankine=-Q_boiler-Q_condenser;
eta=approx((abs(Ws_Rankine)/Q_boiler),3);
disp('(a)Rankine Cycle')
disp(eta,'Thermal Efficiency')

//(b)

eta_b=0.75;

del_H_1=del_Hs_1*eta_b;
Ws_turbine=del_H_1;
H3=H2+del_H_1;
Q_condenser=H4-H3;

//By Example 7.10 for the pump
Ws_pump=del_Hs_2/eta_b;
del_H_2=Ws_pump;
Ws_net=Ws_turbine+Ws_pump;
H1=H4+del_H_2;

Q_boiler=H2-H1;
efficiency=approx(abs(Ws_net)/Q_boiler,4);
disp('(b)Practical cycle with 0.75 efficiency')
disp(efficiency,'Thermal Efficiency')

//(c)
//By rating of Power Cycle
rWs_net=-80000;//[KJ/s] Power Rating
rm=approx(rWs_net/Ws_net,2);

rQ_boiler=approx(rm*Q_boiler/1000,1);//[MW]
rQ_condenser=approx(rm*Q_condenser/1000,1);//[MW]
disp('(c)By rating of Power Cycle');
disp('kg/s',rm,'Steam Rate')
disp('MW',rQ_boiler,'Heat Transfer rate in boiler')
disp('MW',rQ_condenser,'Heat Transfer rate in condenser')

```

```
//End
```

**Scilab code Exa 8.4** Find the Efficiency in a Gas Turbine

```
clear;
clc;

//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

//Example 8.4
//Caption : Program to Find the Efficiency in Various Cycles in a Gas turbine

//Given Values
K=6;//Pb/Pa
T1=298.15;//[K]
Tmax=1033.15;//[K]
Gamma=1.4;

//(a)  Gamma=1.4
//From Eqn(8.12)
eta_a=approx(1-((1/K)^((Gamma-1)/Gamma)),1);
disp('(a)Efficiency of an ideal air cycle')
disp(eta_a,'Efficiency')

//(b)  eta_c=0.83  eta_t=0.86
eta_c=0.83;
eta_t=0.86;
K2=Tmax/T1;
```

```
alpha=(K)^((Gamma-1)/Gamma);

//Using Eqn(8.13)
eta_b=approx(((eta_t*eta_c*K2*(1-(1/alpha)))-(alpha-1))/((eta_c*(K2-1))-(alpha-1)),3);
disp('(b)Thermal efficiency of an air cycle if the Compressor and Turbine Operate adiabatically')
disp(eta_b,'Thermal efficiency')

//End
```

# Chapter 9

# Refrigerator And Liquifaction

**Scilab code Exa 9.1** Find the COP of a Refrigerator

```
clear;
clc;

//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

//Example 9.1
//Caption : Program to Find the COP of a Refrigerator

//Given Values
T1=261.15;//[K] Temgeratureof refrigerated space
T2=294.15;//[K] Temperature of cooling water
dT=5.6;//[K]    Temperature Difference
Qc=35.2;//[kW]  Refrigerant Capacity
eta=0.8;//Efficeincy(b)
```

```

//(a) Carnot Refrigerator
Tc=T1-dT;
Th=T2+dT;
//Using Eqn(9.3)
w=approx(Tc/(Th-Tc),2);
disp(w,'(a)Coefficient of Performance for Carnot Refrigerator')

//(b)  Vapor Compression Cycle

//From Table(9.1)
//@ Tc=255.55K
H2=388.13;//[KJ/Kg]
S2=1.7396;//[KJ/Kg/K]

//@ Th=299.75K
H4=236.76;//[KJ/Kg]

S3=S2;//Isentropic
//Hence
H3=420.27;//[KJ/Kg]
//Step 2 --> 3
del_Hs=H3-H2;
//But Compressor Efficiency = 0.80
del_Hs=del_Hs/eta
//Step 1 --> 4
H1=H4;//isenthalpic
w=approx((H2-H4)/del_Hs,2);
disp(w,'(b)Coefficient of Performance for Vapor Compression Cycle')
rm=approx(Qc/(H2-H4),4);//[Kg/s]
disp('kg/s',rm,'Circulation rate');

//End
```

**Scilab code Exa 9.2** Find Power Requirement For Various seasons

```
clear;
clc;

//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

//Example 9.2
//Caption : Program to Find Power Requirement For Various seasons

//Given Values
Qh_Winter=30;//[KW]
Qc_Summer=60;//[KW]
Tc_Winter=283.15;//[K]
Th_Winter=303.15;//[K]
Tc_Summer=278.15;//[K]
Th_Summer=298.15;//[K]

//For WINTER's
//Using Eqn(5.7)
Qc_Winter=Qh_Winter*(Tc_Winter/Th_Winter);
//Using Eqn(9.1)
W_Winter=approx((Qh_Winter-Qc_Winter),2);//[KW]
disp('KW',W_Winter,'Power Requirement for WINTER''s')

//For SUMMER's
```

```
//Combining Eqn(9.2) And Eqn(9.3)
W_Summer=approx((Qc_Summer*((Th_Summer-Tc_Summer)/
   Tc_Summer)),2);
disp('KW',W_Summer,'Power Requirement for SUMMER''s'
   )

//End
```

**Scilab code Exa 9.3** Find the Temperature of the High Pressure steam

```
clear;
clc;

//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

//Example 9.3
//Caption : Program to Find the Temperature of the
   High Pressure steam

//Given Values

x=0.25;
//For Superheated Methane
//By Perry and Green  by linear interpolation
H4=1140;//[KJ/Kg]  @ 300K and 60 Bar
H15=1188.9;//[KJ/Kg]  @ 295K and 1 Bar
//By interpolation based on lnP
T_sat=111.5;//[K]
H9=285.4;//[KJ/Kg]  Saturated Liquid
```

```
H12=769.9;//[KJ/Kg] Saturated Vapor
S12=9.521;//[KJ/Kg/K] Saturated vapor

T5=253.6;//[K]
H5=1009.8;//[KJ/Kg]  @ 60 Bar

//From Eqn(9.7)
z=((x*(H12-H5))+H4-H15)/(H9-H15);

H14=((H5-H4)/(1-z))+H15;//[KJ/Kg]
//Whence
T14=227.2;//[K]  @ 1Bar

H7=H5-((1-z)/(1-x)*(H14-H12));//[KJ/Kg]
T7=197.6;//[K]  @ 60Bar

//From Eqn(9.8)
z=approx((H4-H15)/(H9-H15),4);

H7=H4-((1-z)*(H15-H12));
T7=206.6;//[K]

disp('%',z*100,'Fraction of methane liquefied')
disp('K',T7,'Temperature of High Pressure steam entering the throttle valve')

//End
```

# Chapter 10

# Vapor Liquid Equillibrium Introduction

**Scilab code Exa 10.1** Plot the Graphs of P vs x1 y1 and t vs x1 y1

```
clear;
clc;

//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

//Example 10.1
//Caption : Program to Plot the Graphs of P vs x1,y1 and t vs x1,y1

//Antoinie Equations

//ln P1_sat=14.2724-(2945.47/(T-49.15))   [KPa]
//ln P2_sat=14.2043-(2972.64/(T-64.15))   [KPa]
```

```

//(a) Graph Showing P vs x1 and P vs y1 for T=348.15 K
T=348.15;//[K]
//using BUBL P calculations

//Calculation of P1_sat and P2_sat at T=348.15K
P1_sat=approx(exp(14.2724-(2945.47/(T-49.15))),2) //KPa
P2_sat=approx(exp(14.2043-(2972.64/(T-64.15))),2) //KPa

//Using Eqn P=P2_sat+(P1_sat-P2_sat)x1

x=[0:0.2:1];
P=approx(P2_sat+((P1_sat-P2_sat)*x),2);
y=approx(x*P1_sat./P,4);

disp('Explanations Of graph')

Ans=[x',y',P'];
disp(Ans,'   x1        y1         P/PKa')

y1=0.6;
y2=1-y1;
P_dew=approx(1/((y1/P1_sat)+(y2/P2_sat)),2)
x1=approx(y1*P_dew/P1_sat,4)

// Plotting the graph
subplot(1,2,1);
T=348.15;//[K]

P1_sat=approx(exp(14.2724-(2945.47/(T-49.15))),2) //KPa
P2_sat=approx(exp(14.2043-(2972.64/(T-64.15))),2) //KPa

x=[0:0.2:1];
```

```
P=approx(P2_sat+((P1_sat-P2_sat)*x),2);
y=approx(x*P1_sat./P,4);

mtlb_axis('auto');
plot(x,P,'g-')  //P vs x1
plot(y,P,'b-')  //P vs y1
x=[0,0.1];
P=[P2_sat,P2_sat];
plot(x,P,'--')  //P2_sat
x=[0.9,1];
P=[P1_sat,P1_sat];
plot(x,P,'r--') //P1_sat

x1=0.6;
P_b=approx(P2_sat+((P1_sat-P2_sat)*x1),2);
y1=approx(x1*P1_sat/P_b,4);
x=[x1,y1];
P=[P_b,P_b];
plot(x,P,'bo-')  //b--b'

y1=0.6;
y2=1-y1;
P_c=approx(1/((y1/P1_sat)+(y2/P2_sat)),2)
x1=approx(y1*P_c/P1_sat,4)

x=[x1,y1];
P=[P_c,P_c];
plot(x,P,'ro-')  //c'--c

P=[(P_b+10),P_b,P_c,(P_c-10)];
x=[0.6,0.6,0.6,0.6];
plot(x,P,'go-')  //a--b--c--d--0.6

P=[(P_c-10),30];
x=[0.6,0.6];
plot(x,P,'yo--')

P=[110,80];
```

```
x=[0.6,0.6];
plot(x,P,'w')
legend('P vs x1(Liquid)','P vs y1(Vapor)','P2_sat','P1_sat',"b—b''","c''--c",'a—b—c—d--0.6')
xtitle('(a)T/t=348.15K','x1,y1','P/Kpa')

disp("This is the liquid-phase composition at point c''")

//(b) Graph showing (t vs x1) and (t vs y1) for a pressure of 70KPa
//Example 10.2(b)
P=70;//[KPa]

T1_sat=approx(2945.47/(14.2724-log(P))+49.15,2);
T2_sat=approx(2972.64/(14.2043-log(P))+64.15,2);

T=[T1_sat,347.15,351.15,355.15,359.15,T2_sat];

P1_sat=approx(exp(14.2724-(2945.47./(T-49.15))),2);  //KPa
P2_sat=approx(exp(14.2043-(2972.64./(T-64.15))),2);  //KPa

x=approx((P-P2_sat)./(P1_sat-P2_sat),3);
y=approx((x.*P1_sat)/P,3);

Ans=[x',y',T'];
disp(Ans,'    x1          y1          T/t(K/C`)')

//at x1=0.6;
x1_b=0.6;
x2_b=1-x1_b;

T_a=347.15;// Intermediate Temperature  (Point a in graph)
P1_sat_a=approx(exp(14.2724-(2945.47./(T_a-49.15))),2);  //KPa
```

```
P2_sat_a=approx(exp(14.2043-(2972.64./(T_a-64.15))),2);  //KPa
alpha=P1_sat_a/P2_sat_a;  //Initial
a=T_a;
i=-1;
while(i==-1)
  P2_sat_b=P/((x1_b*alpha)+x2_b);
  b=approx(2972.64/(14.2043-log(P2_sat_b))+64.15,2);
  dT=abs(a-b);
  if(dT==0)
    i=0;
    T_b=b;
  end
  alpha=exp(0.0681-(2945.47/(b-49.15))+(2972.64/(b-64.15)));  //Eqn C
  a=b;
end
P1_sat_b=approx(exp(14.2724-(2945.47./(T_b-49.15))),2);  //KPa
y1_b=approx((x1_b*P1_sat_b)/P,4);  //b`

disp('K',T_b,'Hence by iteration Temp(Temp at b) at x1=0.6 is ')
disp('KPa',P1_sat_b,'Hence by iteration P1_sat at x1=0.6 is ')
disp(y1_b,'Composition of Vapor(b`) at x1=0.6')


//At y1=0.6
y1_c=0.6;
y2_c=1-y1_c;
T_d=355.15;// Intermediate Temperature  (Point a in graph)
P1_sat_d=approx(exp(14.2724-(2945.47./(T_d-49.15))),2);  //KPa
P2_sat_d=approx(exp(14.2043-(2972.64./(T_d-64.15))),2);  //KPa
alpha=P1_sat_d/P2_sat_d;  //Initial
```

```
d=T_d;
i=-1;
while(i==-1)
  P1_sat_c=P*(y1_c+(y2_c*alpha));
  c=approx(2945.47/(14.2724-log(P1_sat_c))+49.15,2);
  dT=abs(d-c);
  if(dT==0)
    i=0;
    T_c=c;
  end
  alpha=exp(0.0681-(2945.47/(c-49.15))+(2972.64/(c-64.15)));  //Eqn C
  d=c;
end
P1_sat_c=approx(exp(14.2724-(2945.47./(T_c-49.15))),2);  //KPa
x1_c=approx((y1_c*P)/P1_sat_c,4);  //c‘

disp('K',T_c,'Hence by iteration Temp(Temp at b) at y1=0.6 is ')
disp('KPa',P1_sat_c,'Hence by iteration P1_sat at y1=0.6 is ')
disp(x1_c,'Composition of liqiud(c‘) at y1=0.6')

//Graph
subplot(1,2,2);
T=linspace(T1_sat,T2_sat,10);

P1_sat=approx(exp(14.2724-(2945.47./(T-49.15))),2);  //KPa
P2_sat=approx(exp(14.2043-(2972.64./(T-64.15))),2);  //KPa

x=approx((P-P2_sat)./(P1_sat-P2_sat),3);
y=approx((x.*P1_sat)/P,3);

plot(x,T,'g-');
plot(y,T,'b-');
```

```

xsat=[0,0.1];
T2sat=[T2_sat,T2_sat];
plot(xsat,T2sat,'−−')  //T2_sat

xsat=[0.9,1];
T1sat=[T1_sat,T1_sat];
plot(xsat,T1sat,'r——') //T1_sat

Tcc=[T_c,T_c];
xc=[x1_c,y1_c];
plot(xc,Tcc,'ro−')  //c——c'

Tbb=[T_b,T_b];
xb=[x1_b,y1_b];
plot(xb,Tbb,'bo−')  //b——b'

Tabcd=[T_d,T_c,T_b,T_a];
xabcd=[0.6,0.6,0.6,0.6];
plot(xabcd,Tabcd,'go−')  //a——b——c——d−−0.6

Tao=[T_a,340];
xao=[0.6,0.6];
plot(xao,Tao,'yo——')
legend('T vs x1(Liquid)','T vs y1(Vapor)','T2_sat','
   T1_sat',"c''−−c","b——b''",'d——c——b——a−−0.6')
xtitle('(b)P=70KPa','x1,y1','T(K)')

//End
```

**Scilab code Exa 10.2** Find the Composition of the vapor and Liquid phase

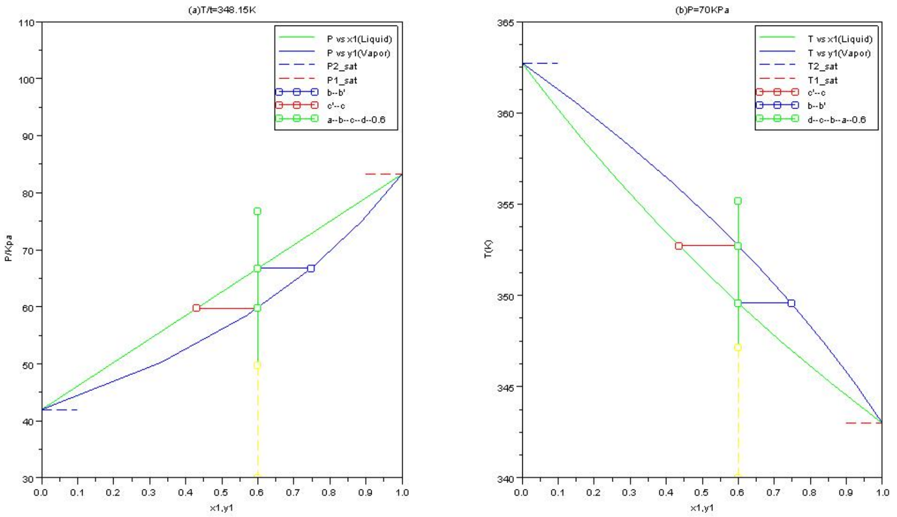

Figure 10.1: Plot the Graphs of P vs x1 y1 and t vs x1 y1

```
clear;
clc;

//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

//Example 10.2
//Caption : Program to Find the Composition of the
   vapor and Liquid phases

//Taking CO2 as Species 1 and Water as Species 2
H=990;//[Bar] Henry's Law const
T=283.15;//[K]
P2_sat=0.01227;//[Bar]  from Steam Tables
x1=0.01;//Assumed
x2=1-x1;
```

```
y1=1;
P=approx((x1*H)+(x2*P2_sat),3);
x1=approx((y1*P)/H,4);
x2=1-x1;
y2=approx((x2*P2_sat)/P,4);
y1=1-y2;
disp(x1,'Composition in liquid Phase')
disp(y1,'Composition in vapor Phase')
disp('Bar',P,'Pressure Exerted on Can')
disp('Hence Vapor phase chosen is nearly pure')

//End
```

**Scilab code Exa 10.3** Find Pressure Temperature and Composition

```
clear;
clc;

//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

//Example 10.3
//Caption : Program to Find Pressure,Temperature and Composition for a system

//Equations to be Used
// ln v1=A*(x2^2)  ln v2=A*(x1^2)  Where A =2.771-0.00523T

//Antoine Equations
```

```
//ln P1_sat = 16.59158-(3643.31/(T-33.424))
//ln P2_sat = 14.25326-(2665.54/(T-53.424))
//P = E(xi * Vi * Pi_sat)  E—Summation         Eqn 10.6
//P = 1/E(yi / (vi * Pi_sat))  E—Summation    Eqn 10.7

//(a) Calculate P and (yi) , for T=318.15K and x1=0.25

//BULB P Calculation
T=318.15;//[K]  Given
x1=0.25; //Given
x2=1-x1;
P1_sat = approx(exp(16.59158-(3643.31/(T-33.424)))
,2);//[KPa]
P2_sat = approx(exp(14.25326-(2665.54/(T-53.424)))
,2);//[KPa]
A=approx(2.771-(0.00523*T),3);
v1=approx(exp(A*(x2^2)),3);
v2=approx(exp(A*(x1^2)),3);

//Form Eqn(10.6)
P_a=approx((x1*v1*P1_sat)+(x2*v2*P2_sat),2);//[KPa]
y1_a=approx((x1*v1*P1_sat)/P_a,3);
y2_a=approx((x2*v2*P2_sat)/P_a,3);

disp('(a)P and [yi] for T=318.15K and x1=0.25')
disp('BUBL P calculations')
disp('KPa',P_a,'P = ')
disp(y1_a,'y1 = ')
disp(y2_a,'y2 = ')

//(b) Calculate P and (xi) , for T=318.15K and y1=0.60

//DEW P calculation
y1=0.6;
```

```
y2=1-y1;
T=318.15;//[K]
P1_sat = approx(exp(16.59158-(3643.31/(T-33.424)))
    ,2);//[KPa]
P2_sat = approx(exp(14.25326-(2665.54/(T-53.424)))
    ,2);//[KPa]
A=approx(2.771-(0.00523*T),3);
v1=0.1;//Assumed
v2=0.1;//Assumed
a1=v1;
a2=v2;
i=-1;
while(i==-1)
  P=approx(1/((y1/(a1*P1_sat))+(y2/(a2*P2_sat))),2);
  x1=approx(y1*P/(a1*P1_sat),4);
  x2=1-x1;
  b1=approx(exp(A*(x2^2)),4);
  b2=approx(exp(A*(x1^2)),4);
  dt=abs(b1-a1);
  if(dt==0)
    i=0;
    v1=b1;
    v2=b2;
    break;
  end
  a1=b1;
  a2=b2;
end
x1_b=x1;
x2_b=1-x1_b;
P_b=P;
v1_b=v1;
v2_b=v2;
disp('(b)P and [xi] for T=318.15K and y1=0.60')
disp('DEW P calculations')
disp('kPa',P_b,'P = ')
disp(x1_b,'x1 = ')
disp(x2_b,'x2 = ')
```

```

//(c) Calculate T and (yi) for P = 101.33 KPa and x1=0.85

//BUBL T calculation
P=101.33;
x1=0.85;
x2=1-x1;
T1_sat=approx((3643.31/(16.59158-log(P)))+33.424,2);
T2_sat=approx((2665.54/(14.25326-log(P)))+53.424,2);
T=(x1*T1_sat)+(x2*T2_sat);
a=T;//Initial
i=-1;
while(i==-1)
  A=approx(2.771-(0.00523*a),4);
  v1=approx(exp(A*(x2^2)),4);
  v2=approx(exp(A*(x1^2)),4);
  P1_sat = approx(exp(16.59158-(3643.31/(a-33.424))),2);//[KPa]
  P2_sat = approx(exp(14.25326-(2665.54/(a-53.424))),2);//[KPa]
  alpha=P1_sat/P2_sat;
  P1_sat=approx(P/((x1*v1)+(x2*v2/alpha)),2);
  b=approx((3643.31/(16.59158-log(P1_sat)))+33.424,2);
  dt=abs(b-a);
  if(dt==0)
    i=0;
    T=b;
    break;
  end
  a=b;
end
T_c=T;
y1_c=approx(x1*v1*P1_sat/P,3);
y2_c=1-y1_c;
disp('(c)T and [yi] for P=101.33kPa and x1=0.')
disp('BUBL T calculations')
disp('K',T_c,'Temperature = ')
disp(y1_c,'y1 = ')
disp(y2_c,'y2 = ')

//(d) Calculate T and (xi) for P = 101.3 KPa and y1 =0.4
P=101.3;
y1=0.4;
y2=1-y1;
T1_sat=approx((3643.31/(16.59158-log(P)))+33.424,2);
T2_sat=approx((2665.54/(14.25326-log(P)))+53.424,2);
T=(y1*T1_sat)+(y2*T2_sat);
v1=1;  //Initially
v2=1;  //Initially
a=T;//Initial
i=-1;
while(i==-1)
  A=approx(2.771-(0.00523*a),4);
  P1_sat = approx(exp(16.59158-(3643.31/(a-33.424))),2);//[KPa]
  P2_sat = approx(exp(14.25326-(2665.54/(a-53.424))),2);//[KPa]
  alpha=P1_sat/P2_sat;
  x1=approx((y1*P)/(v1*P1_sat),4);
  x2=1-x1;
  v1=approx(exp(A*(x2^2)),4);
  v2=approx(exp(A*(x1^2)),4);
  P1_sat=P*((y1/v1)+(y2*alpha/v2));
  b=approx((3643.31/(16.59158-log(P1_sat)))+33.424,2);
  dt=abs(a-b);
  if(dt==0)
    T=a;
    i=0;
    break;
  end
  a=b;
end
```

```
T_d=T;
x1_d=x1;
x2_d=x2;
disp('(d)T and [xi] for P=101.33kPa and y1=0.40')
disp('DEW T calculations')
disp('K',T,'T = ')
disp(x1_d,'x1 = ')
disp(x2_d,'x2 = ')

//(e) Taz , (xi_az) and (yi_az)  for T = 318.15K
T = 318.15;
// Relative Volatility   alpha_12=(y1/x1)/(y2/x2)
//At Azeotrope y1=x1 and y2=x2 and alpha_12=1
P1_sat = approx(exp(16.59158-(3643.31/(T-33.424))),2);//[KPa]
P2_sat = approx(exp(14.25326-(2665.54/(T-53.424))),2);//[KPa]
//From eqn (10.5) alpha_12=(v1*P1_sat)/(v2*P2_sat)
A=approx(2.771-(0.00523*T),4);

//When x1=0 v2=1 and v1=exp(A)
alpha_12_x10=P1_sat*exp(A)/P2_sat;

//When x1=1 v1=1 and v2=exp(A)
alpha_12_x11=P1_sat/(P2_sat*exp(A));

//But this is not Azeotrope  (at Azeotrope alpha_12=1)

//v1_az/v2_az=(P2_sat/P1_sat)=K
K=P2_sat/P1_sat;

//ln(v1/v2)=ln(K)=A(1-(2*x1))
x1_az=approx((A-log(K))/(2*A),3);
x2_az=1-x1_az;
y1_az=x1_az;
y2_az=x2_az;
v1_az=approx(exp(A*(x2_az^2)),3);
```

```
v2_az=approx(exp(A*(x1_az^2)),3);
P_az=approx(v1_az*P1_sat,2);

disp('Azeotropic Pressure and Azeotropic Composition for T = 318.15K')
disp('KPa',P_az,'Azeotropic Pressure = ')
disp(x1_az,'x1_az')
disp(y1_az,'y1_az')

//End
```

**Scilab code Exa 10.4** Find the Dewpoint and Bubblepoint Pressure

```
clear;
clc;

//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

//Example 10.4
//Caption : Program To Find the Dewpoint and Bubblepoint Pressure

T=283.15;//[K]
//(a) Dew Point Pressure
//Species=[" Methane ";" Ethane ";" Propane "];
y=[0.1,0.2,0.7];

P1=6.9;//[bar]
K1=[20,3.25,0.92];
```

```
x1=approx(y./K1,3);

P2=10.34;//[bar]
K2=[13.2,2.25,0.65];
x2=approx(y./K2,3);

P3=8.7;//[bar]
K3=[16,2.65,0.762];
x3=approx(y./K3,3);

i=1;
j=1;
P=[P1,P2,P3];
x=[x1;x2;x3];
E1=zeros(1,3);
for(i=1:3)
  for(j=1:3)
    E1(i)=E1(i)+x(i,j);//Summation
    //j=j+1;
  end
  //i=i+1;
end
P_dew = 8.7;
Ans=[y',K1',x1',K2',x2',K3',x3';1,0,E1(1),0,E1(2),0,E1(3)];
disp('                    P=6.9 bar        P=10.34 bar        P=8.7 bar')
disp(Ans,'   yi        Ki       yi/Ki       Ki       yi/Ki        Ki        yi/Ki')
disp('Last Row Represents the summation')
disp('KPa',P_dew,'The dew Point Pressure')

T=283.15;//[K]
//(b) Bubble Point Pressure
//Species=[" Methane ";" Ethane ";" Propane "];
x=[0.1,0.2,0.7];

P1=26.2;//[bar]
```

```
K1=[5.6,1.11,0.335];
y1=approx(x.*K1,3);

P2=27.6;//[bar]
K2=[5.25,1.07,0.32];
y2=approx(x.*K2,3);

P3=26.54;//[bar]
K3=[5.49,1.1,0.33];
y3=approx(x.*K3,3);

i=1;
j=1;
P=[P1,P2,P3];
y=[y1;y2;y3];
E2=zeros(1,3);
for(i=1:3)
  for(j=1:3)
    E2(i)=E2(i)+y(i,j);//Summation
    //j=j+1;
  end
  //i=i+1;
end
P_Bubble = 26.54;
Ans=[x',K1',y1',K2',y2',K3',y3';1,0,E2(1),0,E2(2),0,E2(3)];
disp('                    P=26.2 bar        P=27.6 bar        P=26.54 bar')
disp(Ans,'    xi       Ki       xiKi       Ki       xiKi       Ki       xiKi')
disp('Last Row Represents the summation')
disp('KPa',P_Bubble,'The Bubble Point Pressure')

//End
```

**Scilab code Exa 10.5** Find L V xi and yi for a System

```
clear;
clc;

//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

//Example 10.5
//Caption : Program to Find L V {xi} and {yi} for a System

z1=0.45;
z2=0.35;
z3=0.2;
P=110;//[KPa]
T=353.15;//[K]
P1_sat=195.75;//[KPa]
P2_sat=97.84;//[KPa]
P3_sat=50.32;//[KPa]

//BUBL Calculation
x1=z1;
x2=z2;
x3=z3;
P_BUBL=(x1*P1_sat)+(x2*P2_sat)+(x3*P3_sat);

//DEW Calculation
y1=z1;
```

```
y2=z2;
y3=z3;
P_Dew=1/((y1/P1_sat)+(y2/P2_sat)+(y3/P3_sat));

//Since P_Bubl<P<P_dew
//Flash Calculation
K1=P1_sat/P;
K2=P2_sat/P;
K3=P3_sat/P;

//Finding V from Eqn(10.17)
//E((zi*Ki)/(1+(V*(Ki-1))))=1

x=0;
F_x=(((z1*K1)/(1+((K1-1)*x)))+((z2*K2)/(1+((K2-1)*x)))+((z3*K3)/(1+((K3-1)*x)))-1);
F_a=F_x;

x=0.9;
F_x=(((z1*K1)/(1+((K1-1)*x)))+((z2*K2)/(1+((K2-1)*x)))+((z3*K3)/(1+((K3-1)*x)))-1);
F_b=F_x;
A=0;
B=0.9;
i=1;
while(i==1)
  a=A;
  F_a=(((z1*K1)/(1+((K1-1)*a)))+((z2*K2)/(1+((K2-1)*a)))+((z3*K3)/(1+((K3-1)*a)))-1);
  b=B;
  F_b=(((z1*K1)/(1+((K1-1)*b)))+((z2*K2)/(1+((K2-1)*b)))+((z3*K3)/(1+((K3-1)*b)))-1);
  x1=((a*F_b)-(b*F_a))/(F_b-F_a);
  F_x1=(((z1*K1)/(1+((K1-1)*x1)))+((z2*K2)/(1+((K2-1)*x1)))+((z3*K3)/(1+((K3-1)*x1)))-1);

  if((F_a*F_x1)<0) then
    flag=1;
    A=a;
    B=x1;
  else((F_x1*F_b)<0)
    flag=2;
    A=x1;
    B=b;
  end
  x1_a=approx(x1,4);
  b_a=approx(b,4);
  a_a=approx(a,4);
  if(x1_a==b_a)
    V=approx(x1,4);
    i=0;
    break;
  elseif(x1_a==a_a)
    root=approx(x1,4);
    i=0;
    break;
  end

end
disp(V,'Hence By solving the polynomial V = ')
L=1-V;
//from eqn 10.16
//yi=(zi*Ki)/(1+(V*(Ki-1)))
y1=approx((z1*K1)/(1+((K1-1)*V)),4);
y2=approx((z2*K2)/(1+((K2-1)*V)),4);
y3=approx((z3*K3)/(1+((K3-1)*V)),4);
x1=approx(y1/K1,4);
x2=approx(y2/K2,4);
x3=approx(y3/K3,4);
y=[y1 y2 y3];
x=[x1 x2 x3];
disp(L,'Moles Of liquid')
disp(V,'Moles Of vapor')
disp(x,'Mole fraction Of liquid')
disp(y,'Mole fraction Of vapor')

```

```
//End
```

**Scilab code Exa 10.6** Find the Composition of Vapor and Liquid Phases

```
clear;
clc;

//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

//Example 10.6
//Caption : Program To Find the Composition of Vapor and Liquid Phases

//Given Values
z=[0.1,0.2,0.7];
K=[10,1.76,0.52];

V_01=[0.1:0.1:1]
for(i=1:10)
  for(j=1:3)
    y_01(i,:)=approx((z.*K)./(1+(V_01(i)*(K-1))),3);
  end
  Sum(i)=sum(y_01(i,:));
end

for(i=1:10)
  if(Sum(i+1)<1)
    a1=V_01(i);
    i=-1;
    break;
  end
end

V_001=[a1:0.01:a1+0.1]
for(i=1:10)
  for(j=1:3)
    y_001(i,:)=approx((z.*K)./(1+(V_001(i)*(K-1))),3);
  end
  Sum(i)=sum(y_001(i,:));
end

for(i=1:10)
  if(Sum(i+1)<1)
    a01=V_001(i);
    i=-1;
    break;
  end
end

V_0001=[a01:0.001:a01+0.01];

for(i=1:10)
  for(j=1:3)
    y_0001(i,:)=approx((z.*K)./(1+(V_0001(i)*(K-1))),3);
  end
  Sum(i)=sum(y_0001(i,:));
end

for(i=1:10)
  if(Sum(i+1)<1)
    a001=V_0001(i);
    i=-1;
    break;
  end
end
```

```
V=a001;
y_02=approx((z.*K)./(1+(a1*(K-1))),3);
y_03=approx((z.*K)./(1+((a1+0.1)*(K-1))),3);
y_0273=approx((z.*K)./(1+(V*(K-1))),3);
x_0273=approx(y_0273./K,3);

Ans=[z',K',y_02',y_03',y_0273',x_0273';1,0,sum(y_02),sum(y_03),sum(y_0273),approx(sum(x_0273),2)];
disp(Ans,'    z        K        y,V=0.2   y,V=0.3   y,V=0.273  x,V=0.273')
disp('NOTE : Last Row represents the summation')
disp('Hence for V = 0.273 E(yi) = 0 and E(xi) = 0')
disp(V,'Fraction of Vapor (V) = ')

//End
```

# Chapter 11

# Solution Thermodynamics Theroy

**Scilab code Exa 11.4** Find the Expression For Enthalpies

```
clear;
clc;

//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

//Example 11.4
//Caption : Program To Find the Expression For Enthalpies

//H=400x1 + 600x2 + x1x2(40x1 + 20x2)  Given

//Substituting x2=1-x1

```

```
H=poly([600 -180 0 -20],'x1','c')      //(A)

//K=dH/dx1

K=poly([-180 0 -60],'x1','c')

//Using Eqn 11.15  H1=H+x2*K

//substituting x2=1-x1

H1=poly([420 0 -60 40],'x1','c')      //(B)

//Similarly for H2

H2=poly([600 0 0 40],'x1','c')        //(C)

//Now to calculate H1_inf and H2_inf

//x1=0 in (B)
H1_inf=420;//[J/mol]

//x2=0 in (C) i.e. x1=1
H2_inf=640;//[J/mol]

disp(H1,'H1 = ');
disp(H2,'H2 = ');
disp('J/mol',H1_inf,'H1_inf = ')
disp('J/mol',H2_inf,'H2_inf = ')

//End
```

**Scilab code Exa 11.5** Plot the Fugacity and Fugacity Coefficient Vs P

```
clear;
clc;

//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

//Example 11.5
//Caption : Program to Plot the Fugacity and
   Fugacity Coefficient Vs P

//Using Eqn 11.30

//G=t(T)+RT ln f
//G`=t(T)+rt ln f`

//Hence ln(f/f`) = (1/RT)*(G-G`)

//G=H-TS
//G`=H-TS`

//ln (f/f`)=(n/R)*(((H-H`)/T)-(S-S`))    (A)

R=8.314;
n=18.015;
f_=1;//[kPa]
P_=f_;
H_=3076.8;//[J/g]
S_=10.3450;//[J/g/K]
T=573.15;//[K]
P=[10 50 100 200 500 1000 1500 2000 2500 3000 3500
   4000 4500 5000 5500 6000 6500 7000 7600 8000
   8400];
H=[3076.6 3075.7 3074.2 3072.1 3064.8 3052.1 3038.9
   3025 3010.4 2995.1 2979 2962 2944.2 2925.5 2905.8
    2885 2862.9 2839.4 2808.8 2786.8 2763.1];
```

```
S=[9.282 8.5380 8.2166 7.8937 7.4614 7.1251 6.9207
    6.7696 6.6470 6.5422 6.4491 6.3642 6.2852 6.2105
    6.1388 6.0692 6.0008 5.9327 5.8503 5.7942
    5.7366];

K=approx(exp((n/R).*(((H-H_)/T)-(S-S_))),0);

f=K*f_;
P(22)=8592.7;//[kPa]
P_sat=P(22)
f(22)=6738.9;
f_sat=f(22)

si=approx(f./P,4);
si_sat=si(22)

Vl=approx(1.403*n,2)//[cm^3/mol]
//Using Eqn 11.41
P_new=linspace(8592.7,10000,10);
f_new=approx(f_sat.*exp(Vl.*(P_new-P_sat)/(R*1000*T)
    ),1);
si_new=f_new./P_new;
subplot(1,2,1)
plot(P/1000,f/1000,'b')
plot(P_new/1000,f_new/1000,'g')
dotsx=[0 P_sat/1000];
dotsy=[f_sat/1000 f_sat/1000];
plot(dotsx,dotsy,'b--')
dotsx=[0 f_sat/1000];
dotsy=[P_sat/1000 P_sat/1000];
plot(dotsy,dotsx,'g--')
dotsx=[11,8];
dotsx=[6,6];
plot(dotsx,dotsy,'w')
legend('f vs P(till P_sat)','f vs P(Beyond P_sat)','
    f_sat','P_sat')
xtitle('f vs P','P X 10^-3 /kPa','f X 10^-3 /kPa')
subplot(1,2,2)
```

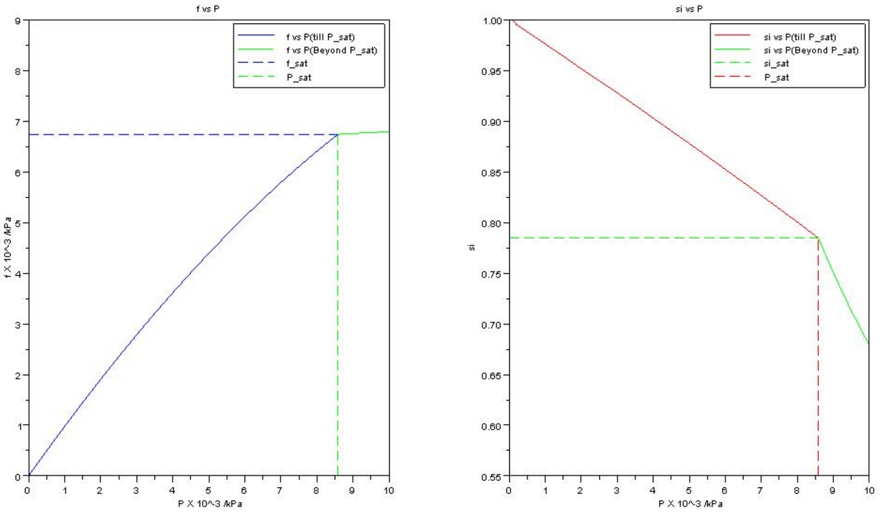

Figure 11.1: Plot the Fugacity and Fugacity Coefficient Vs P

```
plot(P/1000,si,'r')
plot(P_new/1000,si_new,'g')
dotsx=[0 P_sat/1000];
dotsy=[si_sat si_sat];
plot(dotsx,dotsy,'g--')
dotsx=[0.55 si_sat];
dotsy=[P_sat/1000 P_sat/1000];
plot(dotsy,dotsx,'r--')

legend('si vs P(till P_sat)','si vs P(Beyond P_sat)'
    ,'si_sat','P_sat')
xtitle('si vs P','P X 10^-3 /kPa','si')

//End
```

**Scilab code Exa 11.7** Find the Fugacity Coefficient for the mixture

```
clear;
clc;

//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

//Example 11.7
//Caption : Program to Find the Fugacity Coefficient for the mixture

T=200;//[K]
P=30;//[bar]
R=83.14;
x1=0.4;//[N2]
x2=1-x1;//[CH4]

B11=-35.2;//[cm^3/mol]
B22=-105;//[cm^3/mol]
B12=-59.8;//[cm^3/mol]

delta_12=approx((2*B12)-B11-B22,1);
si_1=approx(exp((P/(R*T))*(B11+(x2^2*delta_12))),4);
si_2=approx(exp((P/(R*T))*(B22+(x1^2*delta_12))),4);

B=approx((x1^2*B11)+(2*x1*x2*B12)+(x2^2*B22),2);
Z=approx(1+((B*P)/(R*T)),2);

```

```
disp(si_1,si_2,'Fugacity Coefficients are ')
disp(B,'Second Viral coefficient is ')
disp(Z,'Compressibility Factor is ')

//End
```

**Scilab code Exa 11.8** Find the Fugacity of 1 butene vapor

```
clear;
clc;

//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

//Example 11.8
//Caption : Program to Find the Fugacity of 1–butene
    vapor

T=473.15;//[K]
P=70;//[bar]
Tc=420;//[K]
Pc=40.43;//[bar]
omega=0.191;

//By interpolation in Tables E.15 and E.16
si_0=0.627;
si_1=1.096;
//Using Eqn(11.64)
si=approx(si_0*(si_1^omega),3);
f=approx(si*P,1);
```

```
disp(si,'Fugacity coefficient is ')
disp('bar',f,'fugacity is ')

//End
```

**Scilab code Exa 11.9** Find the Fugacity Coefficients for mixture

```
clear;
clc;

//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

//Example 11.9
//Caption : Program to Find the Fugacity Coefficients for mixture

P=25;//[KPa]
T=323.15;//[K]
R=83.14;
x1=0.5;
x2=1-x1;

ij=[11,22,12];
Tc_ij=[535.5,591.8,563.0];
Pc_ij=[41.5,41.1,41.3];
Vc_ij=[267,316,291];
Zc_ij=approx((Pc_ij.*Vc_ij)./(R*Tc_ij),3);
omega_ij=[0.323,0.262,0.293];

```

```
Tr_ij=approx(T./Tc_ij,3);
B0=approx(0.083-(0.422./(Tr_ij.^1.6)),3)
B1=approx(0.139-(0.172./(Tr_ij.^4.2)),3)
B_ij=round((R*Tc_ij./Pc_ij).*(B0+(omega_ij.*B1)));

delta_12=(2*B_ij(3))-B_ij(1)-B_ij(2);
R=8314;
si_1=approx(exp((P/(R*T))*(B_ij(1)+(x2^2*delta_12)))
    ,3);
si_2=approx(exp((P/(R*T))*(B_ij(3)+(x1^2*delta_12)))
    ,3);

Ans=[ij',Tc_ij',Pc_ij',Vc_ij',Zc_ij',omega_ij',Tr_ij
    ',B0',B1',B_ij'];
disp(Ans,'    ij        Tcij        Pcij      Vcij        Zcij
            Wij        Trij          B0          B1          Bij')

disp(si_1,si_2,'Fugacity Coefficients are ')

//End
```

**Scilab code Exa 11.10** Find the Excess Properties for a mixture

```
clear;
clc;

//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

//Example 11.10
```

```
//Caption : Program to Find the Excess Properties for a mixture

T0=298.15;//[K]
T=323.15;//[K]
Cp_E=-2.86;//[J/mol/K]
Ho_E=897.9;//[J/mol]
Go_E=384.5;//[J/mol]

//(a)  Derivations

//G_E=-a*(T ln T - T)+ bT + c
//S_E=a ln T - b
//H_E=aT + c

//Where

//a=Cp_E
//c=Ho_E-aT0
//b=((Go_E+a(T ln T0 - T0)-c)/T0)

//(b)
a=Cp_E;
c=approx(Ho_E-(a*T0),1);
b=approx((Go_E+(a*((T0*log(T0))-T0)-c))/T0,4);
G_E=approx((-a*(T*log(T)-T))+(b*T)+c,1);
S_E=approx((a*log(T))-b,3);
H_E=approx((a*T)+c,1);

disp('J/mol',G_E,'G_E = ')
disp('J/mol/K',S_E,'S_E = ')
disp('J/mol',H_E,'H_E = ')

//End
```

# Chapter 12

# Solution Thermodynamics Applications

**Scilab code Exa 12.1** Reduce the set of VLE Data and Plot the Graphs

```
clear;
clc;

//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

//Example 12.1
//Caption : Program to Reduce the set of VLE Data and Plot the Graphs

P=[90.15,91.78,88.01,81.67,78.89,76.82,73.39,66.45,62.95,57.70,50.
x1
```

```
   =[0.000,0.063,0.248,0.372,0.443,0.508,0.561,0.640,0.702,0.763,0.8
y1
   =[0.000,0.049,0.131,0.182,0.215,0.248,0.268,0.316,0.368,0.412,0.4
x2=1-x1;
y2=1-y1;
P1_sat=P(13);
P2_sat=P(1);
K=zeros(1,13);
for(i=1:13)
  if(i ~= 1)
    ln_V1(i)=approx(log(y1(i)*P(i)/(x1(i)*P1_sat))
       ,3);
  end
  if(i ~= 13)
    ln_V2(i)=approx(log(y2(i)*P(i)/(x2(i)*P2_sat))
       ,3);
  end
end
ln_V1(1)=%nan;
ln_V2(13)=%nan;
for(i=2:12)
  K(i)=approx(((x1(i)*ln_V1(i))+(x2(i)*ln_V2(i)))/(
     x1(i)*x2(i)),3);  //K=G_E/(x1*x2*R*T)
  k(i)=approx(((x1(i)*ln_V1(i))+(x2(i)*ln_V2(i))),3)
     ;  //K=G_E/(R*T)

end
K(1)=%nan;
k(1)=%nan;
K(13)=%nan;
k(13)=%nan;
A21=0.70;
A12=1.35;
K_new=approx((A21.*x1)+(A12.*x2),3);
//Using Eqn (12.10(a) and 12.10(b))
ln_V1_new=approx((x2.*x2).*(A12+(2*(A21-A12).*x1))
   ,3);
V1_new=approx(exp(ln_V1_new),3);
ln_V2_new=approx((x1.*x1).*(A21+(2*(A12-A21).*x2))
   ,3);
V2_new=approx(exp(ln_V2_new),3);
//Using Eqn (12.11)
P_new=(x1.*V1_new*P1_sat)+(x2.*V2_new*P2_sat);

A21_new=0.596;
A12_new=1.153;

K_new1=approx((A21_new.*x1)+(A12_new.*x2),3);
//Using Eqn (12.10(a) and 12.10(b))
ln_V1_new1=approx((x2.*x2).*(A12_new+(2*(A21_new-
   A12_new).*x1)),3);
V1_new1=approx(exp(ln_V1_new1),3);
ln_V2_new1=approx((x1.*x1).*(A21_new+(2*(A12_new-
   A21_new).*x2)),3);
V2_new1=approx(exp(ln_V2_new1),3);
//Using Eqn (12.11)
P_new1=(x1.*V1_new1*P1_sat)+(x2.*V2_new1*P2_sat);

subplot(1,2,1)
plot(x1,P,'bo')
plot(y1,P,'gs')

plot(x1,P_new,'b–')
plot(y1,P_new,'g–')

plot(x1,P_new1,'b—')
plot(y1,P_new1,'g—')

legend('Actual(P vs x1)','Actual(P vs y1)','By Gibbs
    Duhem(P vs x1)','By Gibbs Duhem(P vs y1)','By
   Barkers Method(Accurate)')

xtitle('(a)','x1,y1','P/kPa')

```

```
subplot(1,2,2)
plot(x1,ln_V1,'bs')
plot(x1,ln_V2,'gv')

plot(x1,K,'ro')

plot(x1,K_new,'r-')
plot(x1,ln_V1_new,'b-')
plot(x1,ln_V2_new,'g-')

plot(x1,K_new1,'r--')
plot(x1,ln_V1_new1,'b--')
plot(x1,ln_V2_new1,'g--')

legend('Actual(ln V1 vs x1)','Actual(ln V2 vs x1)','G_E/x1x2RT vs x1','By Gibbs Duhem(G_E/x1x2RT vs x1)','By Gibbs Duhem(ln V1 vs x1)','By Gibbs Duhem(ln V2 vs x1)','By Barkers Method(Accurate)')
xtitle('(b)','x1')

//End
```

**Scilab code Exa 12.2** Find the Excess Enthalpy as function of x1

```
clear;
clc;

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

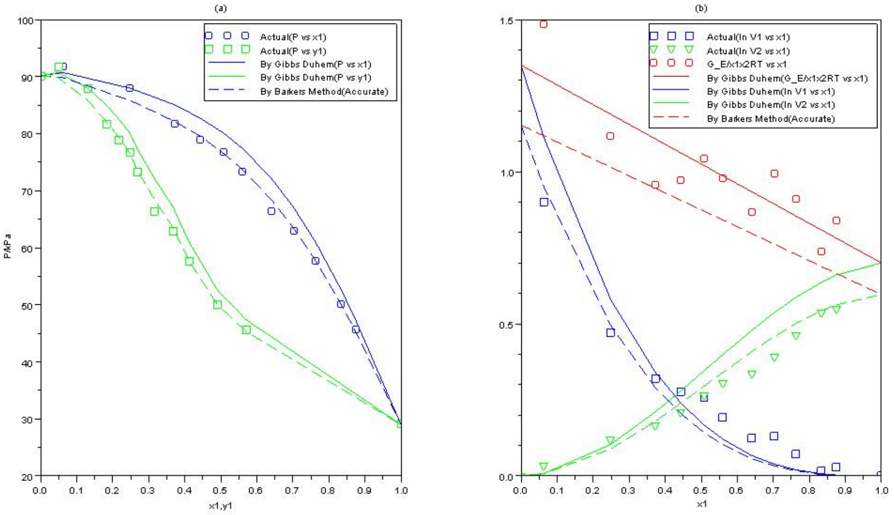

Figure 12.1: Reduce the set of VLE Data and Plot the Graphs

```
  funcprot(0)
endfunction

//Example 12.2
//Caption : Program to Find the Excess Enthalpy as function of x1

//H_E=x1x2(40x1+20x2)    (A)
//Find H1_E and H2_E

//H1_E=H_E+((1-x1)*(dH_E/dx1))  let d=dH_E/dx1

//H2_E=H_E-(x1*(dH_E/dx1))  let d=dH_E/dx1

//Replacing x2=1-x1 in (A)

H_E=poly([0 20 0 -20],'x1','c');
d=poly([20 0 -60],'x1','c');
H1_E=poly([20 0 -60 40],'x1','c');
```

```
H2_E=poly([0 0 0 40],'x1','c');

disp(H1_E,'Expression For H1_E(x1) is ')
disp(H2_E,'Expression For H2_E(x1) is ')


//End
```

**Scilab code Exa 12.4** Find the Heat of Formation of LiCl

```
clear;
clc;

//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

//Example 12.4
//Caption : Program to Find the Heat of Formation of LiCl

//           Li + 0.5Cl2 --> LiCL(s)        (A)

//    LiCl(s) + 12H2O(l) --> LiCl(12H2O)    (B)

//Net Reaction
//Li + 0.5Cl2 +12H2O(l) --> LiCl(12H2O)    (Net)

//From Table C.4
Hf_A=-408610;//[J]
Hf_B=-33614;//[J]
```

```
Hf_Net=Hf_A+Hf_B;//[J]

disp('J',Hf_Net,'Heat of formation of LiCl in 12mol H2O at 298.15K is')

//End
```

**Scilab code Exa 12.5** Calculate the Heat transfer rate in th evaporator

```
clear;
clc;

//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

//Example 12.5
//Caption : Program to Calculate the Heat transfer rate in th evaporator

M_LiCl=42.39;
M_H2O=18.015;
T1=298.15;//[K]
T2=405.15;//[K]
//Step a
m_LiCl=0.15*2;
m_H2O=2-m_LiCl;
n_LiCl=(m_LiCl*1000)/M_LiCl
n_H2O=(m_H2O*1000)/M_H2O;
dH_LiCl=-33800;
dH_a=-n_LiCl*dH_LiCl//[J/s]
```

```

//Step b
m_LiCl=0.15*2;
m_H2O=0.45;
n_LiCl=(m_LiCl*1000)/M_LiCl;
n_H2O=(m_H2O*1000)/M_H2O;
dH_LiCl=-23260;
dH_b=n_LiCl*dH_LiCl//[J/s]

//Step c
m_LiCl=0.75;
Cp=2.72;
dT=T2-T1;
dH_c=m_LiCl*Cp*dT*1000//[J/s]

//step d
m_H2O=2-m_LiCl;
dH_T2=2740.3;//[KJ/s/mol] form Steam Tables
dH_T1=104.8;//[KJ/s/mol]  from Steam Tables
dH_d=m_H2O*(dH_T2-dH_T1)*1000//[J/s]

dH=approx((dH_a+dH_b+dH_c+dH_d)/1000,1);

disp('kW or KJ/s',dH,'The required Heat Transfer rate is ')

//End
```

**Scilab code Exa 12.6** Calculate Heat Transfer Rate in a evaporator

```
clear;
clc;

```

```
//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

//Example 12.6
//Caption : Program to Calculate Heat Transfer Rate in Single effect Evaporator

T0=298.15;//[K]
T=361.5;//[K]
mT=1.25;//[Kg/s]  10% NaOH
m_steam=1;//[Kg/s] at P=76 torr and 361.5K
m_50NaOH=mT-m_steam;//[Kg/s]  at 361.5K

//From Steam tables
//at 76 torr and 361.15K
H_steam=2666;//[KJ/kg]
//for 10% NaOH soln at 294.15K
H_10NaOH=79;//[KJ/Kg]
//for 50% NaOH soln at 361.15K
H_50NaOH=500;//[KJ/Kg]

dH=(m_steam*H_steam)+(m_50NaOH*H_50NaOH)-(mT*H_10NaOH);
Q=dH;
disp('kW or kJ/s',Q,'Heat Transfer rate')

//End
```

**Scilab code Exa 12.9** Calculate the Heat Transformed per Kg of Solution

```
clear;
clc;

//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

//Example 12.9
//Caption : Program to Calculate the Heat Transformed per Kg of Solution formed

T=294.15;//[K]
m_NaOH_soln=1;//[kg]
m_NaOH_solid=0.45*m_NaOH_soln;//[Kg]
m_H2O=0.55*m_NaOH_soln;//[Kg]

//From Steam Tables
H_NaOH_soln=216;//[kJ/Kg]
H_NaOH_solid=1113;//[kJ/Kg]
H_H2O=88;//[kJ/Kg]

dH=m_NaOH_soln*H_NaOH_soln-(m_NaOH_solid*H_NaOH_solid)-(m_H2O*H_H2O);
Q=dH;

disp('kW or kJ/kg',Q,'Heat Transferred per Kg of NaOH Soln')

//End
```

# Chapter 13

# Chemical Reaction Equilibria

**Scilab code Exa 13.1** Determine the Expressions for mole Fractions yi

```
clear;
clc;

//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

//Example 13.1
//Caption : Program to determine the Expressions for
    mole Fractions yi

//CH4 + H2O --> CO + 3H2

n_CH4=2;//Moles of CH4
n_H2O=1;//Moles of H20
n_CO=1;//Moles of CO
n_H2=4;//Moles of H2
```

```

v_CH4=-1;
v_H2O=-1
v_CO=1;
v_H2=3;

v=v_CH4+v_H2O+v_CO+v_H2;
n=n_CH4+n_H2O+n_CO+n_H2;

//y_CH4=(n_CH4+(v_CH4e)/n+(v*e))
//y_H2O=(n_H2O+(v_H2Oe)/n+(v*e))
//y_CO=(n_CO+(v_CO*e)/n+(v*e))
//y_H2=(n_H2+(v_H2*e)/n+(v*e))

y_CH4='(n_CH4+(v_CH4e)/n+(v*e))';
y_H2O='(n_H2O+(v_H2Oe)/n+(v*e))';
y_CO='(n_CO+(v_CO*e)/n+(v*e))';
y_H2='(n_H2+(v_H2*e)/n+(v*e))';



//Hence

y_CH4='(2-e/8+2e)';
y_H2O='(1-e/8+2e)';
y_CO='(1+e/8+2e)';
y_H2='(4+3e/8+2e)';

disp(y_CH4,'y_CH4 = ')

disp(y_H2O,'y_H2O = ')

disp(y_CO,'y_CO = ')

disp(y_H2,'y_H2 = ')

//End
```

**Scilab code Exa 13.3** Determine the Expression for yi for two reactions

```
clear;
clc;

//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

//Example 13.3
//Caption : Program to Determine the Expression for yi for two reactions

//CH4 + H2O  --> CO + 3H2     (A)

//CH4 + 2H2O --> CO2 + 4H2    (B)

Species=['CH4','H2O','CO','CO2','H2','sum'];
v_A=['-1','-1','1','0','3','2'];
v_B=['-1','-2','0','1','4','2'];
m_CH4=2;
m_H2O=3;
mt=m_CH4+m_H2O;
y=['(m_CH4+vie1+vje2)/(mt+vie1+vje2)','(m_H2O+vie1+vje2)/(mt+vie1+vje2)','(vie1)/(mt+vie1+vje2)','(vje2)/(mt+vie1+vje2)','(vie1+vje2)/(mt+vie1+vje2)',' '];

//Hence

```

```
yf=['(2-e1-e2)/(5+2e1+2e2)','(3-e1-2e2)/(5+2e1+3e2)','e1/(5+2e1+2e2)','e2/(5+2e1+2e2)','(3e1+4e2)/(5+2e1+2e2)',' '];

Ans=[Species',v_A',v_B',y',yf'];

disp(Ans,' i    v_A   v_B        y(Before substitution)           y_species')

//End
```

**Scilab code Exa 13.4.a** Alternate Program to 13 iv

```
clear;
clc;

//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

//Example 13.4  Alternate
//Caption : Alternate Program to 13.4

T=[298.15,418.15,593.15];
t=approx(T/T(1),4);
R=8.314;


//C2H4(g) + H2O(g) -->  C2H5OH(g)

//Values From Table C.1 At T=298.15K
```

```

A_ethanol=3.518;
A_ethene=1.424;
A_water=3.470;

B_ethanol=20.001*10^-3;
B_ethene=14.394*10^-3;
B_water=1.450*10^-3;

C_ethanol=-6.002*10^-6;
C_ethene=-4.392*10^-6;
C_water=0;

D_ethanol=0;
D_ethene=0;
D_water=0.121*10^5;

dA=A_ethanol-A_ethene-A_water
dB=B_ethanol-B_ethene-B_water
dC=C_ethanol-C_ethene-C_water
dD=D_ethanol-D_ethene-D_water

// Values from Table C.4 at T=298.15K
H_ethanol=-235100;//[J/mol]
H_ethene=52510;//[J/mol]
H_water=-241572;//[J/mol]

G_ethanol=-168490;//[J/mol]
G_ethene=68460;//[J/mol]
G_water=-228572;//[J/mol]

dHo=H_ethanol-H_ethene-H_water
dGo=G_ethanol-G_ethene-G_water

//Using Eqn(13.21)
Ko=approx(exp(-dGo./(R*T(1))),3)
K0=Ko*ones(1,3);
//Using Eqn(13.22)
```

```
K1=exp((dHo/(R*T0))*(1-(T(1)./T)));
//Using Eqn(13.24)
K2=approx(exp((dA.*(log(t)-((t-1)./t)))+(0.5*dB*T(1)
    .*((t-1).^2)./t)+((1/6)*dC*T(1)*T(1).*((t-1).^2)
    .*(t+2)./t)+(0.5*dD.*((t-1).^2)./((T(1)^2).*(t)
    .^2))),4);

K=K0.*K1.*K2;

Ans=[T',t',K0',K1',K2',K'];
disp(Ans,'      T/K          t                K0              K1
              K2            K')

//End
```

**Scilab code Exa 13.4** Find the equillibrium constant for Vapor Phase

```
clear;
clc;

//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

function[Q]=IDCPH(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=(dA+((dB/2)*T0*(t+1))+((dC/3)*T0*T0*((t^2)+t+1))
     +(dD/(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction

```

```
function[Q]=IDCPS(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=((dA)*log(t))+(((dB*T0)+(((dC*T0*T0)+(dD/(t*t*T0*T0)))*(t+1)/2))*(t-1))
  funcprot(0);
endfunction

//Example 13.4
//Caption : Program to Find the equillibrium constant for Vapor Phase Hydration

T0=298.16;//[K]
T1=418.15;//[K]
T2=593.15;//[K]
R=8.314;

//C2H4(g) + H2O(g) --> C2H5OH(g)
//Values From Table C.1 At T=298.15K

A_ethanol=3.518;
A_ethene=1.424;
A_water=3.470;

B_ethanol=20.001*10^-3;
B_ethene=14.394*10^-3;
B_water=1.450*10^-3;

C_ethanol=-6.002*10^-6;
C_ethene=-4.392*10^-6;
C_water=0;

D_ethanol=0;
D_ethene=0;
D_water=0.121*10^5;

dA=A_ethanol-A_ethene-A_water
dB=B_ethanol-B_ethene-B_water
dC=C_ethanol-C_ethene-C_water
```

```
dD=D_ethanol-D_ethene-D_water

// Values from Table C.4 at T=298.15K
H_ethanol=-235100;//[J/mol]
H_ethene=52510;//[J/mol]
H_water=-241572;//[J/mol]

G_ethanol=-168490;//[J/mol]
G_ethene=68460;//[J/mol]
G_water=-228572;//[J/mol]

dHo=H_ethanol-H_ethene-H_water
dGo=G_ethanol-G_ethene-G_water

I1=approx(IDCPH(T0,T1,dA,dB,dC,dD),3)
I2=approx(IDCPS(T0,T1,dA,dB,dC,dD),5)

//Using Eqn 13.18
//dG_418/RT=((dGo - dHo)/RTo)+(dHo/RT)+((1/T)*I1)-I2 c1=dG_418/RT

c1=approx(((dGo-dHo)/(R*T0))+(dHo/(R*T1))+((1/T1)*I1)-I2,4)

I3=approx(IDCPH(T0,T2,dA,dB,dC,dD),3)
I4=approx(IDCPS(T0,T2,dA,dB,dC,dD),5)

//Using Eqn 13.18
//dG_593/RT=((dGo - dHo)/RTo)+(dHo/RT)+((1/T)*I1)-I2 c2=dG_593/RT

c2=approx(((dGo-dHo)/(R*T0))+(dHo/(R*T2))+((1/T2)*I3)-I4,4)

K_413=approx(exp(-c1),4);
K_593=exp(-c2);

disp('X 10^-1',K_413*10,'Equilibrium Constant at T =
    413.15K is ')
disp('X 10^-3',approx(K_593*1000,3),'Equilibrium
   Constant at T = 593.15K is ')

//End
```

**Scilab code Exa 13.5** Calculate the Fraction of Heat Reacted

```
clear;
clc;

//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

//Example 13.5
//Caption : Program to Calculate the Fraction of
   Heat Reacted for Various Cases

//CO(g) + H2O(g) --> CO2(g) + H2(g)

v_CO=-1;
v_H2O=-1;
v_CO2=1;
v_H2=1;
v=v_CO+v_H2O+v_CO2+v_H2;

//Calculate e(Fraction of Stream) in each case

//(a)
n_H2O_a=1;//mol
```

```
n_CO_a=1;//mol
T_a=1100;//[K]
P_a=1;//[bar]

x=10^4/T_a;
//at this x the value of ln K=0 form Graph
y=0;
nt=n_H2O_a+n_CO_a;
K=exp(y);

//y_H2O=(n_H2O+(v_H2O*e))/nt
//y_CO=(n_CO+(v_CO*e))/nt
//y_H2=(v_H2*e)/nt
//y_CO2=(v_CO2*e)/nt


y_H2O='(1-e)/2'
y_CO='(1-e)/2'
y_H2='e/2'
y_CO2='e/2'


//K=(y_H2*y_CO2)/(y_CO*y_H2O)

K='e^2/((1-e)^2)=1';


//Solving
e_a=0.5;

//(b) same as in (a) P_b=10bar

//Pressure has no effect on fraction of stream
e_b=e_a;

//(c) same as in (a) N2=2mols included

//Since N2 just act as diluent
```

```
//It only changes the total moles fraction remains the same
e_c=e_a;

//(d)
n_H2O_d=2;//mol
n_CO_d=1;//mol
T_d=1100;//[K]
P_d=1;//[bar]

x=10^4/T_d;
//at this x the value of ln K=0 form Graph
y=0;
nt=n_H2O_d+n_CO_d;
K=exp(y);

//y_H2O=(n_H2O+(v_H2O*e))/nt
//y_CO=(n_CO+(v_CO*e))/nt
//y_H2=(v_H2*e)/nt
//y_CO2=(v_CO2*e)/nt

y_H2O='(1-e)/3'
y_CO='(2-e)/3'
y_H2='e/3'
y_CO2='e/3'

//K=(y_H2*y_CO2)/(y_CO*y_H2O)

K='e^2/((1-e)(2-e))=1';

//Solving
e=approx(2/3,3);
e_d=approx(e/2,3);

//(e)
//Here the y_CO and y_H2O are interchanged

//No change in Fraction of stream
```

```
e_e=e_d;

//(f)
n_H2O_f=1;//mol
n_CO_f=1;//mol
n_CO2_f=1;;//[mol]
T_f=1100;//[K]
P_f=1;//[bar]

x=10^4/T_f;
//at this x the value of ln K=0 form Graph
y=0;
nt=n_H2O_f+n_CO_f+n_CO2_f;
K=exp(y);

//y_H2O=(n_H2O+(v_H2O*e))/nt
//y_CO=(n_CO+(v_CO*e))/nt
//y_CO2=(n_CO2+(v_CO2*e))/nt
//y_H2=(v_H2*e)/nt


y_H2O='(1-e)/3'
y_CO='(1-e)/3'
y_H2='(1+e)/3'
y_CO2='e/2'


//K=(y_H2*y_CO2)/(y_CO*y_H2O)

K='(e*(e+1))/((1-e)^2)=1';

//Solving
e_f=approx(1/3,3);

//(g)
n_H2O_g=1;//mol
n_CO_g=1;//mol
T_g=1650;//[K]
```

```
P_g=1;//[bar]

x=10^4/T_g;
//at this x the value of ln K=0 form Graph
y=-1.15;
nt=n_H2O_g+n_CO_g;
K=exp(y);

//y_H2O=(n_H2O+(v_H2O*e))/nt
//y_CO=(n_CO+(v_CO*e))/nt
//y_H2=(v_H2*e)/nt
//y_CO2=(v_CO2*e)/nt


y_H2O='(1-e)/2'
y_CO='(1-e)/2'
y_H2='e/2'
y_CO2='e/2'


//K=(y_H2*y_CO2)/(y_CO*y_H2O)

Exp='e^2/((1-e)^2)=0.316';

//Solving
p=poly([K -2*K K-1],'e','c');

root=roots(p);
e_g=approx(root(1),2);

//Other Root is negative and the Fraction of steam cannot be negative


disp('(a)1mol H20 and 1 mol CO T=1100K  P=1bar')
disp('(b)1mol H20 and 1 mol CO T=1100K  P=10bar')
disp('(c)1mol H20 and 1 mol CO 2mol N2 T=1100K  P=1bar')
disp('(d)2mol H20 and 1 mol CO T=1100K  P=1bar')
disp('(e)1mol H20 and 2 mol CO T=1100K  P=1bar')
disp('(f)1mol H20 and 1 mol CO 1mol CO2 T=1100K  P=1bar')
disp('(g)1mol H20 and 1 mol CO T=1650K  P=1bar')
e=[e_a e_b e_c e_d e_e e_f e_g];
disp(e,'Fraction Of Steam Reacted in each case')

//End
```

**Scilab code Exa 13.6** Find the Maximum Conversion of Ethylene to ethanol

```
clear;
clc;

//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

function[Q]=IDCPH(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=(dA+((dB/2)*T0*(t+1))+((dC/3)*T0*T0*((t^2)+t+1))+(dD/(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction

function[Q]=IDCPS(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=((dA)*log(t))+(((dB*T0)+(((dC*T0*T0)+(dD/(t*t*T0*T0)))*(t+1)/2))*(t-1))
  funcprot(0);
```

```
endfunction

function[si]=PHIB(Tr,Pr,omega)
  B0=0.083-(0.422/(Tr^1.6));
  B1=0.139-(0.172/(Tr^4.2));
  si=exp((Pr/Tr)*(B0+(omega*B1)));
  funcprot(0);

endfunction


//Example 13.6
//Caption : Program to find the Maximum Conversion of Ethylene to ethanol

T0=298.16;//[K]
T1=523.15;//[K]
P=35;//[bar]
R=8.314;

//C2H4(g) + H2O(g) --> C2H5OH(g)
//Values From Table C.1 At T=298.15K

A_ethanol=3.518;
A_ethene=1.424;
A_water=3.470;

B_ethanol=20.001*10^-3;
B_ethene=14.394*10^-3;
B_water=1.450*10^-3;

C_ethanol=-6.002*10^-6;
C_ethene=-4.392*10^-6;
C_water=0;

D_ethanol=0;
D_ethene=0;
D_water=0.121*10^5;
```

```

dA=A_ethanol-A_ethene-A_water
dB=B_ethanol-B_ethene-B_water
dC=C_ethanol-C_ethene-C_water
dD=D_ethanol-D_ethene-D_water

// Values from Table C.4 at T=298.15K
H_ethanol=-235100;//[J/mol]
H_ethene=52510;//[J/mol]
H_water=-241572;//[J/mol]

G_ethanol=-168490;//[J/mol]
G_ethene=68460;//[J/mol]
G_water=-228572;//[J/mol]

dHo=H_ethanol-H_ethene-H_water
dGo=G_ethanol-G_ethene-G_water

I1=approx(IDCPH(T0,T1,dA,dB,dC,dD),3)
I2=approx(IDCPS(T0,T1,dA,dB,dC,dD),5)

//Using Eqn 13.18
//dG_418/RT=((dGo - dHo)/RTo)+(dHo/RT)+((1/T)*I1)-I2 c1=dG_418/RT

c1=approx(((dGo-dHo)/(R*T0))+(dHo/(R*T1))+((1/T1)*I1)-I2,4)
K_523=approx(exp(-c1),4);
disp('X 10^-3',approx(K_523*1000,3),'Equilibrium Constant at T = 523.15K is ')

//Values Frm App B
Tc=[282.3,647.1,513.9];
Pc=[50.4,220.55,61.48];
omega=[0.087,0.345,0.645];

Tr=approx(T1./Tc,3);
Pr=approx(P./Pc,3);
```

```
si=approx(PHIB(Tr,Pr,omega),3);

//Using eqn
//(y_ETOH*si_ETOH)/(y_C2H4*si_C2H4*y_H20*si_H2O)=(P/Po)K
//y_ETOH/(y_C2H4*y_H20)=c=((si_C2H4*si_H2O)/si_ETOH)(P/Po)K
c=approx(((si(1)*si(2))/si(3))*(P*K_523),3)

//y_C2H4 = (1-e)/(6-e)
//y_ETOH = (5-e)/(6-e)
//y_H2O = (e)/(6-e)

//Solving we get a Eqn
poly([1.342 -6 1],'e','c')
root=approx(roots(poly([1.342 -6 1],'e','c')),3)

r=root(1)*100;
//Since e > 1 not possible so e=0.233

disp('%',r,'The Maximum Conversion of ethylene to ethanol by Vapor-Phase Hydration is ')

//End
```

**Scilab code Exa 13.7** Find the Composition of Product Steam

```
clear;
clc;

//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

//Example 13.7
//Caption : Program to Find the Composition of
   Product Steam at Equillibrium

T=1393.15;//K
P=1;//[bar]
x=10^4/T;
//C2H2 --> 2C + H2  (I)
//2C + 2H2 --> C2H4 (II)

//Values Of ln K (at  1000/T )for Reactions I and II
    from Graph
K_I=exp(12.9);
K_II=exp(-12.9);
K=K_I*K_II;

//Application in Eqn (13.5)

//y_C2H4/(y_C2H2*y_H2)=c=(P/Po)K
c=P*K;
//y_H2=y_C2H2=(1-e)/(2-e)
//y_C2H4=e/(2-e)


//The Eqn comes out to be
poly([1 -4 2],'e','c')

root=approx(roots(poly([1 -4 2],'e','c')),3)
e=root(1);
//Since e > 1 not possible so e=0.293
y_C2H2=approx((1-e)/(2-e),3);
y_H2=y_C2H2;
y_C2H4=approx(e/(2-e),3);

disp(y_H2,y_C2H2,y_C2H4,'Equilibrium Composition of
   H2 C2H2 and C2H4 Respectively ')

//End
```

**Scilab code Exa 13.8** Find the Mole fraction of Ethyl Acetate

```
clear;
clc;

//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

//Example 13.8
//Caption : Program to Find the Mole fraction of
   Ethyl Acetate

T0=298.15;
T=373.15;//[K]
R=8.314;
//CH3COOH(l)+C2H5OH(l) --> CH3COOC2H5(l) + H2O(l)

//From Table C.4
dHo_EtAc=-480000;//[J]
dHo_H2O=-285830;//[J]
dHo_EtOH=-277690;//[J]
dHo_AcH=-484500;//[J]

dGo_EtAc=-332200;//[J]
dGo_H2O=-237130;//[J]
dGo_EtOH=-174780;//[J]
```

```
dGo_AcH=-389900;//[J]

dHo_298=dHo_EtAc+dHo_H2O-dHo_EtOH-dHo_AcH;
dGo_298=dGo_EtAc+dGo_H2O-dGo_EtOH-dGo_AcH;

K_298=approx(exp(-dGo_298/(R*T0)),4);

//Using Eqn(13.15)
//ln(K_373/K_298)=c=-(dHo_298/R)*((1/373.15)-(1/298.15))
c=approx(-(dHo_298/R)*((1/373.15)-(1/298.15)),4);
K_373=approx(K_298*exp(c),4);

//x_AcH=x_EtOH=(1-e)/2  and  x_EtAc=x_H2O=e/2
//K=(x_EtAc*x_H2O)/(x_AcH*x_EtOH)

//Hence The Eqn is
q=poly([K_373 -2*K_373 K_373-1],'e','c')
root=approx(roots(q),4)
e=root(1);
//Since Other Root is > 1 hence e=0.6879
x_EtAc=approx(e/2,3);

disp(x_EtAc,'Composition of Ethyl Acetate in the Reacting Mixture')

//End
```

**Scilab code Exa 13.9** Determine Composition and Temperature of Steam

```
clear;
clc;

```

```
//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

function[Q]=MCPH(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))
  funcprot(0);
endfunction

function[Q]=IDCPH(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=(dA+((dB/2)*T0*(t+1))+((dC/3)*T0*T0*((t^2)+t+1))+(dD/(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction

function[Q]=IDCPS(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=((dA)*log(t))+(((dB*T0)+(((dC*T0*T0)+(dD/(t*t*T0*T0)))*(t+1)/2))*(t-1))
  funcprot(0);
endfunction

//Example 13.9
//Caption : Program to Determine Composition and Temperature of Product Steam

P=1;//[bar]
T0=298.15;//[K]
R=8.314;

//SO2 + 0.5O2 --> SO3
dHo_298=-98890;//[J/mol]
dGo_298=-70866;//[J/mol]
```

```

n_O2_i=0.5*1.2;//   Moles O2 Entering
n_N2_i=n_O2_i*(79/21);//Moles N2 Entering

//n_SO2=1-e
//n_O2=0.6-(0.5*e)
//n_SO3=e
//n_N2=2.257

//By Energy Balance
//(dHo_298*e)+dHo_P = dH = 0                                    (A)

//dHo_P=Cp*(T-298.15)   Cp=E nCp                                (B)

//Cp_SO2=R*MCPH(T0,T,5.699,0.801E-3,0,-1.015E+5)
//Cp_O2=R*MCPH(T0,T,3.639,0.506E-3,0,-0.227E+5)
//Cp_SO3=R*MCPH(T0,T,8.06,1.056E-3,0,-2.028E+5)
//Cp_N2=R*MCPH(T0,T,3.28,0.593E-3,0,0.04E+5)

//T=(-(dHo_298*e)/Cp)+T0                                        (C)

//K=(e/(1-e))*((3.857-(0.5*e))/(0.6-(0.5*e)))^0.5      (D)

//ln K = ((dHo_298-dGo_298)/(R*T0))-(dHo_298/(R*T))+I1-(I2/T)   (E)

//I1=IDCPS(T0,T,0.5415,0.002E-3,0,-0.8995E+5)
//I2=IDCPH(T0,T,0.5415,0.002E-3,0,-0.8995E+5)

//Iteration
A1=300;//Initial
i=-1;

while(i==-1)
```

```

I1=IDCPS(T0,A1,0.5415,0.002E-3,0,-0.8995E+5);
I2=IDCPH(T0,A1,0.5415,0.002E-3,0,-0.8995E+5);
//Applying in Eqn (E)
K = exp(((dHo_298-dGo_298)/(R*T0))-(dHo_298/(R*
   A1))+I1-(I2/A1));
//Applying in Eqn (D)
if(isreal(K))
  x=0;
  // p=poly([-0.6*(K^2) 1.7*(K^2) 3.857-(1.6*(K
     ^2)) 0.5*((K^2)-1)],'e','c')
  // (0.5*((K^2)-1)*(x^3))+((3.857-(1.6*(K^2)))
     *(x^2))+(1.7*(K^2)*x)+(-0.6*(K^2))
  F_x=(0.5*((K^2)-1)*(x^3))+((3.857-(1.6*(K^2)))
     *(x^2))+(1.7*(K^2)*x)+(-0.6*(K^2));
  F_a=F_x;

  x=1;
  F_x=(0.5*((K^2)-1)*(x^3))+((3.857-(1.6*(K^2)))
     *(x^2))+(1.7*(K^2)*x)+(-0.6*(K^2));
  //F_x=(x^3)-(4*x)+1;
  F_b=F_x;
  root=-100;
  A=0;
  B=1;
  i=1;
  while(i==1)
   a=A;
   F_a=(0.5*((K^2)-1)*(a^3))+((3.857-(1.6*(K^2))
      )*(a^2))+(1.7*(K^2)*a)+(-0.6*(K^2));
   //F_a=(a^3)-(4*a)+1;
   b=B;
   F_b=(0.5*((K^2)-1)*(b^3))+((3.857-(1.6*(K^2))
      )*(b^2))+(1.7*(K^2)*b)+(-0.6*(K^2));
   //F_b=(b^3)-(4*b)+1;
   x1=((a*F_b)-(b*F_a))/(F_b-F_a);
   F_x1=(0.5*((K^2)-1)*(x1^3))+((3.857-(1.6*(K
      ^2)))*(x1^2))+(1.7*(K^2)*x1)+(-0.6*(K^2));
   //F_x1=(x1^3)-(4*x1)+1;

   if((F_a*F_x1)<0) then
     flag=1;
     A=a;
     B=x1;
   else((F_x1*F_b)<0)
    flag=2;
    A=x1;
    B=b;
  end
  x1_a=approx(x1,4);
  b_a=approx(b,4);
  a_a=approx(a,4);
  if(x1_a==b_a)
    root=approx(x1,5);
    i=0;
    break;
  elseif(x1_a==a_a)
    root=approx(x1,5);
    i=0;
    break;
  end

end
e=root;
Cp_SO2=R*MCPH(T0,A1,5.699,0.801E-3,0,-1.015E+5);
Cp_O2=R*MCPH(T0,A1,3.639,0.506E-3,0,-0.227E+5);
Cp_SO3=R*MCPH(T0,A1,8.06,1.056E-3,0,-2.028E+5);
Cp_N2=R*MCPH(T0,A1,3.28,0.593E-3,0,0.04E+5);

n_SO2=1-e;
n_O2=0.6-(0.5*e);
n_SO3=e;
n_N2=2.257;
if(n_SO2<0 | n_O2<0 | n_SO3<0)
  e=0;
end
```

```
    Cp=(n_SO2*Cp_SO2)+(n_O2*Cp_O2)+(n_SO3*Cp_SO3)+(n_N2*Cp_N2);
    //Applying in Eqn (C)
    B=(-(dHo_298*e)/Cp)+T0;
    m=(A1+B)/2;
    dT=approx(abs(m-A1),2);
    if(dT<0.1)
      i=0;
      T=approx(A1,1);
      e=approx(e,2);
      break;
   end
    A1=m;
    i=-1;
  else
    i=-1;
    A1=A1+1;
  end
end
disp(e,'Fraction')

n_SO2=1-e
n_O2=0.6-(0.5*e)
n_SO3=e
n_N2=2.257

nt=n_SO2+n_O2+n_SO3+n_N2;

y_SO2=approx(n_SO2/nt,4);
y_O2=approx(n_O2/nt,4);
y_SO3=approx(n_SO3/nt,4);
y_N2=approx(n_N2/nt,4);

disp(T,'Final Temperature')
disp(y_SO2,'Composition of SO2')
disp(y_O2,'Composition of O2')
disp(y_SO3,'Composition of SO3')
disp(y_N2,'Composition of N2')
```

```

//End
```

**Scilab code Exa 13.12** Find the Product Composition for Two Reactions

```
clear;
clc;


//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

function[Q]=IDCPH(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=(dA+((dB/2)*T0*(t+1))+((dC/3)*T0*T0*((t^2)+t+1))+(dD/(t*T0*T0)))*(T-T0)
  funcprot(0);
endfunction

function[Q]=IDCPS(T0,T,dA,dB,dC,dD)
  t=T/T0;
  Q=((dA)*log(t))+(((dB*T0)+(((dC*T0*T0)+(dD/(t*t*T0*T0)))*(t+1)/2))*(t-1))
  funcprot(0);
endfunction


//Example 13.12
//Caption : Program to Find the Product Composition for Two Reactions
```

```

T0=298.16;//[K]
T1=750;//[K]
R=8.314;
P=1.2;//[bar]

//C4H10 --> C2H4 + C2H6   (I)
//C4H10 --> C3H6 + CH4    (II)

//Values From Table C.1 At T=298.15K

A_butane=1.935;
A_ethene=1.424;
A_ethane=1.131;
A_propene=1.637;
A_methane=1.702;

B_butane=36.915*10^-3;
B_ethene=14.394*10^-3;
B_ethane=19.225*10^-3;
B_propene=22.706*10^-3;
B_methane=9.081*10^-3;

C_butane=-11.402*10^-6;
C_ethene=-4.392*10^-6;
C_ethane=-5.561*10^-6;
C_propene=-6.915*10^-6;
C_methane=-2.164*10^-6;

D_butane=0;
D_ethene=0;
D_ethane=0;
D_propene=0;
D_methane=0;

dA_I=A_ethene+A_ethane-A_butane;
dA_II=A_methane+A_propene-A_butane;

```

```
dB_I=B_ethene+B_ethane-B_butane;
dB_II=B_methane+B_propene-B_butane;

dC_I=C_ethene+C_ethane-C_butane;
dC_II=C_methane+C_propene-C_butane;

dD_I=D_ethene+D_ethane-D_butane;
dD_II=D_methane+D_propene-D_butane;

// Values from Table C.4 at T=298.15K
H_butane=-125790;//[J/mol]
H_ethene=52510;//[J/mol]
H_ethane=-83820;//[J/mol]
H_propene=19710;//[J/mol]
H_methane=-74520;//[J/mol]

G_butane=-16570;//[J/mol]
G_ethene=68460;//[J/mol]
G_ethane=-31855;//[J/mol]
G_propene=62205;//[J/mol]
G_methane=-50460;//[J/mol]

dHo_I=H_ethene+H_ethane-H_butane
dHo_II=H_methane+H_propene-H_butane

dGo_I=G_ethene+G_ethane-G_butane
dGo_II=G_methane+G_propene-G_butane

I1_I=approx(IDCPH(T0,T1,dA_I,dB_I,dC_I,dD_I),3)
I1_II=approx(IDCPH(T0,T1,dA_II,dB_II,dC_II,dD_II),3)
I2_I=approx(IDCPS(T0,T1,dA_I,dB_I,dC_I,dD_I),5)
I2_II=approx(IDCPS(T0,T1,dA_II,dB_II,dC_II,dD_II),5)

//Using Eqn 13.18
//dG_418/RT=((dGo − dHo)/RTo)+(dHo/RT)+((1/T)*I1)−I2
    c1=dG_418/RT

c1_I=approx(((dGo_I-dHo_I)/(R*T0))+(dHo_I/(R*T1))
   +((1/T1)*I1_I)-I2_I,4)
c1_II=approx(((dGo_II-dHo_II)/(R*T0))+(dHo_II/(R*T1)
   )+((1/T1)*I1_II)-I2_II,4)

K_I=approx(exp(-c1_I),4)
K_II=approx(exp(-c1_II),4)

k=(K_II/K_I)^0.5;
e_I=approx(((K_I/P)/(1+(K_I*(1/P)*(1+k)*(1+k))))
   ^0.5,4);

e_II=approx(k*e_I,4);

n_C4H10=1-e_I-e_II;
n_C2H4=e_I;
n_C2H6=e_I;
n_C3H6=e_II;
n_CH4=e_II;
nt=n_C4H10+n_C2H4+n_C2H6+n_C3H6+n_CH4;

y_C4H10=approx(n_C4H10/nt,4);
y_C2H4=approx(n_C2H4/nt,4);
y_C2H6=approx(n_C2H6/nt,4);
y_C3H6=approx(n_C3H6/nt,4);
y_CH4=approx(n_CH4/nt,4);

y=[y_C4H10 y_C2H4 y_C2H6 y_C3H6 y_CH4];
disp(y,'   Y_C4H10    Y_C2H4     Y_C2H6     Y_C3H6
   Y_CH4')

//End
```

**Scilab code Exa 13.13** Find the Composition at different Temperatures

```
clear;
clc;

//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

//Example 13.13
//Caption : Program to Find the Composition at different Temperatures

n_air=2.381//[mol]
n_O2=0.21*n_air;
n_N2=0.79*n_air;
R=8.314;

P=20;//[bar]
T=[1000 1100 1200 1300 1400 1500];
dG_H2O=[-192420 -187000 -181380 -175720 -170020 -164310];
dG_CO=[-200240 -209110 -217830 -226530 -235130 -243740];
dG_CO2=[-395790 -395960 -396020 -396080 -396130 -396160];

KI='y_H2O/((y_O2)^0.5*y_H2)(P/Po)^-0.5'
KII='y_CO/((y_O2)^0.5)(P/Po)^0.5'
KIII='y_CO2/y_O2'

n='3.38+((e2-e1)/2)'
y_H2='-e1/n'
y_CO='e2/n'
y_O2='((0.5(1-e1-e2))-e3)/n'
y_H2O='(1+e1)/n'
y_CO2='e3/n'
y_N2='1.88/n'
```

```

KI='(1+e1)(2n)^0.5*(P/Po)^-0.5'
KII='(e3*(P/Po)^0.5)/(1-e1-e2-2e3)^0.5*(n/2)^0.5'
KIII='2e3/(1-e1-e2-2e3)'

K_I=approx(exp(-dG_H2O./(R.*T)),1)
K_II=approx(exp(-dG_CO./(R.*T)),1)
K_III=approx(exp(-dG_CO2./(R.*T)),1)

//Now since the values of KI KII KIII valyes are so High the mole fraction of O2 must be very small
//Hence We eleminate O2,Hence 2 Eqns are,

//C + CO2 --> 2CO       (a)
//H2O + C --> H2 + CO   (b)

Ka='(y_CO^2/y_CO2)*(P/Po)'
Kb='((y_H2*y_CO)/y_H2O)*(P/Po)'

n='3.38+(e_a+e_b)'
y_H2='e_b/n'
y_CO='(2e_a+e_b)/n'
y_H2O='(1-e_b)/n'
y_CO2='(0.5-e_a)/n'
y_N2='1.88/n'

Ka='(2e_a+e_b)^2/((0.5-e_a)*n)*(P/Po)'
Kb='e_b(2e_a+e_b)/((1-e_b)*n)*(P/Po)'

dG_new_a=(2*dG_CO)-dG_CO2;
dG_new_b=dG_CO-dG_H2O;

Ka=approx(exp((-dG_new_a./(R.*T))),3);
Kb=approx(exp((-dG_new_b./(R.*T))),3);

//Calculation of e_a and e_b

a=0.1;//Initial Value
```

```

b=0.7;//Initial Value

C1=Ka/20;
C2=Kb/20;

for(i=1:6)
c=-1;
while(c==-1)
  fa=approx((((a^2)*(4+C1(i)))+(b^2)+((4+C1(i))*(a*b))+(2.88*C1(i)*a)-(0.5*C1(i)*b)-(1.69*C1(i))),4);
  dfax=approx(((2*a*(4+C1(i)))+((4+C1(i))*b)+(2.88*C1(i))),4);
  dfay=approx((2*b)+((4+C1(i))*a)-(0.5*C1(i)),4);

  fb=approx(((b^2*(1+C2(i)))+((2+C2(i))*a*b)-(C2(i)*a)+(2.38*C2(i)*b)-(3.38*C2(i))),4);
  dfbx=approx((((2+C2(i))*b)-C2(i)),4);
  dfby=approx(((2*b*(1+C2(i)))+((2+C2(i))*a)+(2.38*C2(i))),4);

  A=[dfax dfay;dfbx dfby];
  B=[-fa;-fb];
  Ans=approx(A\B,4);
  da=Ans(1);
  db=Ans(2);

  if(da==0 & db==0)
    c=0;
    e_a(i)=a;
    e_b(i)=b;
    break;
  end
  a=a+da;
  b=b+db;
end
end
```

```

n=3.38+(e_a+e_b);
y_H2=approx(e_b./n,3);
y_CO=approx(((2*e_a)+e_b)./n,3);
y_H2O=approx((1-e_b)./n,3);
y_CO2=approx((0.5-e_a)./n,3);
y_N2=approx(1.88./n,3);

Ans=[T',Ka',Kb',e_a,e_b];
Ans1=[T',y_H2,y_CO,y_H2O,y_CO2,y_N2];

plot(T',y_H2,'r-')
plot(T',y_CO,'b-')
plot(T',y_H2O,'g-')
plot(T',y_CO2,'m-')
plot(T',y_N2,'y-')

legend('H2','CO','H2O','CO2','N2',)
xtitle('Equllibrium Compositions','T/K','yi')



disp(Ans,'     T/K          Ka              Kb                e_a                  e_b')

disp(Ans1,'     T/K          y_H2         y_CO        y_H2O           y_CO2        y_N2')

//End
```

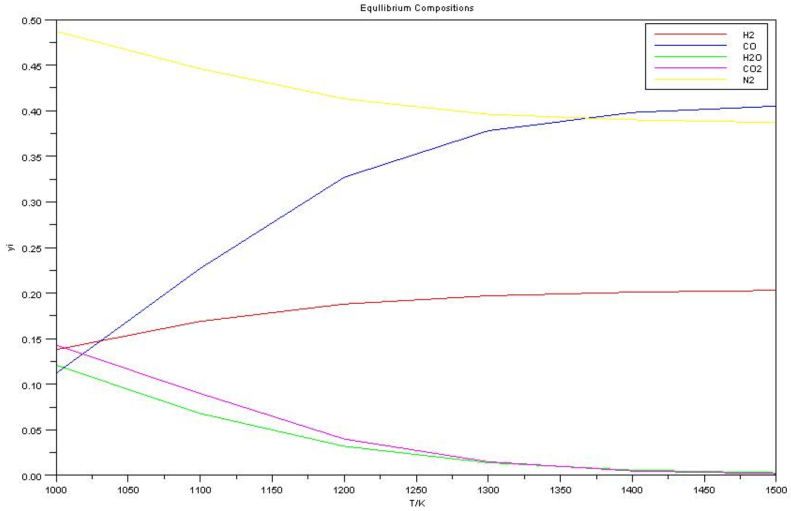

Figure 13.1: Find the Composition at different Temperatures

# Chapter 14

# Topics In Phase Equilibria

**Scilab code Exa 14.1** Find the Fugacity Coefficients of N2 and CH4

```
clear;
clc;

//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

//Example 14.1
//Caption : Program to Find the Fugacity Coefficients of Nitrogen and Methane

Tc=[126.2 190.6];
T=200;//[K]
Tr=T./Tc;
Pc=[34 45.99];
P=30;//[Bar]
Pr=P./Pc;
```

```
R=83.14;
bi=approx(0.08664.*R.*Tc./Pc,3);
ai=approx(((0.42748.*(R^2).*(Tc.^2).*(Tr.^(-0.5))./
   Pc)/(10^5)),3);  //10^-5ai
y=[0.4 0.6];
a=approx(((y(1)^2)*ai(1))+(2*y(1)*y(2)*sqrt((ai(1)*
   ai(2))))+((y(2)^2)*ai(2)),2);  //10^-5a
b=approx((y(1)*bi(1))+(y(2)*bi(2)),3);

q=(a*10^5)/(b*R*T);
Beta=0.051612;
//Z=1+Beta-(q*(Z-Beta)/(Z*(Z+Beta)))

Z=1;//initial
A=Z;
for i=0:10
  B=1+Beta-((q*Beta)*(A-Beta)/(A*(A+Beta)));
   if((B-A)==0.0001)
     break;
   end
   A=B;
   i=i+1;
end
Z=approx(B,5);

I=log((Z+Beta)/Z)
a1=approx((2*y(1)*ai(1))+(2*y(2)*sqrt((ai(1)*ai(2)))
   -a),2);   //10^-5a1
a2=approx((2*y(2)*ai(2))+(2*y(1)*sqrt((ai(2)*ai(1)))
   -a),2);   //10^-5a2
b1=bi(1);
b2=bi(2);
q1=approx(q*(((a1+a)/a)-(b1/b)),5);
q2=approx(q*(((a2+a)/a)-(b2/b)),5);
ln_si1=approx((((b1/b)*(Z-1))-(log(Z-Beta))-(q1*I))
   ,5);   //ln si1
ln_si2=approx((((b2/b)*(Z-1))-(log(Z-Beta))-(q2*I))
   ,5);   //ln si2
```

```
si1=approx(exp(ln_si1),5);
si2=approx(exp(ln_si2),5);
q=[q1 q2];
ln_si=[ln_si1 ln_si2];
si=[si1 si2];
a_=[a1 a2];
b_=[b1 b2];
q_=[q1 q2];

disp(’bar cmˆ6 molˆ−2’,a,’a = ’)
disp(’cmˆ3 mol6−1’,b,’b = ’)
disp(q,’q = ’)

Ans=[Tc’,Tr’,Pc’,bi’,ai’,a_’,b_’,q_’,ln_si’,si’];
disp(Ans,’         Tc          Tr           Pc           bi
            ai          a            b            q           ln
   si          si’)

//End
```

**Scilab code Exa 14.5** Derive the equations from LLE data

```
clear;
clc;

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

//Example 14.5
//Caption : Program to derive the equations from LLE
```

```
    data

function[Root]=RF(A,B,K)

    //By Regula Falsi Method
    i=1;
   while(i==1)
    a=A;
    F_a=log((1-a)/a)+(2*a*K)-K;
    b=B;
    F_b=log((1-b)/b)+(2*b*K)-K;
    x1=((a*F_b)-(b*F_a))/(F_b-F_a);
    F_x1=log((1-x1)/x1)+(2*x1*K)-K;

    if((F_a*F_x1)<0) then
      flag=1;
      A=a;
      B=x1;
    else((F_x1*F_b)<0)
      flag=2;
      A=x1;
      B=b;
    end
    x1_a=approx(x1,4);
    b_a=approx(b,4);
    a_a=approx(a,4);

    if(x1_a==b_a)
      Root=approx(x1,4);
      i=0;
      break;
    elseif(x1_a==a_a)
      Root=approx(x1,4);
      i=0;
      break;
    end
  end
endfunction
```

```

//Example 14.5

//G_E/RT = Ax1x2                                        (A)

//ln V1=A*x2^2=A(1-x1)^2
//ln V2=A*x1^2

//A[(1-x1_a)^2 - (1-x1_b)^2] = ln(x1_b/x1_a)            (B)

//A[(x1_a)^2-(x1_b)^2] = ln((1-x1_b)/(1-x1_a))          (C)

//x1_b=1-x1_a                                           (D)

//A(1 - 2*x1) = ln((1-x1)/x1)                           (E)

//A=a/T + b - clnT                                      (F)

//H_E=R(a + cT)x1x2                                     (G)

//Cp_E=(dH_E/dT) = Rcx1x2                               (H)


T=linspace(250.1,450,20);
A=(-975.*(T.^-1)) + 22.4 - (3.*log(T));

subplot(3,2,1)
plot(T,A)
x=[250.001 450];
y=[2 2];
plot(x,y,'b--')

x=[272.9 272.9];
y=[1.9001 2.01];
plot(x,y,'r--')

x=[391.2 391.2];
y=[1.9001 2.01];
```

```
plot(x,y,'g--')

legend('A vs T(K)','T=272.9,A=2','T=391.2,A=2')

xtitle('(a)A vs T','T(K)','A')

subplot(3,2,2)

clear;

T=linspace(272.9,391.2,100);
K=approx((-975*(T.^-1))+22.4+(-3.*log(T)),4);

root=zeros(100,1);
for(z=1:13)
  root(z)=RF(0.4,0.49,K(z));
end

for(z=14:80)
  root(z)=RF(0.01,0.49,K(z));
end

for(z=81:100)
  root(z)=RF(0.4,0.49,K(z));
end
x1=root';
plot2d(x1,T,rect=[0,250,1,450])

x=[0 0.55];
y=[272.9 272.9];
plot2d(x,y,style=3)

x=[0 0.55];
y=[391.2 391.2];
plot2d(x,y,style=4)

legend('T vs x1','T=272.9K(LCST)','T=391.2K(UCST)')
xtitle('(b)T vs x1','x1','T(K)')
```

```

root=1-x1;
x1=root;
plot2d(x1,T,rect=[0,250,1,450])

x=[0.5 0.51];
y=[272.9 272.9];
plot2d(x,y)

x=[0.5 0.51];
y=[391.2 391.2];
plot2d(x,y)

clear;
//xset('window',1)


T=linspace(250.1,450,20);
A=(-540.*(T.^-1)) + 21.1 - (3.*log(T));

subplot(3,2,3)
plot(T,A)
x=[250.001 450];
y=[2 2];
plot(x,y,'b--')

x=[346 346];
y=[1.51 2.2];
plot(x,y,'r--')

legend('A vs T(K)','A=2','T=346K(UCST)')
xtitle('(a)A vs T','T(K)','A')
subplot(3,2,4)
clear;
T=linspace(250,346,100);
K=approx((-540*(T.^-1))+21.1+(-3.*log(T)),4);

root=zeros(100,1);
```

```
for(z=1:100)
  root(z)=RF(0.1,0.49,K(z));
end
x1=root';
plot2d(x1,T,rect=[0,250,1,450])
x=[0 0.55];
y=[346 346];
plot2d(x,y,style=3)
legend('T vs x1','T=346K(UCST)')
xtitle('(b)T vs x1','x1','T(K)')
root=1-x1;
x1=root;

plot2d(x1,T,rect=[0,250,1,450])
x=[0.49 0.51];
y=[345.4 345.4];
plot2d(x,y)

clear;
//xset('window',2)


T=linspace(250.1,450,20);
A=(-1500.*(T.^-1)) + 23.9 - (3.*log(T));

subplot(3,2,5)
plot(T,A)
x=[250.001 450];
y=[2 2];
plot(x,y,'b--')

x=[339.7 339.7];
y=[1.35 2.2];
plot(x,y,'r--')

legend('A vs T(K)','A=2','T=339.7K(LCST)')
xtitle('(a)A vs T','T(K)','A')
subplot(3,2,6)
```

```
clear;
T=linspace(339.7,450,100);
K=approx((-1500*(T.^-1))+23.9+(-3.*log(T)),4);

root=zeros(100,1);
for(z=1:100)
  root(z)=RF(0.1,0.49,K(z));
end
x1=root';
plot2d(x1,T,rect=[0,300,1,480])
x=[0 0.55];
y=[339.7 339.7];
plot2d(x,y,style=3)
legend('T vs x1','T=339.7K(LCST)')
xtitle('(b)T vs x1','x1','T(K)')
root=1-x1;
x1=root;

plot2d(x1,T,rect=[0,300,1,480])
x=[0.49 0.51];
y=[339.7 339.7];
plot2d(x,y)

//End
```

**Scilab code Exa 14.8** Determine the Phase equlibrium data for the System

```
clear;
clc;

```

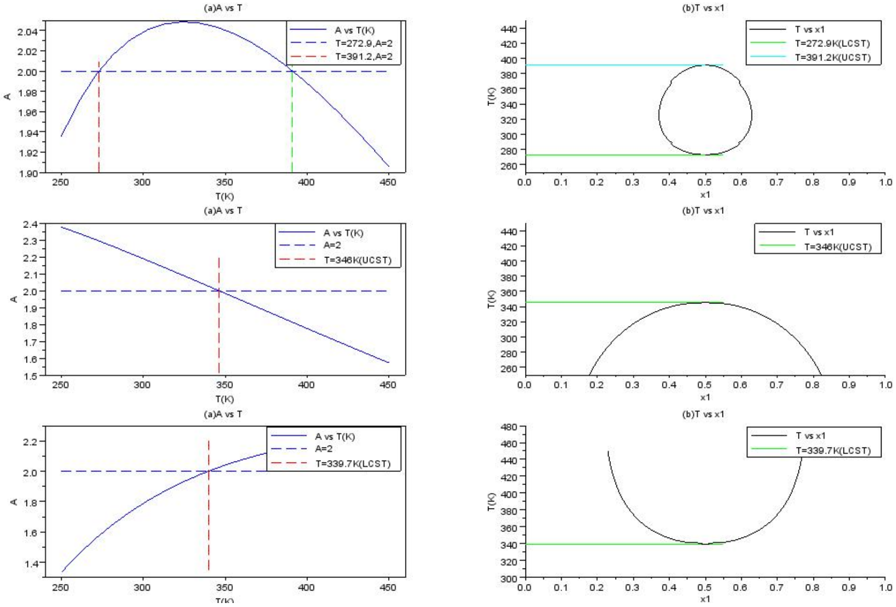

Figure 14.1: Derive the equations from LLE data

```
//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

//Exampl_14.8
//Solution : Program to Determine the Phase
   equlibrium data for the System

A12=4.62424;
A21=3.35629;
alpha12=3.78608;
alpha21=1.81775;
B11=-996;
B22=-1245;
B12=-567;

P1_sat=103.264;//[kPa]
```

```
P2_sat=5.633;//[kPa]

T=308.15;//[K]
R=8314;

//G_E/RT = T1 = A21*x1 + A12*x2 - Q

//V1=exp[(x2^2)*[A12 + (2*(A21-A12)*x1) - Q - (x1*(dQ/dx1))]]

//V2=exp[(x1^2)*[A21 + (2*(A12-A21)*x2) - Q + (x2*(dQ/dx1))]]

//Q=(alpha12*x1*alpha21*x2)/((alpha12*x1) + (alpha21*x2))

//dQ/dx1=dQ_x1=(alpha12*alpha21*(alpha21*x2^2 - alpha12*x1^2))/((alpha12*x1 + alpha21*x2)^2)

//P=(x1*V1*P1_sat)/si1 + (x2*V2*P2_sat)/si2

//d12=2B12-B11-B22

//si1=exp[((B11*(P-P1_sat)) + (P*y2^2*d12)))/RT]

//si2=exp[((B22*(P-P2_sat)) + (P*y1^2*d12)))/RT]

//y1=(x1*V1*P1_sat)/(si1*P)

//y2=(x2*V2*P2_sat)/(si2*P)


//BUBL P

x1=[0.01:0.01:0.99];
x2=1-x1;

for(i=1:99)
```

```

  si1=1; //Assumed
  si2=1; //Assumed

  dP=100;
  while(dP>0.0001)

    Q=approx(((alpha12*x1(i)*alpha21*x2(i))/((alpha12*x1(i)) + (alpha21*x2(i)))),4);
    dQ_x1=approx((alpha12*alpha21*((alpha21*((x2(i))^2)) - (alpha12*((x1(i))^2))))/(((alpha12*x1(i)) + (alpha21*x2(i)))^2),4);
    V1=approx(exp((x2(i)^2)*(A12 + (2*(A21-A12)*x1(i)) - Q - (x1(i)*dQ_x1))),4);
    V2=approx(exp((x1(i)^2)*(A21 + (2*(A12-A21)*x2(i)) - Q + (x2(i)*dQ_x1))),4);

    Pi=approx((((x1(i)*V1*P1_sat)/si1) + ((x2(i)*V2*P2_sat)/si2)),4);

    y1=approx((x1(i)*V1*P1_sat)/(si1*Pi),4);
    y2=approx((x2(i)*V2*P2_sat)/(si2*Pi),4);

    d12=(2*B12)-B11-B22;

    si1=approx(exp(((B11*(Pi-P1_sat))+(Pi*(y2^2)*d12))/(R*T)),4);
    si2=approx(exp(((B22*(Pi-P2_sat))+(Pi*(y1^2)*d12))/(R*T)),4);

    Pf=approx(((x1(i)*V1*P1_sat)/si1) + ((x2(i)*V2*P2_sat)/si2),4);

    dP=abs(Pf-Pi);
  end
  P(i)=Pf;
  y(i)=y1;
end
```

```

for(i=1:99)
  if(P(i)>104.61)
    P(i)=%nan;
  end
end
x1(100)=1;
y(100)=1;
P(100)=P1_sat;

subplot(1,2,1)
P_=[5.633 104.6];
x=[0 0.0117];
plot2d(x,P_,rect=[0,0,0.02,104.6])

P_=[104.6 104.6];
x=[0 0.02];
plot(x,P_,'r')

P_=[5.633 5.633];
y1=[0 0.02];
plot(y1,P_,'b')

P_=[104.6 120];
xa=[0.0117 0.0117];
plot(xa,P_,'g--')

legend('P vs x1','P* = 104.6kPa','P vs y1','x1_a=0.0117')
xtitle('P-x-y','x1,y1','P/kPa')

P_=[100 120];
y1=[0.02 0.02];
plot(y1,P_,'w')

subplot(1,2,2)

P_=[104.6 104.6];
```

```
x=[0.943 0.96];
plot(x,P_,'r')

P_=[104.3 104.6];
y1=[0.946 0.946];
plot(y1,P_,'b--')

P_=[104.6 104.8];
xb=[0.95 0.95];
plot(xb,P_,'g--')

plot2d(x1,P,rect=[0.943,103,1,105])
plot2d(y,P,style=3,rect=[0.943,103,1,105])

legend('P*=104.6kPa','y1*=0.946','x1_b=0.95','P vs x1','P vs y1')
xtitle('P-x-y(Ether Rich Region)','x1,y1','P/kPa')

//End
```

**Scilab code Exa 14.9** Prepare a Table of Temperature and Compostion Data

```
clear;
clc;

//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
```

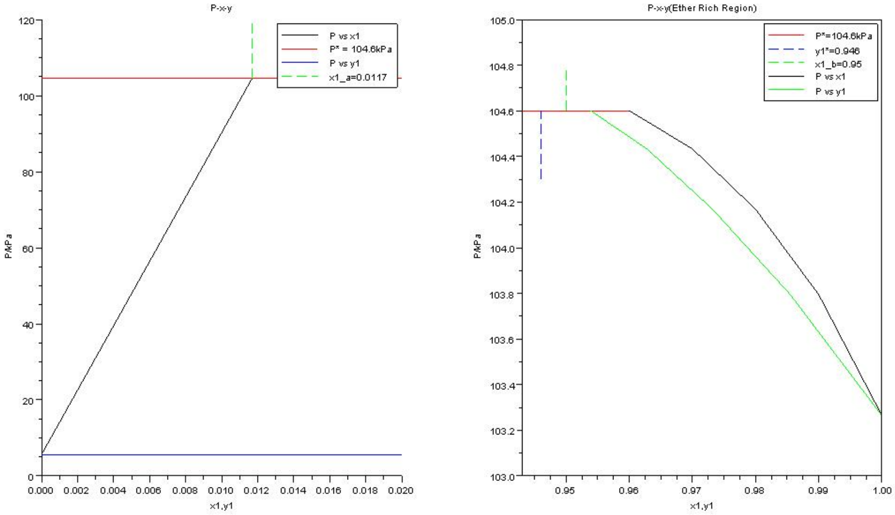

Figure 14.2: Determine the Phase equlibrium data for the System

```

//Example 14.9
//Caption : Program to Prepare a Table of Temperature/Compostion Data
subplot(1,2,1)
P=101.33;//[kPa]
T=[333.15 343.15 348.15 353.15 353.25 363.15 373.15];
P1_sat=[52.22 73.47 86.40 101.05 101.33 136.14 180.04];
P2_sat=[19.92 31.16 38.55 47.36 47.56 70.11 101.33];
P_=P1_sat+P2_sat;
plot(P_,T,'b');

Ans=[T',P1_sat',P2_sat',P_'];
disp(Ans,'      T          P1_sat      P2_sat     P1_sat+P2_sat')
//Hence P lies between T=333.15 and 343.15
P=[101.33 101.33];
```

```
Tp=[330.15 343.15];
xgrid();
plot(P,Tp,'r--')

//Thus by interpolation
P=[50.14 104.63];
T_=[342.15 342.15];

plot(P,T_,'g--');

legend('P* vs T','P=101.33kPa','T=342.15K')
xtitle('T vs P1_sat + P2_sat','P1_sat + P2_sat(kPa)'
   ,'T(K)')

T_=342.15;//[K]

subplot(1,2,2)

plot(P1_sat,T,'b')

//Hence P1_sat @ T=T_=342.15 by interpolation
P=[41 70];
Tp=[342.15 342.15];
xgrid();
plot(P,Tp,'r--')

//Thus by interpolation  P1_sat=71.3kPa
P=[71.3 71.3];
T_=[330.15 342.15];

plot(P,T_,'g--');


legend('P1_sat vs T','T=342.15K','P=71.3kPa')
xtitle('T vs P1_sat','P1_sat(kPa)','T(K)')

P_sat=71.3;
T(1)=342.15;
```

```
P=101.33;//[kPa]
P1_sat(1)=P_sat;
P2_sat(1)=P-P_sat;

y_I=approx(P1_sat/P,3);
y_II=approx(1-(P2_sat/P),3);
for(i=1:7)
  if(y_I(i)>1)
    y_I(i)=%nan;
  elseif(y_II(i)>1)
    y_II(i)=%nan;
  end
end

Ans=[T',y_I',y_II'];
disp(Ans,'      T       y1_I        y1_II')

//End
```

**Scilab code Exa 14.10** Illustrate the Concepts of Pure Gas Adsorption

```
clear;
clc;

//Example 14.10
//Caption : Program to illustrate the Concepts of Pue Gas Adsorption

subplot(2,1,1)
m=4.7087;
b=2.1941;
```

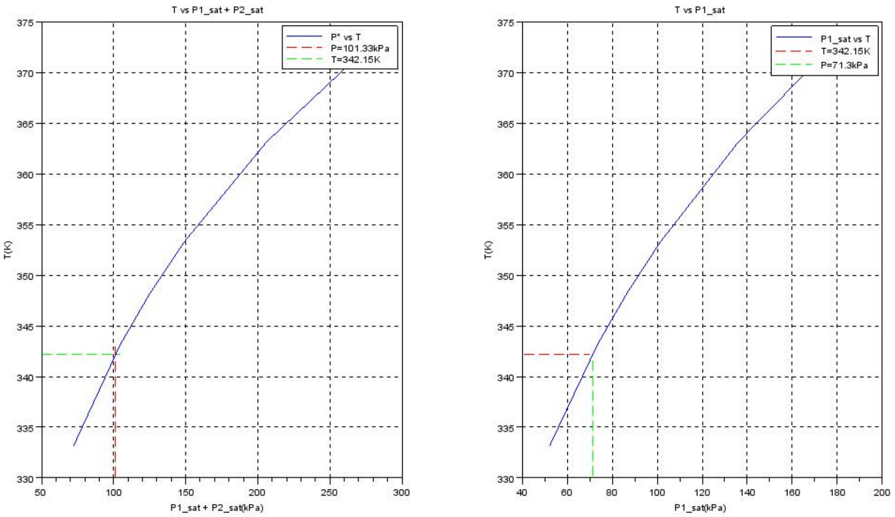

Figure 14.3: Prepare a Table of Temperature and Compostion Data

```
t=0.3984;
P=linspace(0,40,10);
N=(m.*P)./((b+(P.^t)).^(1/t));
plot(P,N)
m=0.6206;
b=1.5454;
t=1;
n=(m.*P)./((b+(P.^t)).^(1/t));
plot(P,n,'b—')
legend('Toth Equation','Langmuir Equation')
xtitle('Adsorption Isotherm(n vs P)','P(kPa)','n(mol
   /kg)')

subplot(2,1,2)
C0=0.4016;
C1=-0.6471;
C2=0.4567;
C3=-0.12;
n=linspace(0,1.6,20);
```

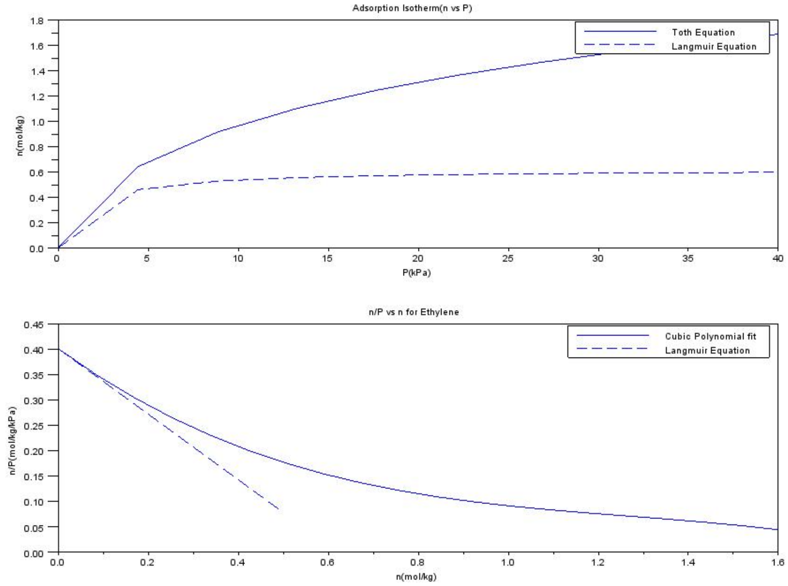

Figure 14.4: Illustrate the Concepts of Pure Gas Adsorption

```
K=C0+(C1*n)+(C2*(n^2))+(C3*(n^3));
plot(n,K)
n=linspace(0,0.5,20);
K=C0+(C1*n);
plot(n,K,'b—')
legend('Cubic Polynomial fit','Langmuir Equation')
xtitle('n/P vs n for Ethylene','n(mol/kg)','n/P(mol/
   kg/kPa)')

//End
```

# Chapter 15

# Thermodynamic Analysis Of Process

**Scilab code Exa 15.1** Do a Thermodynamic Analysis of Steam Power Plant

```
clear;
clc;

//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

function[Q]=MCPS(T0,T,A,B,C,D)
  t=T/T0;
  Q=(A)+(((B*T0)+(((C*T0*T0)+(D/(t*t*T0*T0)))*(t+1)/2))*((t-1)/log(t)))
  funcprot(0);
endfunction

function[Q]=MCPH(T0,T,A,B,C,D)
```

```
  t=T/T0;
  Q=(A+((B/2)*T0*(t+1))+((C/3)*T0*T0*((t^2)+t+1))+(D/(t*T0*T0)))
  funcprot(0);
endfunction

//Example 15.1
//Caption : Program to do a Thermodynamic Analysis of Steam Power Plant

State=['Supercooled Liquid','Superheated Vapor','Wet Vapor,x=0.9378','Saturated Liqiud'];
T=[318.98 773.15 318.98 318.98];
P=[8600 8600 10 10];
H=[203.4 3391.6 2436 191.8];
S=[0.6580 6.6858 7.6846 0.6493];
T0=298.15;
T1=460;//[K]
R=8.314;
T_sigma=T0;
//CH4 + 2O2 --> CO2 + 2H2O
dH_CO2=-393509;
dH_H2O=-241818;
dH_CH4=-74520;

dG_CO2=-394359;
dG_H2O=-228572;
dG_CH4=-50460;

dH_298=dH_CO2+(2*dH_H2O)-dH_CH4
dG_298=dG_CO2+(2*dG_H2O)-dG_CH4

dS_298=approx((dH_298-dG_298)/T0,3);

//Moles Entering
ni_O2=2*1.25;
ni_N2=approx(ni_O2*(79/21),3);
ni=ni_O2+ni_N2;
```

```

//Moles After Combustion
n_CO2=1;
n_H2O=2;
n_O2=0.5;
n_N2=ni_N2;
n=n_CO2+n_H2O+n_O2+n_N2;
m=[n_CO2 n_H2O n_N2 n_O2];

y_CO2=approx(n_CO2/n,4);
y_H2O=approx(n_H2O/n,4);
y_O2=approx(n_O2/n,4);
y_N2=approx(n_N2/n,4);

y=[y_CO2 y_H2O y_O2 y_N2];
yT=sum(y);

//Step(a)
dH_a=0
dS_a=approx(ni*R*((0.21*log(0.21))+(0.79*log(0.79)))
    ,3)//[J/K]

//Step(b)
dH_b=dH_298
dS_b=dS_298//[J/K]

//Step(c)
dH_c=0
dS_c=approx(-n*R*sum(y.*log(y)),3)//[J/K]

//Step(d)
//For CO2
CpH_CO2=approx(R*MCPH(T0,T1,5.457,1.045*(10^-3)
    ,0,-1.157*(10^5)),3);
//For H2O
CpH_H2O=approx(R*MCPH(T0,T1,3.470,1.450*(10^-3)
    ,0,0.121*(10^5)),3);
//For O2
```

```
CpH_O2=approx(R*MCPH(T0,T1,3.639,0.506*(10^-3)
   ,0,-0.227*(10^5)),3);
//For N2
CpH_N2=approx(R*MCPH(T0,T1,3.280,0.593*(10^-3)
   ,0,0.040*(10^5)),3);

//For CO2
CpS_CO2=approx(R*MCPS(T0,T1,5.457,1.045*(10^-3)
   ,0,-1.157*(10^5)),3);
//For H2O
CpS_H2O=approx(R*MCPS(T0,T1,3.470,1.450*(10^-3)
   ,0,0.121*(10^5)),3);
//For O2
CpS_O2=approx(R*MCPS(T0,T1,3.639,0.506*(10^-3)
   ,0,-0.227*(10^5)),3);
//For N2
CpS_N2=approx(R*MCPS(T0,T1,3.280,0.593*(10^-3)
   ,0,0.040*(10^5)),3);

CpH=[CpH_CO2 CpH_H2O CpH_N2 CpH_O2];
CpS=[CpS_CO2 CpS_H2O CpS_N2 CpS_O2];

Comp=['CO2' 'H2O' 'N2' 'O2'];

Ans=[CpH',CpS'];
disp(Ans,'     CpH          CpS',Comp')

CpHt=approx(sum(m.*CpH),3)//[J/K]
CpSt=approx(sum(m.*CpS),3)//[J/K]

dH_d=approx(CpHt*(T1-T0),0)//[J]
dS_d=approx((CpSt*log(T1/T0)),3)//[J/K]

dH=dH_a+dH_b+dH_c+dH_d//[J]
dS=dS_a+dS_b+dS_c+dS_d//[J/K]

rm=84.75;//[kg/s]

```

```
rn_CH4=approx((rm*(H(1)-H(2))*1000)/dH,2)//[mol/s]

rW_ideal=approx(rn_CH4*((dH/1000)-(T0*dS/1000))/1000,2)*1000//[KW]

//(a) Furnace/Boiler
rS_a=approx((rn_CH4*dS/1000)+(rm*(S(2)-S(1))),2)//[kJ/s/K]

rW_a=approx(T_sigma*rS_a/1000,2)*1000//[kW]

//(b) Turbine
rS_b=approx(rm*(S(3)-S(2)),2)//[kW/K]

rW_b=approx(T_sigma*rS_b/1000,2)*1000//[kW]

//(c) Condenser
Q_c=H(4)-H(3);//[kJ/kg]
rQ_c=approx(rm*Q_c/1000,1)*1000//[kJ/s]
rS_c=approx((rm*(S(4)-S(3)))-(rQ_c/T_sigma),2)//[kW/K]
rW_c=approx(T_sigma*rS_c/1000,2)*1000//[kW]

//(d) Pump
rS_d=approx(rm*(S(1)-S(4)),2)//[kW/K]
rW_d=approx(T_sigma*rS_d/1000,2)*1000//[kW]

rS=[rS_a rS_b rS_c rS_d];
pS=approx(rS/sum(rS)*100,1);
T=[sum(rS) sum(pS)];
Process=['Furnace/boiler' 'Turbine' 'Condenser' 'Pump'];
Ans=[rS',pS'];
disp(Ans,'   S(kW/K)    %',Process')
disp(T)
rW_ideal=80000;
rW=[rW_ideal rW_a rW_b rW_c rW_d]/1000;
pW=approx(rW/sum(rW)*100,1);
```

```
T=[sum(rW) sum(pW)];
Process=['Ideal' 'Furnace/boiler' 'Turbine' 'Condenser' 'Pump'];
Ans=[rW',pW'];
disp(Ans,' W(kW/K)*10^-3   %',Process')
disp(T)

eta=pW(1);

disp('%',eta,'Efficiency of the power plant is')

//End
```

**Scilab code Exa 15.2** Prepare a Thermodynamic Analysis of Linde System

```
clear;
clc;

//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

//Example 15.2
//Caption : Program to Prepare a Thermodynamic Analysis of Linde System


State=['Superheated Vapor','Superheated Vapor','Superheated Vapor','Saturated Liqiud','Saturated Vapor','Superheated Vapor'];
```

```
T=[300 300 207.1 111.5 111.5 295];
P=[1 60 60 1 1 1];
H=[1199.8 1140 772 285.4 796.9 1188.9];
S=[11.629 9.359 7.798 4.962 9.523 11.589];
Given=[T',P',H',S'];
disp(Given,'   T/K    P/kPa    H/kJ/Kg    S/kJ/kg/K',State')
T_sigma=300;//[K]
rQ=5;//[KJ]
rW=1000;//[KJ/s]
z=approx((H(6)-H(2)-rQ)/(H(6)-H(4)),4);

//rW_ideal = (dH*rm) - (T_sigma(dS*rm))
rW_ideal=approx(((z*H(4))+((1-z)*H(6))-H(1))-((T_sigma)*((z*S(4))+((1-z)*S(6))-S(1))),1);

//(a) Compression/cooling
rQ_a=(H(2)-H(1))-rW;//[kJ]
rS_a=approx((S(2)-S(1))-(rQ_a/T_sigma),4);//[kJ/Kg/K]

rW_a=T_sigma*rS_a;//[KJ/Kg]

//(b) Exchanger
rS_b=approx(((S(6)-S(5))*(1-z))+(S(3)-S(2))-(rQ/T_sigma),4);//[kJ/Kg/K]
rW_b=T_sigma*rS_b;//[KJ/Kg]

//(c) Throttle
rS_c=approx(((S(4)*z)+(S(5)*(1-z))-S(3)),4);//[KJ/Kg/K]
rW_c=T_sigma*rS_c;//[KJ/kg]

S=[rS_a rS_b rS_c];
pS=approx((S/sum(S))*100,1);
ES=[sum(S) sum(pS)];

W=approx([rW_ideal rW_a rW_b rW_c],1);
```

```
pW=approx((W/sum(W))*100,1);
EW=[sum(W) sum(pW)];
Ans=[S',pS'];
Process=['Compression/Cooling';'Exchanger';'Throttle'];

disp(Ans,'        Si       %',Process)
disp(ES,'Sum')
Ans=[W',pW'];

Process=['Ideal';'Compression/Cooling';'Exchanger';'Throttle'];
disp(Ans,'        Wi       %',Process)
disp(EW,'Sum')
```