# Scilab Textbook Companion for
# A Textbook Of Chemical Engineering Thermodynamics
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# Book Description

**Title:** A Textbook Of Chemical Engineering Thermodynamics

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

**Exa** Example (Solved example)

**Eqn** Equation (Particular equation of the above book)

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

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

# Contents

# List of Scilab Codes

# Chapter 1

# Introduction and Basic Concepts

**Scilab code Exa 1.1** To find mans mass and weight on earth

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 1
//Introduction and Basic Concepts
//Example 1

clear all;
clc;


//Given:
F = 300; //[N]
g_local = 4.5; //local gravitational acceleration[m/s^2]
g_earth = 9.81; //earth's gravitational acceleration[m/s^2]


//To find man's mass and weight on earth
m = F/g_local;//mass of man[kg]
```

```
w = m*g_earth; // weight of man on earth[N]
mprintf('Mass of man is %f kg',m);
mprintf('\nWeight of man on earth is %f N',w);


//end
```

**Scilab code Exa 1.2** To find height of manometer fluid

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 1
//Introduction and Basic Concepts
//Example 2

clear all;
clc;


//Given:
p1 = 1.15*10^5; //measured pressure[N/m^2]
p2 = 1.01325*10^5; //atmospheric pressure[N/m^2]
sg = 2.95; //specific gravity of fluid

//To find height of manometer fluid
p = p1-p2; //difference in pressure
//Using equation 1.2 (Page no. 6)
h = p/(sg*(10^3)*9.8067); //height of manometer fluid[m]
mprintf('Height of manometer fluid is %f m',h);


//end
```

**Scilab code Exa 1.3** To find height from ground and Kinetic Energy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 1
//Introduction and Basic Concepts
//Example 3

clear all;
clc;


//Given
PE = 1.5*10^3; //potential energy[J]
m = 10; //mass in kg
u = 50; // velocity in m/s

//To find height from ground and kinetic energy
//Using equation 1.8 (Page no. 8)
h = PE/(m*9.8067);// height from ground in m

//Using equation 1.9 (Page no. 8)
KE = 0.5*m*(u^2);// Kinetic energy in J
mprintf('Height from ground is %f m',h);
mprintf('\nKinetic Energy of body is %3.2e J',KE);


//end
```

---

**Scilab code Exa 1.4** To determine the power developed in man

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 1
//Introduction and Basic Concepts
//Example 4

```

```
clear all;
clc;


//Given
F = 600; //weight in N
t = 120; //time in sec
h = 0.18; //height of stairs in m

//To determine the power developed in man
S = 20*h; //total vertical displacement in m
W = F*S; //work done in J
P = W/t; //power developed
mprintf('Power developed is %i W',P);


//end
```

**Scilab code Exa 1.5** To determine the force exerted pressure work done and change in potential energy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 1
//Introduction and Basic Concepts
//Example 5

clear all;
clc;


//Given:
A = (%pi/4)*(0.1^2); //area in m^2
P = 1.01325*10^5; //pressure in N/m^2
m = 50; //mass of piston and weight in kg
g = 9.81; //acceleration due to gravity (N/m^2)
```

```
//To determine the force exerted pressure work done
   and change in potential energy
//(a)
Fa = P*A; //force exerted by atmosphere in N
Fp = m*g; //force exerted by piston and weight in N
F = Fp+Fa; //total force exerted in N
mprintf('Total force exerted by the atmosphere, the
   piston and the weight is %f N',F);

//(b)
Pg = F/A; //pressure of gas in N/m^2
mprintf('\nPressure of gas is %5.4e Pa',Pg);

//(c)
S = 0.4; //displacement of gas in m
W = F*S; //work done by gas in J
mprintf('\nWork done by gas is %f J',W);

//(d)
PE = m*g*S; //change in potential energy in J
mprintf('\nChange in potential energy is %f J',PE);

//end
```

**Scilab code Exa 1.6** To determine work done by gas

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 1
//Introduction and Basic Concepts
//Example 6


clear all;
```

```
clc;


//Given:
//P/D = constant, where P is pressure and D is diameter
//P =(2*10^5)*D
Df = 2.5; //final diameter (m)
Di = 0.5; //initial diameter(m)

//To determine work done by gas
//Work done = integral(PdV)
//W = intg((2*10^5*D)d(pi/6)(D^3))....that is
W = (%pi/4)*10^5*((Df^4)-Di^4);
mprintf('Work done by gas is %6.4e J',W);

//end
```

**Scilab code Exa 1.7** To find the work done on surrounding

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 1
//Introduction and Basic Concepts
//Example 7


clear all;
clc;


//Given:
T = 300; //temperature in K
P = 6.5*10^5; //pressure in N/m^2
Pa = 1.01325*10^5; //atmospheric pressure in N/m^2
R = 8.314; //ideal gas constant
```

```
m = 2; //mass of gas (kg)
M = 44; //molecular weihgt of gas

//To find the work done on surrounding
n = m/M; // n is number of kmoles
Vi = (n*R*10^3*T)/P; // initial volume in m^3
Vf = 2*Vi; //final volume in m^3
V = Vf-Vi; //change in volume
Ps = Pa+(5000*9.8067); //pressure on surroundings
W = Ps*V; //work done on the surroundings
mprintf('Work done on surroundings is %5.2e J',W);


//end
```

# Chapter 2

# First Law of Thermodynamics

**Scilab code Exa 2.1** To find change in internal energy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 1


clear all;
clc;


//Given
W = -2.25*745.7; //work done on system in J/s
Q = -3400*(10^3)/3600; //heat transferred to the
    surrounding in J/s

//To find the change in internal energy
//Using equation 2.4 (Page no. 26)
U = Q-W; //change in internal energy in J/s
mprintf('Internal energy of system increases by %f J
    /s',U);

```

```
//end
```

---

**Scilab code Exa 2.2** To find heat liberated work done and change in internal energy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 2


clear all;
clc;


//Given
T = 298; //temperature in K
P = 101; //pressure in kPa
n_iron = 2; //moles of iron reacted
Q = -831.08; //heat liberated in kJ
R = 8.314; //ideal gas constant

//To find heat liberated work done and change in internal energy
mprintf('Heat liberated during the reaction is %f kJ',Q);
n_oxygen = 1.5; //moles of oxygen reacted

//Using ideal gas equation P(Vf-Vi)=nRT and W=P(Vf-Vi)
W = -1.5*R*T; //work done by system in J

//Using equation 2.4 (Page no. 26)
U = (Q*10^3)-W; //change in internal energy in J
mprintf('\nWork done by gas is %f J',W);
```

```
mprintf('\nChange in internal energy is %6.3e J',U);

//end
```

**Scilab code Exa 2.3** To find the heat energy dissipated by brakes

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 3


clear all;
clc;


//Given
u = 20; //speed of car in m/s
z = 30; //height vertically above the bottom of hill in m
m = 1400; //mass of car in kg

//To find the heat energy dissipated by brakes
//Using equation 2.3 (Page no. 26)
KE = -0.5*m*(u^2); //change in kinetic energy in J
PE = -m*9.81*z; //change in potential energy in J
Q = -(KE+PE); //heat dissipated by brakes in J
mprintf('Heat dissipated by brakes is %3.2e J',Q);

//end
```

**Scilab code Exa 2.4** To find internal energy change during each step and work done during adiabatic process

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 4


clear all;
clc;


//Given:
//Step 1: constant pressure process
//Step 2: costant volume process
//Step 3: adibatic process

//To find internal energy change during each step and work done during adiabatic process

//For step 1
W1 = -50; //work received in J
Q1 = -25; //heat gven out in J
U1 = Q1-W1; //internal energy change in J
mprintf('Change in internal energy for constant pressure process is %i J',U1);

//For step 2
W2 = 0; //work done for constant volume process is zero
Q2 = 75; //heat received in J
U2 = Q2; //internal energy change in J
mprintf('\nChange in internal energy for constant volume process is %i J',U2);

//For step 3
Q3 = 0; //no heat exchange in adiabatic process
//Since the process is cyclic
//U3+U2+U1 = 0;
U3 = -(U1+U2);
```

```
W3 = -U3; //work done in J
mprintf('\nWork done during adiabatic process is %i J',W3);

//end
```

**Scilab code Exa 2.5** To find change in internal energy and enthalpy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 5


clear all;
clc;


//Given:
n_water = 10^3; //moles of water
T = 373; //tempearture(K)
P = 101.3; //pressure(kPa)
sv_liquid = 0.00104; //specific volume of liquid(m^3/kmol)
sv_vapour = 1.675; //specific volume of vapour(m^3/kmol)
Q = 1.03*10^3; //heat added in kJ

//To find change in internal energy and enthalpy
W = P*n_water*(sv_vapour-sv_liquid)*10^-3; //expansion work done in kJ
U = Q-W; //change in internal energy in kJ

//For constant pressure process
H = Q; //enthalpy change in kJ
```

```
mprintf('Change in internal energy is %f kJ',U);
mprintf('\nChange in enthalpy is %3.2e kJ',H);

//end
```

---

**Scilab code Exa 2.6** To find internal energy of saturated liquid and internal energy and enthalpy of saturated vapour

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 6


clear all;
clc;


//Given:
T = 233; //temperature in K
VP = 1.005*10^3; //vapour pressure of CO2 in kPa
sv_liquid = 0.9*10^-3; //specific volume of liquid
   CO2 in m^3/kg
sv_vapour = 38.2*10^-3; //specicific volume of CO2
   vapour in m^3/kg
L = 320.5; //latent heat of vaporisation of CO2 in
   kJ/kg
//Assuming at these conditions CO2 is saturated
   liquid so
H1 = 0; //enthalpy in liquid state

//To find internal energy of saturated liquid and
   internal energy and enthalpy of saturated vapour
//For saturated liquid
U1 = H1-(VP*sv_liquid); // internal energy in liquid
```

```
    state in kJ/kg
//For saturated vapour
Hv = H1+L; //enthalpy of saturated vapour in kJ/kg
Uv = Hv-(VP*sv_vapour); //internal energy in vapour
    state in kJ/kg
mprintf('Internal Energy of saturated liquid is %f
    kJ/kg',U1);
mprintf('\nEnthalpy of vapour state is %f kJ/kg',Hv)
    ;
mprintf('\nInternal Energy of vapour state is %f kJ/
    kg',Uv);

//end
```

---

**Scilab code Exa 2.7** To calculate molar internal energy change and molar enthalpy change

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 7


clear all;
clc;


//Given:
I = 0.5; //current in Amperes
V = 12; //voltage in volts
t = 5*60; //time in sec
m = 0.798; //mass of water vaporised in g
M = 18; //molecular mass of water in g

//To calculate molar internal energy change and
```

```
molar enthalpy change
Q = (I*V*t/1000); //electric energy supplied in kJ
//Referring equation 2.10 (Page no. 29)
H = (Q*M)/m; //molar enthalpy change in kJ/mole

//BY ideal gas equation PV=RT
//Referring equation 2.9 for constant pressure process (Page no. 29)
U = H-(8.314*10^-3*373); //molar internal energy change in kJ/mole
mprintf('Molar Enthalpy change during the process is %i kJ/mole',H);
mprintf('\nMolar Interanl Energy change during the process is %f kJ/mole',U);

//end
```

---

**Scilab code Exa 2.8** To determine the theoretical horsepower developed

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 8


clear all;
clc;


//Given:
m = 1650; //mass of steam used in kg/hr
H1 = 3200; //enthalpy at 1368 kPa and 645 K in kJ/kg
H2 = 2690; //enthalpy at 137 kPa and 645 K in kJ/kg

//To determine the theoretical horsepower developed
```

```
//Using equation 2.13 (Page no.32)
Q = 0; //since the process is adiabatic
z = 0; //assuming that inlet and discharge of
    turbine are at same level
u = 0; //feed and discharge velocities being equal
Ws = -(H2-H1);
Wj = Ws*10^3*m/3600; //work done by turbine in J
W = Wj/745.7; //work done by turbine in hp
mprintf('Work done by turbine is %f hp',W);

//end
```

---

**Scilab code Exa 2.9** To find temperature of water delivered to second storage tank

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 9

clear all;
clc;


//Given:
m = 25*10^3; //mass flow rate of water in kg/h
P = 2; //power supplied by motor in hp
q = 42000; //heat given in kJ/min
z = 20; //elevation in m
T = 368; //temperature in K
To = 273; //standard temperature in K
Cp = 4.2; //specific heat of water in kJ/kg K

//To find temperature of water delivered to second
    storage tank
```

```
W = (P*745.7*10^-3*3600)/m; //work done per kg of water pumped in kJ/kg
Q = q*60/m; //heat given out per kg of fluid
PE = 09.81*z*10^-3; //change in potential energy in kJ/kg

//Using equation 2.13 (Page no. 32)
H = -Q+W-PE;
//H = H2-H1
H1 = Cp*(T-To);
H2 = H1+H;
//Let T1 be the temperature at second storage tank
T1 = To+(H2/Cp);
mprintf('Temperature of water at second storage tank is %i K',T1);

//end
```

---

**Scilab code Exa 2.10** To find change in enthalpy and maximum enthalpy change

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 10


clear all;
clc;


//Given:
D1 = 25; //internal diameter of pipe in mm
u1 = 10; //upstream velocity in m/s
D2 = 50; //downstream diameter of pipe in mm
```

```
//Since there is no external device for adding or
   removing energy as work
//Q = 0, Ws = 0

//To find change in enthalpy and maximum enthalpy
   change

//(a)
//Let A1 nad A2 be upstream and downstream
   crosssectional areas of pipe
u2 = ((D1/D2)^2)*u1; //downstream velocity in m/s
H = 0.5*(u1^2-u2^2); //change in enthalpy in J/kg
mprintf('Change in enthalpy is %f J/kg',H);

//(b)
//For maximum enthalpy change
u2 = 0;
Hmax = 0.5*u1^2; //(J/kg)
mprintf('\nMaximum enthalpy chnage for a sudden
   enlargement in pipe is %f J/kg',Hmax);

//end
```

**Scilab code Exa 2.11** To determine heat transfer rates

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 11


clear all;
clc;


```

```
//Given:
//At inlet:
T1 = 293; //Temperature(K)
P1 = 300+136.8; //Pressure(kPa)

//At exit:
T2 = 453; //Temperature(K)
P2 = 136.8; //Pressure(kPa)
Cp = 29.4; //specific heat capacity at constant
    pressure in kJ/kmol
m = 1000; //mass of hydrogen in kg
M = 2.02; //molecular mass of hydrogen

//To determine heat transfer rates
//Neglecting the kinetic nd potential energy changes
//Assuming the process to be occuring through a
    number of steps

//Step 1 be isothermal and step 2 be isobaric
H1 = 0; //change in enthalpy for step 1
H2 = (m/M)*Cp*(T2-T1)/1000; //change in enthalpy for
     step 2 in kJ
H = H2+H1;
Q = H; //heat transferred in coils in kJ
mprintf('Heat transferred in coils is %f kJ', Q);

//end
```

**Scilab code Exa 2.12** To find change in internal energy enthalpy heat supplied and work done

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 12
```

```
clear all;
clc;


//Given:
m = 10; //mass of air in kg
P1 = 100; //initial pressure(kPa)
T1 = 300; //initial temperature(K)
T2 = 600; //final temperature(K)
R = 8.314; //ideal gas constant(kJ/kmol K)
Cp = 29.099; //specific heat capacity at constant
   pressure (kJ/kmol K)
Cv = 20.785; //specific heat capacity at constsant
   volume (kJ/kmol K)
M = 29; //molecular weight of air

//To determine change in internal energy enthalpy
   heat supplied and work done
n = m/M; //number of moles of gas(kmol)
V1 = (n*R*T1)/P1; //initial volume of air (m^3)

//(a)
//Constant volume process
V2 = V1; //final volume
//Change in internal energy U = n*intg(CvdT)...so
U = n*Cv*(T2-T1); //change in internal energy(kJ)
Q = U; //heat supplied(kJ)
W = 0; //work done
H = U+(n*R*(T2-T1)); //change in enthalpy(kJ)
disp('For constant volume process');
mprintf('\nChange in internal energy is %i kJ',U);
mprintf('\nHeat supplied is %i kJ',Q);
mprintf('\nWork done is %i kJ',W);
mprintf('\nChange in enthalpy is %i kJ',H);

//(b)
```

```
//Constant pressure process
//Change in enthalpy H = n*intg(CpdT)...so
H = n*Cp*(T2-T1); //change in enthalpy(kJ)
Q = H;//heat supplied(kJ)
U = H-(n*R*(T2-T1));//change in internal energy(kJ)
W = Q-U; //work done(kJ)
mprintf('\n\nFor constant pressure process');
mprintf('\n\nChange in internal energy is %i kJ',U);
mprintf('\nHeat supplied is %i kJ',Q);
mprintf('\nWork done is %i kJ',W);
mprintf('\nChange in enthalpy is %i kJ',H);

//end
```

**Scilab code Exa 2.13** To determine change in internal energy and change in enthalpy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 2
//First Law of Thermodynamics
//Example 13


clear all;
clc;


//Given:
R = 8.314; //ideal gas constant(kJ/kmol K)
Cv = 20.8; //specific heat capacity at constant volume(kJ/kmol K)
Cp = 29.1; //specific heat capacity at constant pressure(kJ/kmol K)
P1 = 10; //initial pressure(bar)
T1 = 280; //initial temperature in K
```

```
P2 = 1; //final pressure(bar)
T2 = 340; //final temperature(K)

//To determine the change in internal energy and
    change in enthalpy
//Solution
n = 1; //basis: 1 kmol of ideal gas
V1 = (n*R*T1)/(P1*100); //initial volume in m^3
V2 = (n*R*T2)/(P2*100); //final volume in m^3

//Assuming the change in state is occuringalong the
    following two step process
//1. A constant volume process in which the pressure
     is reduced to the final value P2 and the
    temperature gets reduced to T2
//Let Po and Vodenote the pressure and volume of
    system after this step
Po = P2;
Vo = V1;
To = (Po*100*Vo)/(n*R);
U1 = Cv*(To-T1);
H1 = U1+(V1*100*(P2-P1));
W1 = 0;
Q1 = U1;

//2. A constant pressure process in which the gas is
     heated to the final temperature T2 and the final
     volume V2
H2 = Cp*(T2-To);
U2 = H2-100*(V2-V1);
Q2 = H2;
W2 = Q2-U2;

//For actual process
U = U1+U2; //change in internal energy(kJ)
H = H1+H2; //change in enthalpy(kJ)
mprintf('Change in internal energy is %f kJ',U);
mprintf('\nChange in enthalpy is %f kJ',H);
```

```

//end
```

# Chapter 3

# PVT Behaviour And Heat Effects

**Scilab code Exa 3.1** To find the molar volume of air

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P–V–T Behaviour and Heat Effects
//Example 1


clear all;
clc;


//Given:
T = 350; //temperature in K
P = 10^5; //pressure in N/m^2
R = 8.314; //ideal gas constant

//To find the molar volume of air

V = (R*T)/P; //molar volume in m^3
mprintf('Molar volume of air is %3.2e cubic m/mol',V
```

```
    );

//end
```

---

**Scilab code Exa 3.2** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 2


clear all;
clc;


//Given:


//The given problem is theoretical and does not
    involve any numerical computation

//end
```

---

**Scilab code Exa 3.3** To determine heat and work effects for each step

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 3


clear all;
```

```
clc;


//Given:
Cp = 29.3; //specific heat at constant pressure(kJ/kmol K)
R = 8.314; //ideal gas constant

//To determine heat and work effects for each step

//Step 1: Gas is heated at constant volume
T1 = 300; //temperature in K
P1 = 1; //initial pressure in bar
P2 = 2; //final pressure in bar
T2 = (P2/P1)*T1; //final temperature in K
Cv = Cp-R; //specific heat at constant volume
W1 = 0; //work done is zero as volume remains constant
Q1 = Cv*(T2-T1); //heat supplied in kJ/kmol
mprintf('For step 1');
mprintf('\nWork done in step 1 is %i',W1);
mprintf('\nHeat supplied in step 1 is %f kJ/kmol',Q1);

//Step 2: The process is adiabatic
Q2 = 0; //the process is adiabatic
P3 = 1; //pressure after step 2 in bar
gama = (Cp/Cv);
T3 = ((P3/P2)^((gama-1)/gama))*T2; //temperature after step 2
W2 = (Cv*(T2-T3)); //work done by system
mprintf('\n\nFor step 2');
mprintf('\nHeat supplied in step 2 is %i', Q2);
mprintf('\nWork done by system in step 2 is %f kJ/kmol',W2);

//Step 3: The process is isobaric
T4 = 300; //temperature after step 3 (K)
```

```
Q3 = Cp*(T4-T3); //heat supplied during step 3(kJ/kmol)
U = (Cv*(T4-T3)); //change in internal energy during step 3(kJ/kmol)
W3 = Q3-U; //Using first law of thermodynamics
mprintf('\n\nFor step 3');
mprintf('\nHeat given out by the system in step 3 is %f kJ/kmol',Q3);
mprintf('\nWork done on the system in step 3 is %f kJ/kmol',W3);

//end
```

---

**Scilab code Exa 3.4** To calculate change in internal energy change in enthalpy work done and heat supplied

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P–V–T Behaviour and Heat Effects
//Example 4


clear all;
clc;


//Given:
R = 8.314; //ideal gas constant
Cp = 30; //specific heat at constant pressure(J/mol K)

//To calculate change in internal energy change in enthalpy work done and heat supplied
```

```

//(a): Gas is expanded isothermally
T = 600; //temperature in K
P1 = 5; //initial pressure in bar
P2 = 4; //final pressure in bar
U1 = 0; //since the process is isothermal
H1 = 0; //since the process is isothermal
W1 = (R*T*log(P1/P2)); //work done during the process
Q1 = W1; //heat supplied during the process
mprintf('When gas is expanded isothermally');
mprintf('\nChange in internal energy in isothermal process is %i',U1);
mprintf('\nChange in enthalpy in isothermal process is %i',H1);
mprintf("\nWork done during the process is %f kJ/kmol",W1);
mprintf('\nHeat supplied during the process is %f kJ/kmol',Q1);

//(b): Gas is heated at constant volume
V = 0.1; //volume (m^3)
P1 = 1; //initial pressure(bar)
T1 = 298; //initial temperature(K)
T2 = 400; //final temperature(K)
n = ((P1*V*10^5)/(R*T1)); //number of moles of gas
Cv = Cp-R; //specific heat at constant volume(J/mol K)
U2 = n*Cv*(T2-T1); //change in internal energy(J)
H2 = n*Cp*(T2-T1); //change in enthalpy(J)
W2 = 0; //isochoric process
Q2 = U2+W2; //heat supplied(J)
mprintf('\n\nWhen gas is heated at constant volume');
mprintf('\nChange in internal energy is %f J',U2);
mprintf('\nChange in enthalpy is %f J',H2);
mprintf('\nWork done during the process is %i ', W2);
```

```
mprintf('\nHeat supplied during the process is %f J',Q2);

//end
```

---

**Scilab code Exa 3.5** To determine work done and amount of heat transferred

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P–V–T Behaviour and Heat Effects
//Example 5


clear all;
clc;


//Given:
function[y] = Cv(T);
    y = 27.4528+(6.1839*(10^-3)*T)-(8.9932*(10^-7)*(T^2))-R;
endfunction

m = 20; //mass of air(kg)
n = 1.25; //polytropic constant
P1 = 1; //initial pressure(bar)
P2 = 5; //final pressure(bar)
T1 = 300; //temperature(K)
R = 8.314; //ideal gas constant
M = 29; //molecular wt of air

//To determine work done and amount of heat
```

```
    transferred

//(a): Work done by the compressor per cycle
n_mole = m/M; //moles of air(kmol)
V1 = ((n_mole*10^3*R*T1)/(P1*10^5)); //initial volume(m^3)
V2 = (V1*((P1/P2)^(1/n))); //final volume(m^3)

//Since the process is polytropic P(V^n)=c(say constant)
c = P1*10^5*(V1^n);
//function[z] = f(V);
//     z = c/(V^1.25);
//endfunction
//W1 = intg(V1,V2,f); so
W = (c/(1-n))*((V2^(-n+1))-(V1^(-n+1)))/1000;
mprintf('Work done by compressor is %4.3e J',W*1000);

//(b): Amount of heat transferred to surrounding
T2 = ((T1*V2*P2)/(V1*P1)); //final temp in K
U1 = intg(T1,T2,Cv);
U = U1*n_mole; //change in internal energy(kJ)
Q = U+W; //heat supplied
mprintf('\nChnage in internal energy is %f kJ',U);
mprintf('\nHeat supplied is %f kJ',Q);

//end
```

**Scilab code Exa 3.6** To compare the pressures

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P–V–T Behaviour and Heat Effects
//Example 6
```

```


clear all;
clc;


//Given:
V = 0.3821*10^-3 //molar volume(m^3/mol)
T = 313; //temperature (K)
R = 8.314; //ideal gas constant
a = 0.365; b = 4.28*10^-5; //Vander Waals constant

//To compare the pressures

//(a): Ideal gas equation
P = ((R*T)/(V*10^5)); //pressure in bar
mprintf('Pressure obtained by ideal gas equation is %f bar',P);

//(b): Van der Waals equation
P = ((((R*T)/(V-b))-(a/(V^2)))/(10^5));
mprintf('\nPressure obtained by Van der Waals equation is %f bar',P);

//end
```

---

**Scilab code Exa 3.7** To calculate the volume

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 7


clear all;
```

```
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


//Given:
T = 300; //temperature(K)
P = 100; //pressure(bar)
R = 8.314; //ideal gas constant
a = 0.1378; b = 3.18*10^-5; //Van der waals constant

//To calculate the volume

//(a): Ideal gas equation
V_ideal = approx(((R*T)/(P*10^5)),6);
mprintf('Volume calculated by ideal gas equation is %4.2e cubic m',V_ideal);

//(b): Van der Waals equation
function [y]=f(V);
    y=((P*10^5)+(a/(V^2)))*(V-b)-(R*T); //function to calculate difference between calculated and assumed volume
endfunction

V_real = 0;
for i = 0.20:0.01:0.30 //Van der waals volume should be nearly equal to Ideal gas valoume
    res = approx(f(i*10^-3),0);
    for j = -5:5
        if(j==res) //for very small difference i may be taken as exact volume
            V_real = i*10^-3;
    end
```

```
end
end
mprintf('\nVolume calculated by Van der Waals
   equation is %3.2e cubic m',V_real);

//end
```

---

**Scilab code Exa 3.8** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 8


clear all;
clc;

//Given:

//The given problem is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 3.9** To calculate compressibility factor and molar volume

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 9


```

```
clear all;
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


//Given:
T = 500; //temperature (K)
P = 10; //pressure(bar)
R = 8.314; //ideal gas constant
B = -2.19*10^-4; C=-1.73*10^-8; //Virial coeffecients
Tc = 512.6; //critical temperature
Pc = 81; //critical pressure

//To calculate compressibility factor and molar volume

//(a): Truncated form of virial equation
V_ideal = approx(((R*T)/(P*10^5)),7); //ideal gas volume
function [z] = f1(V)
    z = (((R*T)/(P*10^5))*(1+(B/V)+(C/(V^2)))); //function for obtaining volume by virial equation
endfunction

//loop for hit and trial method
flag = 1;
while(flag==1)
    V_virial = approx(f1(V_ideal),7);
    if(approx(V_ideal,5)==approx(V_virial,5))
        flag = 0;
        break;
```

```
        else
    V_ideal = V_virial;
end
end
mprintf('Volume obtained vy virial equation is %4.3e cubic m',V_virial);
Z = approx(((P*10^5*V_virial)/(T*R)),3); //compressibility factor
mprintf('\nCompressibilty factor for virial equation is %f ',Z);

//(b): Redlich Kwong Equation
//Constants in Redlich Kwong equation
a = approx(((0.4278*(R^2)*(Tc^2.5))/(Pc*10^5)),4);
b = approx(((0.0867*R*Tc)/(Pc*10^5)),9);

V_ideal = approx(((R*T)/(P*10^5)),7); //ideal gas volume

//Function to find volume by Redlich Kwong equation
function [x] = f2(V)
    x = ((R*T)/(P*10^5))+b-((a*(V-b))/((T^0.5)*(P*10^5)*V*(V+b)));
endfunction

//loop for hit and trial method
flag = 1;
while(flag==1)
    V_redlich = approx(f2(V_ideal),7);
    if(approx(V_ideal,5)==approx(V_redlich,5))
        flag = 0;
        break;
        else
    V_ideal = V_redlich;
end
end
mprintf('\n\nVolume obtained by Redlich Kwong Equation is %4.3e cubic m/mol',V_redlich);
```

```
Z = approx(((P*10^5*V_redlich)/(T*R)),3); //compressibility factor
mprintf('\nCompressbility factor by Redlich Kwong equation is %f',Z);

//end
```

**Scilab code Exa 3.10** To calculate heat of formation of methane gas

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P–V–T Behaviour and Heat Effects
//Example 10


clear all;
clc;


//Given:
Ha = -890.94; //standard heat for reaction a (kJ)
Hb = -393.78; //standard heat for reaction b (kJ)
Hc = -286.03; //standard heat for reaction c (kJ)

//To calculate heat of formation of methane gas
//c*2 + b - a gives the formation of methane from elements
Hf = (2*Hc)+Hb-Ha;
mprintf('Heat of formation of methane is %f kJ/mol',Hf);

//end
```

**Scilab code Exa 3.11** To calculate heat of formation of chloroform

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 11


clear all;
clc;


//Given:
Ha = -509.93; //heat of combustion of reaction a (kJ)
Hb = -296.03; //heat of combustion of reaction b (kJ)
Hc = -393.78; //heat of combustion of reaction c (kJ)
Hd = -167.57; //heat of combustion of reaction d (kJ)

//To calculate heat of formation of chloroform
//c + (3*d) -a -b gives chloroform from its elements
Hf = Hc+(3*Hd)-Ha-Hb;
mprintf('Heat of formation of chloroform is %f kJ/mol',Hf);

//end
```

---

**Scilab code Exa 3.12** To calculate standard heat of reaction at 773 K

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
```

```
//Example 12


clear all;
clc;


//Given:
Ho = -164987; //standard heat of reaction at 298 K in J
T1 = 298;
T2 = 773; //temperature(K)

//To calculate standard heat of reaction at 773 K
alpha = (2*29.16)+13.41-26.75-(4*26.88);
betta = ((2*14.49)+77.03-42.26-(4*4.35))*10^-3;
gama = ((2*-2.02)-18.74+14.25+(4*0.33))*10^-6;

//Using equation 3.54 (Page no. 67)
H1 = Ho-(alpha*T1)-(betta*(T1^2)/2)-(gama*(T1^3)/3);

//At 773 K
Hr = H1+(alpha*T2)+(betta*(T2^2)/2)+(gama*(T2^3)/3);
mprintf('Heat of reaction at 773 K is %f kJ',Hr/1000);

//end
```

---

**Scilab code Exa 3.13** To determine heat added or removed

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 13

```

```

clear all;
clc;


//Given:
To = 298; //standard temperature(K)
T1 = 400; //temperature of reactants(K)
T2 = 600; //temperature of products (K)
Ho = -283.028; //standard heat of reaction(kJ/mol)

//To determine heat added or removed
//Basis:
n_CO = 1; //moles of CO reacted
n_O2 = 1;//moles of oxygen supplied
n_N2 = 1*79/21; //moles of nitrogen
n1_O2 = 0.5; //moles of oxygen required
n_CO2 = 1; //moles of carbon di oxide formed

H1 = ((n_O2*29.70)+(n_N2*29.10)+(n_CO*29.10))*(To-T1
    )/1000; //enthalpy of cooling of reactants
H2 = ((n1_O2*29.70)+(n_N2*29.10)+(n_CO2*41.45))*(T2-
    To)/1000; //enthalpy of heating the products
Hr = H1+Ho+H2;
mprintf('Heat supplied is %f kJ',Hr);

//end
```

**Scilab code Exa 3.14** To calculate theoretical flame temperature

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 3
//P-V-T Behaviour and Heat Effects
//Example 14

```

```

clear all;
clc;


//Given:
To = 298; //standard temperature (K)
T1 = 373; //temperature of reactants (K)
Ho = 283178; //standard heat of combustion(J/mol)

//To calculate theoretical flame temperature
//Basis:
n_CO = 1; //moles of CO
n_O2 = 1; //moles of oxygen supplied
n1_O2 = 0.5; //moles of oxygen reacted
n_CO2 = 1; //moles of carbon di oxide formed
n_N2 = 79/21; //moles of nitrogen

H1 = ((n_O2*34.83)+(n_N2*33.03)+(n_CO*29.23))*(To-T1
    ); //enthalpy of cooling of reactants
//Using equation 3.55 (Page no. 69)
H2 = Ho-H1;
Tf = H2/((n1_O2*34.83)+(n_N2*33.03)+(n_CO2*53.59))
    +298; //flame temperature
mprintf('Theoretical flame temperature is %f K',Tf);

//end
```

# Chapter 4

# Second Law of Thermodynamics

**Scilab code Exa 4.1** To calculate the maximum efficiency

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 1


clear all;
clc;


//Given:
T1 = 700; //temperature of heat source(K)
T2 = 300; //temperature of heat sink(K)

//To calculate the maximum efficiency
eff=((T1-T2)/T1); //efficiency of a heat engine
mprintf('Maximum efficiency of heat engine is %f',
   eff);

```

```

//end
```

---

**Scilab code Exa 4.2** To determine minimum amount of work done and heat given to surrounding

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 2


clear all;
clc;

//Given:
m = 1; //mass of water(kg)
T1 = 300; //temperature of surrounding(K)
T2 = 273; //temperature of water(K)
Hf = 334.11; //latent heat of fusion of ice(kJ/kg)


//To determine minimum amount of work and heat given upto surrounding

//(a)
Q2 = m*Hf; //heat absobed at temperature T2
W = ((Q2*(T1-T2))/T2); //minimumm amount of work required
mprintf('Minimum amount of work required is %f kJ',W);

//(b)
//Q1 is the heat given up the surrounding
Q1 = W+Q2;
```

```
mprintf('\nHeat given upto surrounding is %f kJ',Q1);


//end
```

---

**Scilab code Exa 4.3** To determine efficiency of proposed engine

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 3


clear all;
clc;


//Given:
P_out = 4.5; //output power(hp)
P_in = 6.25; //input power(kW)
T1 = 1000; //source temperature(K)
T2 = 500; //sink temperature(K)

//To determine efficiency of proposed engine
ep = ((P_out*745.7)/(P_in*1000)); //proposed efficiency
mprintf('Efficiency of proposed engine is %f',ep);

em = ((T1-T2)/T1); //maximum efficiency
mprintf('\nThe maximum efficieny is %f',em);
mprintf('\nHence the claim of the proposed engine is impossible');


```

```
//end
```

---

**Scilab code Exa 4.4** To calculate entropy of evaporation

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 4


clear all;
clc;


//Given:
P = 500; //pressure of dry saturated steam(kPa)

//From steam tables
Hv = 2106; //latent heat of vaporisation(kJ/kg)
T = 425; //saturation temperature(K)

//To calculate the entropy of evaporation
//By equation 4.25 (Page no. 93)
Sv = (Hv/T); //entropy change accompanying
   vaporisation
mprintf('Entropy of evaporation is %f kJ/kg K',Sv);

//end
```

---

**Scilab code Exa 4.5** To determine change in entropy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
```

```
//Second Law of Thermodynamics
//Example 5


clear all;
clc;


//Given:
m = 2; //mass of gas(kg)
T1 = 277; //initial temperature(K)
T2 = 368; //final temperature(K)
Cv = 1.42; //specific geat at constant volume(kJ/kg
   K)

//To determine change in entropy
//Using equation 4.31 (Page no. 94)
S = (m*Cv*log(T2/T1)); //change in entropy(kJ/K)
mprintf('Change in entropy is %f kJ/K',S);


//end
```

**Scilab code Exa 4.6** To calculate the entropy change

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 6


clear all;
clc;


```

```
//Given:
T = 300; //temperature in K
P1 = 10; //initial pressure(bar)
P2 = 1; //final pressure(bar)
R = 8.314; //ieal gas constant

//To calculate the entropy change
//Using equation 4.33(Page no. 94)
S = (R*log(P1/P2)); //(kJ/kmol K)
mprintf('Entopy change is %f kJ/kmol K',S);


//end
```

---

**Scilab code Exa 4.7** To determine change in entropy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 14


clear all;
clc;


//Given:
T1 = 335; //initial temperature in K
T2 = 300; //final temperature in K
P1 = 10; //initial pressure(bar)
P2 = 1; //final pressure(bar)
Cp = 29.3; //specific heat constant at constant
    pressure(kJ/kmol K)
R = 8.314; //ideal gas constant

```

```
//To determine change in entropy
//Using equation 4.30 (Page no. 94)
S = ((Cp*log(T2/T1))-(R*log(P2/P1))); //entropy
   change(kJ/kmol K)
mprintf('Entropy change in the process is %f kJ/kmol
    K',S);


//end
```

---

**Scilab code Exa 4.8** To determine the change in entropy

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 8


clear all;
clc;


//Given:
m1 = 10; //mass of water at 375 K (kg)
m2 = 30; //mass of water at 275 K (kg)
c = 4.2; //specific heat of water (kJ.kg K)


//To determine the change in entropy

//Let T be the final temperature(K)
T = ((m1*375)+(m2*275))/(m1+m2);
//S1 be change in entropy for hot water
S1 = (m1*c*log(T/375)); //[kJ/K]
//S2 be the change in entropy for cold water
```

```
S2 = (m2*c*log(T/275)); //[kJ/K]
//S be the total entropy change
S = S1+S2;
mprintf('The total entropy change is %f kJ/K',S);
//end
```

---

**Scilab code Exa 4.9** To calculate the total entropy change

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 9


clear all;
clc;


//Given:
m1 = 35; //mass of steel in kg
m2 = 150; //mass of oil in kg
T1 = 725; //temperature of steel(K)
T2 = 275; //temperature of oil(K)
c1 = 0.88; //specific heat of steel (kJ/kg K)
c2 = 2.5; //specific heat of oil(kJ/kg K)


//To calculate the total entropy change
//Let T be the final temperature
T = (((m1*c1*T1)+(m2*c2*T2))/((m1*c1)+(m2*c2)));
//S1 be the in entropy for steel
S1 = (m1*c1*log(T/T1)); //[kJ/K]
//S2 be the change in entropy for oil
S2 = (m2*c2*log(T/T2)); //[kJ/K]
//S be the total entropy change
```

```
S = S1+S2;
mprintf('The total entropy change is %f kJ/K',S);

//end
```

**Scilab code Exa 4.10** To calculate entropy of 1 kmole of air

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 10


clear all;
clc;

//Given:
n1 = 0.21; //volume % of oxygen in air
n2 = 0.79; //volume % of nitrogen in air
R = 8.314; //ideal gas constant


//To calculate entropy of 1 kmol of air
//Using equation 4.35 (Page no. 96)
S = (-R*(n1*log(n1)+n2*log(n2))); //[kJ/kmol K]
mprintf('The total entropy change is %f kJ/kmol K',S
   );
//end
```

**Scilab code Exa 4.11** To determine change in entropy for the reaction

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
```

```
//Second Law of Thermodynamics
//Example 11


clear all;
clc;

//Given:
//For the reaction
//CO + 1/2O2 -> CO2
H = -2.8318*10^5; //heat of reaction (J/mol)
T = 298; //temperature of reaction in K
//Absolute entropies for CO, O2, CO2 are (in J/mol K)
S_CO = 198;
S_O2 = 205.2;
S_CO2 = 213.8;

//To determine the change in entropy for the reaction
//Referring equation 4.36 (Page no. 96)
S_reactant = S_CO + 0.5*S_O2; //entropy change for reactants
S_product = S_CO2; //entropy change for products
S = S_product-S_reactant; //total entropy change
mprintf('The total entropy change for the reaction is %f J/mol',S);
mprintf('\nSince the reaction is highly irreversible, entropy change cannot be calculated as the ratio of heat of reaction to the temperature');

//The energy available for useful work is the difference between heat of reaction and entropy energy due to ireversible nature of the process
W_useful = -H+(T*S); //energy available for useful work (J)
mprintf('\nEnergy available for useful work is %3.2e J', W_useful);
```

```

//end
```

**Scilab code Exa 4.12** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 12


clear all;
clc;

//Given

//This is a theoretical question and does not
   involve any numerical computation

//end
```

**Scilab code Exa 4.13** To calculate change in entropy and check whether the process is reversible

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 13


clear all;
clc;

```

```
//Given:
H_steam = 2923.5; //enthalpy of superheated steam (kJ/kg)
S_steam = 6.71; //entropy of superheated steam (kJ/kg K)
H_liquid = 845; //enthalpy of saturated liquid (kJ/kg)
S_liquid = 2.32; //entropy of saturated liquid (kJ/kg K)
T = 300; //temperature of system (K)

//To calculate change in entropy and check whether the process is reversible

S_system = S_liquid-S_steam; //change in entropy of steam

//Let Q be the heat given out during condensation
Q = -(H_liquid-H_steam);
S_surrounding = Q/T; //change in entropy of the surrounding
S_total = S_system+S_surrounding; //total entropy change
mprintf('The total entropy change is %f kJ/kg',S_total);
mprintf('\nSince total entropy change is positive, the process is irreversible');

//end
```

**Scilab code Exa 4.14** To determine the change in entropy of system

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

```
//Example 14


clear all;
clc;

//Given:
V = 1; //volume of each compartment in cubic meters
P_sat = 683.6; //pressure of saturated steam (kPa)
P_steam = 101.3; //pressure of supereated steam (kPa)
T_sat = 437.2; //temperature of system (K)

//Referring steam tables
//For saturated steam at pressure 683.6 kPa and temp 437.2 K
H_sat = 2761; //enthalpy of saturated steam (kJ/kg)
S_sat = 6.7133; //entropy of saturated steam (kJ/kg K)
spvol_sat = 278.9*10^-3; //specific volume of saturated steam (cubic m/kg)
U_sat = 2570.4; //specific internal energy of saturated steam (kJ/kg)

//For superheated steam at 101.3 kPa and 437.2 K
H_steam = 2804; //enthalpy of superheated steam (kJ/kg)
S_steam = 7.6712; //entropy of superheated steam (kJ/kg K)
spvol_steam = 1976.2*10^-3; //specific volume of superheated steam (cubic m /kg)
U_steam = 2603.3; //specific internal energy of superheated steam (kJ/kg)


//To determine the change in entropy of system

m_sat = V/spvol_sat; //mass of satureated steam(kg)
```

```
m_steam = V/spvol_steam; //mass of superheated steam
    (kg)
m_sys = m_sat+m_steam; //mass of system (kg)
spvol_sys = (2*V)/m_sys; //specific volume of system
    (cubic m/kg)
//Since no heat exchange and work interaction occurs
    so internal energy after mixing remains the same
U1_sat = m_sat*U_sat; //internal energy of saturated
    steam (kJ)
U1_steam = m_steam*U_steam; //internal enegy of
   superheated steam (kJ)
U_sys = (U1_sat+U1_steam)/m_sys; //specific internal
    energy of system (kJ/kg)

//Referring steam tables
//At calculated U_sys and spvol_sys
S_sys = 6.9992; //specific entropy of system (kJ/kg
   K)
Si = ((m_sat*S_sat)+(m_steam*S_steam)); //initial
   entropy of system (kJ/K)
Sf = (m_sys*S_sys); //final entropy of system (kJ/K)
S = Sf-Si; //change in entropy
mprintf('The change in entropy of the system is %f
   kJ/K',S);
mprintf('\nSince entropy change is positive, the
   process is irrevresible');

//end
```

**Scilab code Exa 4.15** To calculate entropy change

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 15
```

```


clear all;
clc;

//Given:
V = 1; //volume of each compartment in cubic m
T = 300; //temperature of ideal gas in 1st
    compartment (K)
P = 200; //pressure of ideal gas in 1st compartment
    (kPa)
R = 8.314; //ideal gas constant

//To calculate entropy change
//Let n be the number of moles of gas
n = ((P*V)/(R*T));
//Since gas in vessel exchanges no heat and work
    with surrounding so internal energy remains same
//This implies temperature after mixing is same as
    that before mixing

//Final conditions:
Tf = 300; //final temperature (K)
Vf = 2; //final volume (cubic m)
Pf = 100; //final pressure (kPa)

//Initial conditions:
Ti = 300; //initial temperature (K)
Vi = 1; //initial volume (cubic m)
Pi = 200; //initial pressure (kPa)

//Using equation 4.33 (Page num 94)
S = n*R*log(Vf/Vi); //entropy change of system (kJ/K
    )
//Since entropy of surrounding does not change
S_total = S; //total entropy change
mprintf('The change in total entropy is %f kJ/K',
    S_total);
```

```

//end
```

---

**Scilab code Exa 4.16** To calculate entropy change in the process

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 16


clear all;
clc;

//Given:
m_oil = 5000; //mass flow rate of oil (kg/h)
Tin_oil = 500; //inlet temperature of oil (K)
Tin_water = 295; //inlet temperature of water (K)
c_oil = 3.2; //specific heat of oil (kJ/kg K)
c_water = 4.2; //specific heat of water (kJ/kg K)

//To calculate entropy change in the process

//Assuming oil is cooled to minimum permissible
    temperature
Tout_oil = 305; //exit temperature of oil (K)
Tout_water = 490; //exit temperature of water (K)

//Let m_water be the mass flow rate of water
//By enthalpy balance
m_water = ((m_oil*c_oil*(Tin_oil-Tout_oil))/(c_water
    *(Tout_water-Tin_water))); //(kg/h)
S_oil = m_oil*c_oil*log(Tout_oil/Tin_oil); //entropy
     change of oil (kJ/K)
S_water = m_water*c_water*log(Tout_water/Tin_water);
```

```
    //entropy change of water (kJ/K)
S_tot = S_oil+S_water; //total entropy change
mprintf('The total entropy change in the process is
    %f kJ/K',S_tot);

//end
```

---

**Scilab code Exa 4.17** To calculate loss in capacity of doing work

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 17


clear all;
clc;

//Given:
To = 275; //temperature of quenching oil (K)

//To calculate loss in capacity of doing work

//Referrring example 4.9 (Page no. 95)
S_steel = -26.25; //change in entropy os casting (kJ
    /K)
S_oil = 43.90; //change in entropy of oil (kJ/K)

S_tot = S_steel+S_oil; //total entropy change
//Let W be loss in capacity for doing work
W = To*S_tot; //(kJ)
mprintf('The loss in capacity for doing work is %f
    kJ',W);

//end
```

**Scilab code Exa 4.18** To calculate total change in entropy and available work

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 18


clear all;
clc;

//Given:
m_oil = 5000; //mass flow rate of hydrocarbon oil (kg/h)
Tin_oil = 425; //inlet temperature of oil (K)
Tout_oil = 340; //exit temperature of oil (K)
m_water = 10000; //mass flow rate of water (kg/h)
Tin_water = 295; //inlet temperature of water (K)
c_oil = 2.5; //mean specific heat of oil (kJ/kg K)
c_water = 4.2; //mean specific heat of water (kJ/kg K)

//To determine total change in entropy and available work

//(a)
//By energy balance
Tout_water = ((m_oil*c_oil*(Tin_oil-Tout_oil))/(m_water*c_water))+295; //exit temperature of water (K)
S_oil = m_oil*c_oil*log(Tout_oil/Tin_oil); //change in entropy of oil (kJ/K)
S_water = m_water*c_water*log(Tout_water/Tin_water);
```

```
    //change in entropy of water (kJ/K)
S_tot = S_oil+S_water; //total entropy change
mprintf('The total entropy change is %f kJ/K',S_tot);


//(b)
To = 295; //temperature at which heat is rejected to surrounding (K)
//Let Q be heat given out by the oil on cooling
Q = m_oil*c_oil*(Tin_oil-Tout_oil);
//Heat rejected to the surrounding at To by the Carnot Engine is given by
//Q2 = To(Q/T) = -To*S_oil
Q2 = -To*S_oil; //(kJ)
//Let W be the work output of engine
W = Q-Q2;
mprintf('\nThe work output of the engine would be %4.3e kJ', W);

//end
```

---

**Scilab code Exa 4.19** To calculate the molar entropy of metal

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 19


clear all;
clc;

//Given:
T = 10; //temperature of metal (K)
```

```
Cp = 0.45; //molar heat capacity at 10 K (J/mol K)
//Molar heat capacity of a substance at low
    temperatures can be approximated by the relation
//Cp = a(T^3) where a is constant


//To determine the molar entropy of metal
//Entropy of solid at 10 K is calculated using first
     integral in equation 4.55 (Page no. 108)
S = Cp/3;
mprintf('Molar entropy of meatl at 10 K is %f J/mol
    K',S);

//end
```

---

**Scilab code Exa 4.20** To calculate the absolute entropy of water vapour

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 4
//Second Law of Thermodynamics
//Example 20


clear all;
clc;

//Given:
T = 473; //temperature at entropy is to be
    determined (K)
Tf = 273; //base temperature (K)
Tb = 373; //boiling temperature (K)
Cpl = 4.2; //avearge heat capacity of water (kJ/kg K
    )
Cpg = 1.9; //avearge heat capacity of water vapour
    between 373 K and 473 K
```

```
Hv = 2257; //latent heat of vaporisation at 373 K (kJ/kg)

//To determine the absolute entropy of water vapour
//Entropy of water vapour is calculated using last three terms of equation of 4.55 (Page no. 108)
S = (Cpl*log(Tb/Tf))+(Hv/Tb)+(Cpg*log(T/Tb));
mprintf('Absolute entropy of water vapour at 473 K and 101.3 kPa is %f kJ/kg K',S);
mprintf('\nIt compares favourably with the value reported in steam tables');

//end
```

# Chapter 5

# Some Applications of the Laws of Thermodynamics

**Scilab code Exa 5.1** To calculate the pressure at exit

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 1


clear all;
clc;


//Given:
u1 = 1; //entering velocity of water (m/s)
d_ent = 0.2; //entrance diameter of reducer (m)
d_exit = 0.1; //exit diameter of reducer (m)
P_ent = 105; //pressure at entrance (kPa)
z = 5; //distance between entrance and exit (m)
g = 9.81; //acceleration due to gravity
den = 1000; //density of water (kg/m^3)

```

```
//To calculate the pressure at exit
A1 = (%pi/4)*d_ent^2; //cross section area of
    entrance (m^2)
A2 = (%pi/4)*d_exit^2; //cross section area of exit
    (m^2)

//By the equation of continuity and since density of
     water remains constant
u2 = (A1*u1)/A2;

//By Bernoulli's equation between section 1 and 2 (
    Eq 5.20 Page no. 118)
P_exit = (-((u2^2-u1^2)/2)-(g*z)+(P_ent*10^3/den))*(
    den/10^3);
mprintf('The pressure at exit is %f kPa',P_exit);

//end
```

---

**Scilab code Exa 5.2** To determine quality of steam flowing through the pipe

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 2


clear all;
clc;


//Given:
P = 1000; //pressure of saturated steam (kPa)
T = 398; //temperature of escaping steam (K)

```

```
//Referring steam tables
H_vap = 2778; //enthalpy of saturated vapour at 1000 kPa (kJ/kg)
H_liq = 763; //enthalpy of saturated liquid at 1000 kPa (kJ/kg)
H_steam = 2726; //enthalpy of superheated steam at 398 K (kJ/kg)

//To determine quality of steam flowing through the pipe
//Assuming potential and kinetic energy changes are neglegible
//Using equation 5.10 (Page no. 117)
//H = Q-Ws

//Let section 1 be a point in pipe and x be the fraction of steam that is liquid
//Then H1 = x*H_liq + (1-x)*H_vap

//Let section 2 be the point in steam issuing from the leak in valve
H2 = 2726; //[kJ/kg]

//No work is done and no heat is exchanged between section 1 and 2
//S0, H1 = H2
x = (H2-H_vap)/(H_liq-H_vap);
mprintf('The steam contains %f percent liquid',x*100);

//end
```

**Scilab code Exa 5.3** To determine the discharge velocity

```
//A Textbook of Chemical Engineering Thermodynamics
```

```
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 3


clear all;
clc;


//Given:
m = 10; //mass flow rate of steam (kg/s)
H1 = 3062; //enthalpy of entering steam (kJ/kg)
H2 = 2875; //enthalpy of discharged steam (kJ/kg)
Q = -100/m; //heat loss to the surrounding (kJ/kg)
u1 = 0; //entering velocity of steam

//To determine the discharge velocity
//Using total energy balance (Eq. 5.9, Page no. 117)
//Neglecting change in potential energy and putting
   Ws = 0

H = H2-H1;
u2 = sqrt((Q-H)*1000*2);
mprintf('The discharge velocity is %i m/s',u2);

//end
```

**Scilab code Exa 5.4** To determine thermodynamic properties at throat and critical pressure

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 4

```

```

clear all;
clc;


//Given:
To = 600; //temperature of air (K)
Po = 2000; //pressure of air (kPa)
gama = 1.4;
M = 0.8; //Mach number at throat
m = 29; //molecular mass of air
R = 8.314; //ideal gas constant

//To determine thermodynamical properties at throat and critical pressure

//(a)
//Using equation 5.40 (Page no 123).. u^2 = (M^2)*gama*P*V
//Substituting this in eq. 5.39 (Page no. 123) and on rearranging we get
P = Po/((1+(((gama-1)/2)*M^2))^(gama/(gama-1)));
//Using eq. 5.39 and the relation PoVo = RTo/m
u = sqrt((2*gama*R*To*1000)/(m*(gama-1))*(1-(P/Po)^((gama-1)/gama)));
//Using eq. 3.23 (Page no. 49)
T = To*(P/Po)^((gama-1)/gama);
//Let d be the density
d_o = (Po*m)/(R*To);
//Since P*(V^gama) = P/(den^gama) = constant...so
d = d_o*((P/Po)^(1/gama));
mprintf('(a). At throat');
mprintf('\nPressure = %i kPa',P);
mprintf('\nTemperature = %i K',T);
mprintf('\nVelocity = %f m/s',u);
mprintf('\nDensity = %f kg/cubic m',d);

//(b)
```

```
//Using eq. 5.42 (Page no.124)
Pc = Po*((2/(gama+1))^(gama/(gama-1))); //critical
   pressure
mprintf('\n\n(b).');
mprintf('\nThe critical pressure is %f kPa',Pc);

//end
```

---

**Scilab code Exa 5.5** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 5


clear all;
clc;


//Given:
//The given problem is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 5.6** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 6

```

```

clear all;
clc;


//Given:
//The given numerical is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 5.7** To calculate work required and temperature after compression

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 7


clear all;
clc;


//Given:
P1 = 1; //initial pressure (bar)
T1 = 300; //initial temperature (K)
P2 = 10; //final pressure (bar)
gama = 1.3; //gama for CO2
V_rate = 100; //volumetric flow rate (m^3/h)

//To calculate work required and temperature after
   compression
Ws = (gama/(gama-1))*P1*10^5*(V_rate/3600)*(1-(P2/P1
   )^((gama-1)/gama));
```

```
mprintf('The work required is %f kW',-Ws/1000);

//Using equation 3.23 (Page no.49)
T2 = T1*((P2/P1)^((gama-1)/gama));
mprintf('\nTemperature of gas after compression is
   %f K',T2);

//end
```

---

**Scilab code Exa 5.8** To calculate work required and temperature

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 8


clear all;
clc;



//Given:
P1 = 100; //initial pressure of saturated steam (kPa
   )
P2 = 500; //final pressure (kPa)
eff = 0.8; //compression efficiency

//Referring steam tables
//Properties of steam entering the compressor
H1 = 2675.5; //enthalpy (kJ/kg)
S1 = 7.3594; //entropy (kJ/kg K)

//Properties of compressed steam
H2 = 3008; //enthalpy (kJ/kg)
S2 = S1; //isentropic compression
```

```

//To calculate work required and temperature

Hs = H2-H1;
//Using eq. 5.44 (Page no. 128)
W_isentropic = -Hs;
W_act = W_isentropic/eff;
mprintf('The work required for compression is %f kJ/kg',-W_act);

H = Hs/eff; //actual change in enthalpy
H_act = H1+H; //actual enthalpy of steam leaving the compressor
//From steam tables for superheated steam at 500 kPa and enthalpy of H_act
T = 586; //temperature (K)
mprintf('\nTemperature of exhaust steam is %i K',T);

//end
```

**Scilab code Exa 5.9** To determine the least amount of power

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 9


clear all;
clc;


//Given:
T1 = 288; //temperature of surrounding (K)
T2 = 261; //temperature of solution (K)
```

```
Q2 = 1000; //heat removed (kJ/min)

//To determine the least amount of power
//Using eq. 5.57 (Page no. 137)
W = Q2*((T1-T2)/T2); //power in kJ/min
P = (W*1000)/(746*60); //power in hp
mprintf('Least amount of power necessary is %f hp',P);

//end
```

---

**Scilab code Exa 5.10** To determine COP heat rejected and lowest temperature

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 10


clear all;
clc;


//Given:
T = 290; //operating temperature (K)
W = 1000; //work (J)
tof = 3516.67; //ton of refrigeration (W)

//To determine COP, heat rejected and lowest temperature

//(a)
Q2 = tof;
COP = Q2/W; //coeffecient of performance
```

```
mprintf('(a). COP is %f',COP);

//(b)
Q1 = Q2+W; //heat rejected
mprintf('\n\n (b). Heat rejected is %f kW',Q1/1000);

//(c)
//Let T2 be the lowest temperature
T2 = T1*(Q2/Q1);
mprintf('\n\n (c). Lowest possible temperature in
   refrigerator is %f K',T2);

//end
```

---

**Scilab code Exa 5.11** To determine COP at given conditions

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 11


clear all;
clc;


//Given:
T2 = 266;
T1 = 300; //operating temperatures of vapour
   compression refrigeration cycle(K)

//To determine COP at given conditions
//(a)
Ha = 656; //(kJ/kg)
Hb = 724; //(kJ/kg)
```

```
Hd = 144; //(kJ/kg)
Hc = Hd;
//Using eq. 5.61 (Page no. 139)
COP = (Ha-Hd)/(Hb-Ha);
mprintf('(a). COP = %f',COP);

//(b)
Ha = 652; //(kJ/kg)
Hb = 758; //(kJ/kg)
Hd = 159; //(kJ/kg)
Hc = Hd;
eff = 0.75; //efficiency of compressor
COP = (Ha-Hd)/((Hb-Ha)*(1/eff));
mprintf('\n\n (b). COP = %f',COP);

//(c). Ideal Carnot refrigerator
COP = T2/(T1-T2);
mprintf('\n\n (c). COP = %f',COP);

//end
```

**Scilab code Exa 5.12** To determine power requirement and refrigeration capacity in tonnes

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 12


clear all;
clc;


//Given:
```

```
Tin_cool = 288; //entering temperature of cooling water (K)
Tout_cool = 300; //discharge temperature of cooling water (K)
m_c = 0.25; //mass flow rate of coling water (kg/s)
m = 0.5; //mass flow rate of ammonia (kg/min)
Ha = 1426; //enthalpy of saturated ammonia vapour at 258 K (kJ/kg)
Hd = 281.5; //enthalpy of liquid ammonia at 294 K (kJ/kg)
eff = 0.9; //compressor efficiency
Cp = 4.2; //specific heat of water (kJ/kg K)
tof = 12660; //ton of refrigeration (kJ/h)

//To determine the power requirement and refrigeration capacity in tons
Q1 = m_c*Cp*(Tout_cool-Tin_cool); //heat rejected by compressor at constant pressure (kJ/s)
Q2 = (m/60)*(Ha-Hd); //heat absorbed (kJ/s)
W = Q1-Q2; //work required (kJ/s)
P = (W*1000)/(eff*746); //power requirement of compressor (hp)
mprintf('Power requirement of the compressor is %f hp',P);

rc = Q2*3600/tof; //refrigeration capacity (ton)
mprintf('\n Refrigeration capacity is %f ton',rc);

//end
```

---

**Scilab code Exa 5.13** To calculate the COP and refrigeration circulation rate

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
```

```
//Some Applications of the Laws of Thermodynamics
//Example 13


clear all;
clc;


//Given:
m1 = 10; //machine rating (ton)
//Since 5 K approach is necessary
T1 = 293+5; //temperature of cooling water (K)
T2 = 261-5; //temperature of cold storage (K)
Ha = 181; //enthalpy of saturated vapour at 256 K (
    kJ/kg)
Sa = 0.714; //entropy of saturated vapour at 256K (
    kJ/kg K)
Hc = 62; //enthalpy of saturated liquid at 298 K (kJ
    /kg)
Sc = 0.231; //entropy of saturated liquid at 298 K (
    kJ/kg K)
Hb = 206; //enthalpy of superheated vapour (kJ/kg)
Sb = 0.714; //entropy of superheated vapour (kJ/kg)

//To calculate the COP and refrigerant circulation
    rate
//Referring fig 5.11 (Page no. 143)
//(DA/FA) = (Ha-Hd)/Hv
//(DA/FA) = (Sa-Sd)/Sv
//Hv/Sv = T2

//Combining the three relations , we get
Sd = Sc; //isentropic process
Hd = Ha-(T2*(Sa-Sd));
//Using eq. 5.64 (Page no. 141)
COP = (Ha-Hd)/((Hb-Hc)-(Ha-Hd));
mprintf('COP = %f',COP);

```

```
//Using equation 5.63 (Page no. 140)
m = (12660*m1)/(Ha-Hd); //refrigerant circulation rate (kg/h)
mprintf('\n Refrigerant circulation rate is %f kg/h',m);

//end
```

---

**Scilab code Exa 5.14** To determine the COP and air circulation rate

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 14


clear all;
clc;


//Given:
m1 = 10; //machine rating (ton)
//Assuming 5 K approach in refrigerator and cooler
Ta = 261-5; //temperature of air leaving the refrigerator (K)
Tc = 293+5; //temperature of air leaving the cooler (K)
gama = 1.4;
Cp = 1.008; //sp. heat of air (kJ/kg K)
P1 = 4.052;
P2 = 1.013; //operating pressures in bar

//To determine the COP and air circulation rate
//Using eq. 5.66 (Page no. 145)
Tb = Ta*(P1/P2)^((gama-1)/gama);
```

```
Td = (Tc*Ta)/Tb;

//Using equation 5.68 (PAge no. 146)
COP = Ta/(Tb-Ta);
mprintf('COP = %f',COP);

//Considering energy balance in refrigerator [m*Cp*(Ta-Td) = m1*12660]
m = (m1*12660)/(Cp*(Ta-Td)); //air circulation rate (kg/h)
mprintf('\n Air circulation rate is %i kg/h',m);

//end
```

**Scilab code Exa 5.15** To verify that given heat pump is equivalent to 30 kW pump

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 15


clear all;
clc;


//Given:
T1 = 300; //indoor temperatur (K)
T2 = 290; //outside temperature (K)
W_input = 1; //1 kW heat pump
W_output = 30; //given output (kW)

//To verify that given heat pump is equivalent to 30 kW heater
```

```
Q2 = (T2/(T1-T2))*W_input; //heat absorbed
Q1 = Q2 + W_input; //heat rejected

if(Q1==W_output)
    mprintf('1 kW pump if operated reversibly, is
       equivalent to a 30 kW heater');
else
    mprintf('The given heat pump is not equivalent
       to a 30 kW heater');
end

//end
```

---

**Scilab code Exa 5.16** To determine the amount of fuel burned

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 16


clear all;
clc;


//Given:
T1 = 295; //temperature inside building (K)
T2 = 275; //temperature of outside air (K)
eff = 0.25; //overall efficiency of unit
Hc = 890.9; //heat of combustion of fuel (kJ/mol)
conv = 0.33; //efficiency of conversion of heat of
   combustion to electricity
Q1 = 10^6; //amount of heat to be delivered

//To determine the amount of fuel burned
```

```
COP = T1/(T1-T2);
W = Q1/COP; //work required to deliver Q1 kJ of heat
W_act = W/eff; //actual amount of electrical energy to be supplied
W_heat = W_act/conv; //heat energy required as heat of combustion
n = W_heat/Hc; //number of moles of fuel burned
mprintf('The amount of fuel burned is %f kmol',n/1000);

//end
```

---

**Scilab code Exa 5.17** To calculate fraction of liquid in inlet stream and temperature

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 17


clear all;
clc;


//Given:
//Referring steam tables at 2.54 bar
H1 = 2717; //enthalpy of saturated vapour (kJ/kg)
H2 = 538; //enthalpy of saturated liquid (kJ/kg)
S1 = 7.05; //entropy of saturated vapour (kJ/kg K)
S2 = 1.61; //entropy of saturated liquid (kJ/kg K)

H = 2700; //enthalpy of superheated steam at 1 bar and 385 K (kJ/kg)
S = 7.42; //entropy of superheated steam at 1 bar
```

```
and 385 K (kJ/kg K)

//To determine fraction of liquid in inlet stream and the temperature
//Let the fraction of liquid in inlet stream be x

//(a)..The expansion is isenthalpic
//Applying enthalpy balance around the throttle valve
//(x*H2)+(1-x)*H1 = H
x = (H-H1)/(H2-H1);
//From steam tables
T = 401; //temperature of steam (K)
mprintf('(a). For isenthalpic expansion');
mprintf('\n The fraction of liquid in inlet stream is %f',x);
mprintf('\n The temperature of stream is %i K',T);

//(b)..The expansion is isentropic
//Since entropy of saturated vapour at inlet pressure (S1) is less than entropy of steam leaving the turbine (S)
//So, the inlet stream is superheated, therefore
x = 0;
//From steam tales
T = 478; //temperature of superheated steam having entropy of 7.42 kJ/kg K
mprintf('\n\n(b). For isentropic expansion');
mprintf('\n The fraction of liquid in inlet stream is %i',x);
mprintf('\n The temperature of stream is %i K',T);

//end
```

**Scilab code Exa 5.18** To determine fraction of air liquified and temperature of air

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 18


clear all;
clc;


//Given:
//Referring Fig. 5.15 (Page no. 151)
Hc = 516; //enthalpy of high pressure gas at 120 bar
    and 306 K (kJ/kg)
Ha = 526; //enthalpy of low pressure gas at 2 bar
   and 292 K (kJ/kg)
Hf = 121; //entalpy of saturated liquid at 2 bar (kJ
   /kg)
Hg = 314; //enthalpy of saturated vapour at 2 bar (
   kJ/kg)

//To determine the fraction of air liquified and
   temperature of air

//(a)..
//Using equation 5.73 (Page no. 152)
x = (Hc-Ha)/(Hf-Ha); //fraction of air liquified
mprintf('(a). The fraction of liquified air is %f',x
   );

//(b)..
//Taking enthalpy balance around heat exchanger
Hd = Hc - (1-x)*(Ha-Hg);
//At enthalpy of Hd kJ/kg, from T-S diagram for air
T = 167; //temperature in K
```

```
mprintf('\n (b). Temperature of air on high pressure
    side of throttle valve is %i K',T);

//end
```

---

**Scilab code Exa 5.19** To determine ideal Rankine cycle efficiency thermal efficiency and rate of steam production

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 19


clear all;
clc;


//Given:
P2 = 2800; //pressure of superheated steam (kPa)
P1 = 5; //pressure after expansion (kPa)
e_turbine = 0.85; //isentropic turbine efficiency
e_pump = 0.8; //isentropic pump efficiency
V = 1.005*10^-3; //specific volume of saturated
    liquid at 5 kPaHl =

//From steam tables:
Hl = 138; //enthalpy of saturated liquid at 5 kPa (
    kJ/kg)
Hv = 2562; //enthalpy of saturated vapour at 5 kPa (
    kJ/kg)
H3 = 3063; //enthalpy of superheated steam at 2800
    kPa and 598 K (kJ/kg)
Sl = 0.4764; //entropy of saturated liquid at 5 kPa
    (kJ/kg K)
```

```
Sv = 8.3951; //entropy of saturated vapour at 5 kPa (kJ/kg K)
S3 = 6.6875; //entropy of superheated steam at 2800 kPa and 598 K (kJ/kg K)


//To determine the ideal Rankine cycle efficiency , thermal efficiency and rate of steam production

//(a)..The ideal Rankine cycle efficiency for the stated conditions
//Referring fig 5.19(b) (Page no. 155) and considering feed water pump
Ws = V*(P2-P1); //work done by pump (kJ/kg)
H2 = Hl+Ws;
//Considering isentropic expansion in turbine
S4 = S3;
x = (S4-Sl)/(Sv-Sl); //fraction of steam that is vapour
H4 = Hl + x*(Hv-Hl);
//Using eq. 5.80 (Page no. 155)
e_r = ((H3-H2)-(H4-Hl))/(H3-H2);
mprintf('(a). The ideal Rankine cycle efficiency for the stated conditions is %i percent',e_r*100);

//(b)..The thermal efficiency of plant
W_act = Ws/e_pump; //actual work requirement in pump
H_2 = Hl + W_act; //enthalpy of water leaving the feed water pump
W_out = e_turbine*(H3-H4); //actual work output
H_4 = H3-W_out; //actual enthalpy of steam leaving the turbine
e_act = ((H3-H_2)-(H_4-Hl))/(H3-H_2);
mprintf('\n (b). The actual efficiency is %f percent',e_act*100);

//(c)..The rate of steam production
W_net = e_act*(H3-H_2); //net work output (kJ/kg)
```

```
rate = (3.6*10^6)/W_net; //steam produced in boiler (kg/h)
mprintf('\n (c). The rate of steam production is %f kg/h',rate);

//end
```

---

**Scilab code Exa 5.20** To determine the work output thermal efficiency and rate of steam circulation

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 20


clear all;
clc;


//Given:
P2 = 7600; //pressure of superheated steam (kPa)
P1 = 5; //pressure after expansion (kPa)
V = 1.005*10^-3; //specific volume of saturated liquid (m^3/kg)

//From steam tables:
H_l1 = 138; //enthalpy of saturated liquid at 5 kPa (kJ/kg)
S_l1 = 0.4764; //entropy of saturated liquid at 5 kPa (kJ/kg K)
H_v1 = 2562; //enthalpy of saturated vapour at 5 kPa (kJ/kg)
```

```
S_v1 = 8.3951; //entropy of saturated vapour at 5 kPa (kJ/kg K)
H_l2 = 830; //enthalpy of saturated liquid at 1400 kPa(kJ/kg)
S_l2 = 2.2842; //entropy of saturated liquid at 1400 kPa (kJ/kg K)
H_v2 = 2790; //enthalpy of saturated vapour at 1400 kPa (kJ/kg)
S_v2 = 6.4693; //entropy of saturated vapour at 1400 kPa (kJ/kg K)
H5 = 3226; //enthalpy of superheated steam at 1400 kPa and 658 K
S5 = 7.2558; //entropy of superheated steam at 1400 kPa and 658 K
H3 = 3150; //enthalpy of superheated steam at 7600 kPa and 673 K
S3 = 6.4022; //entropy of superheated steam at 1400 kPa and 673 K

//To determine the work output, thermal efficiency and rate of steam circulation
//(a)
//For high pressure turbine
//Let the fraction of steam in vapour state be x
S4 = S3; //as the expansion process is isentropic
x = (S4-S_l2)/(S_v2-S_l2);
H4 = H_l2 + x*(H_v2-H_l2);
W_high = H3-H4;

//For low pressure turbine
S6 = S5; //isentropic expansion
x = (S6-S_l1)/(S_v1-S_l1);
H6 = H_l1 + x*(H_v1-H_l1);
W_low = H5-H6;

mprintf('(a)');
mprintf('\n The work output of high pressure turbine is %i kJ/kg',W_high);
```

```
mprintf('\n The work output of low pressure turbine is %i kJ/kg',W_low);

//(b)
//Work output of feed pump is [-Ws = intg(VdP)]
Ws = V*(P2-P1);
H2 = H_l1+Ws;
//Using eq. 5.82 (Page no. 159)
eff = ((H3-H2)+(H5-H4)-(H6-H_l1))/((H3-H2)+(H5-H4));
mprintf('\n\n (b)');
mprintf('\n Thermal efficiency is %f percent',eff*100);

//(c)
//The numerator of eq. 5.82 gives net work output
W_net = (H3-H2)+(H5-H4)-(H6-H_l1);
//For 1000 kW of net work output
rate = 3.6*10^6/W_net;
mprintf('\n\n (c)');
mprintf('\n The rate of steam circulation is %f kg/h',rate);

//end
```

**Scilab code Exa 5.21** To determine fraction of steam withdrawn and thermal efficiency of cycle

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 21


clear all;
clc;
```

```


//Given:
P2 = 2800; //pressure of superheated steam (kPa)
P1 = 275; //pressure of withdrawn steam (kPa)
V = 1.070*10^-3; //specific volume of saturated liquid at 275 kPa

//From steam tables:
H6 = 138; //enthalpy of saturated liquid at 5 kPa
S6 = 0.4764; //entropy of saturated liquid at 5 kPa
H_v1 = 2562; //enthalpy of saturated vapour at 5 kPa
S_v1 = 8.3951; //entropy of saturated vapour at 5 kPa
H1 = 549; //enthalpy of saturated liquid at 275 kPa
S1 = 1.6408; //entropy of saturated liquid at 275 kPa
H_v2 = 2721; //enthalpy of saturated vapour at 275 kPa
S_v2 = 7.0209; //entropy of saturated vapour at 275 kPa
H3 = 3063; //enthalpy of superheated steam at 2800 kPa and 598 K
S3 = 6.6875; //entropy of superheated steam at 2800 kPa and 598 K

//To determine the fraction of steam withdrawn and thermal efficiency of cycle
//Referring fig. 5.23 (Page no.161)
S4 = S3; //isentropic expansion
x = (S4-S1)/(S_v2-S1); //quality of steam
H4 = H1 + x*(H_v2-H1);
H7 = H6; //as the power input to the condensate pump is neglegible

//Applying energy balance around feed water heater
m = (H1-H7)/(H4-H7); //fraction of steam extracted
mprintf('Fraction of steam withdrawn is %f',m);
```

```

W_in = V*(P2-P1); //work input to the feed water pump
H2 = H1+W_in;
//Considering isentropic expansion in turbine
S5 = S3;
x = (S5-S6)/(S_v1-S6);
H5 = H6 + x*(H_v1-H6);
//Using eq. 5.85 (Page no.162)
eff = ((H3-H2)-(1-m)*(H5-H6))/(H3-H2);
mprintf('\n Thermal efficiency is %f percent',eff*100);

//end
```

---

**Scilab code Exa 5.22** To determine mean effective pressure

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 22


clear all;
clc;


//Given:
r = 8; //compression ratio
T1 = 290; //temperature at beginning (K)
P1 = 100; //pressure at the beginning (kPa)
Q1 = 450; //heat transferred per cycle (kJ/kg K)
Cp = 1.005; //specific heat of air (kJ/kg K)
Cv = 0.718; //specific heat of air (kJ/kg K)
R = 8.314; //ideal gas constant
```

```
M = 29; //molecular wt of air

//To determine mean effective pressure
//Basis:
m = 1; //mass of air (kg)

//(a)
//Referring fig. 5.24 (Page no. 164)
V1 = (m*R*1000*T1)/(M*P1*10^3);

//Conditions at state 2
V2 = V1/r;
gama = Cp/Cv;
T2 = T1*(r^(gama-1));
P2 = P1*(r^gama);
mprintf('(a)');
mprintf('\n At the end of first process');
mprintf('\n Temperature = %f K',T2);
mprintf('\n Pressure = %f kPa',P2);

//Conditions at state 3
//Constant volume process
V3 = V2;
T3 = Q1/Cv + T2;
P3 = (T3/T2)*P2;
mprintf('\n\n At the end of second process');
mprintf('\n Temperature = %f K',T3);
mprintf('\n Pressure = %f kPa',P3);

//Conditions at state 4
T4 = T3/(r^(gama-1));
P4 = P3/(r^gama);
mprintf('\n\n At the end of third process');
mprintf('\n Temperature = %f K',T4);
mprintf('\n Pressure = %f kPa',P4);
Q2 = Cv*(T4-T1); //heat rejected during the constant
    volume process

```

```
//(b)
//Using eq. 5.88 (Page no. 165)
eff = 1 - ((1/r)^(gama-1));
mprintf('\n\n\n (b)');
mprintf('\n Thermal efficiency is %f',eff);

//(c)
W = Q1-Q2; //work done
mprintf('\n\n\n (c)');
mprintf('\n Work done is %f kJ/kg',W);

//(d)
Pm = W/(V1-V2);
mprintf('\n\n\n (d)');
mprintf('\n Mean effective pressure is %f kPa',Pm);

//end
```

---

**Scilab code Exa 5.23** To determine work done thermal effeciency and mean effective pressure

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 23


clear all;
clc;


//Given:
r = 15; //compression ratio
P1 = 100; //pressure in the beginning (kPa)
T1 = 300; //temperature in thebeginning (K)
```

```
Q1 = 500; //heat transfer rate (kJ/kg)
M = 29; //molecular wt of air
R = 8.314; //ideal gas constant

//Specific heats of air (kJ/kg K)
Cp = 1.005;
Cv = 0.718;

//To determine work done thermal efficiency and mean
    effective pressure
//Referring fig 5.25 (Page no. 167)

//(a)
//Isentropic compression 1-2
V1 = (R*1000*T1)/(M*P1*10^3);
T2 = T1*r^(gama-1);
P2 = P1*r^gama;
V2 = V1/r;
mprintf('(a)');
mprintf('\n At the end of first process');
mprintf('\n Temperature = %f K',T2);
mprintf('\n Pressure = %f kPa',P2);

//Consatnt pressure heat addition 2-3
T3 = Q1/Cp + T2;
V3 = (T3/T2)*V2;
P3 = P2;
mprintf('\n\n At the end of second process');
mprintf('\n Temperature = %f k',T3);
mprintf('\n Pressure = %f kPa',P3);

//Isentropic expansion 3-4
V4 = V1;
T4 = T3/((V4/V3)^(gama-1));
P4 = P3*((V3/V4)^gama);
mprintf('\n\n At the end of third process');
mprintf('\n Temperature = %f K',T4);
mprintf('\n Pressure = %f kPa',P4);
```

```
Q2 = Cv*(T4-T1); //heat rejected 4-1

//(b)
Wnet = Q1-Q2;
mprintf('\n\n (b)');
mprintf('\n Net work done per cycle per kg air is %f
    kJ/kg',Wnet);

//(c)
eff = Wnet/Q1; //thermal efficiency
mprintf('\n\n (c)');
mprintf('\n Thermal efficiency is %f',eff);

//(d)
Pm = Wnet/(V1-V2); //mean effective pressure
mprintf('\n\n (d)');
mprintf('\n Mean effective pressure is %f kPa',Pm);

//end
```

---

**Scilab code Exa 5.24** To determine temperature pressure work and thermal effeciency

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 5
//Some Applications of the Laws of Thermodynamics
//Example 24


clear all;
clc;


//Given:
T1 = 300; //initial temperature (K)
```

```
P1 = 100; //initial pressure (kPa)
T3 = 1200; //max temperature (K)
P3 = 500; //max pressure (kPa)
Cp = 1.005; //(kJ/kg K)
Cv = 0.718; //(kJ/kg K)

//To determine pressure and temperature work and thermal efficiency
gama = Cp/Cv;

//(a)
P4 = P1;
P2 = P3;
//Isentropic compression 1−2
T2 = T1*((P2/P1)^((gama-1)/gama));
mprintf('(a)');
mprintf('\n At the end of first process');
mprintf('\n Temperature = %f K',T2);
mprintf('\n Pressure = %f kPa',P2);

//Process 2−3
mprintf('\n\n At the end of second process');
mprintf('\n Temperature = %f K',T3);
mprintf('\n Pressure = %f kPa',P3);

//Isentropic expansion 3−4
T4 = T3/((P3/P4)^((gama-1)/gama));
mprintf('\n\n At the end of third process');
mprintf('\n Temperature = %f K',T4);
mprintf('\n Pressure = %f kPa',P4);

//(b)
W_comp = Cp*(T2-T1); //work required by compressor
mprintf('\n\n (b)');
mprintf('\n Work required by compressor is %f kJ/kg',W_comp);

//(c)
```

```
W_turb = Cp*(T3-T4); //work done by turbine
mprintf('\n\n (c)');
mprintf('\n Work done by turbine is %f kJ/kg',W_turb);

//(d)
eff = 1-(P1/P2)^((gama-1)/gama);
mprintf('\n\n (d)');
mprintf('\n Thermal efficiency is %f',eff);

//end
```

# Chapter 6

# Thermodynamic Properties of Pure Fluids

**Scilab code Exa 6.1** To determine change in entropy of system

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 1


clear all;
clc;


//Given:
betta = 1.25*10^-3; //coeffecient of expansion (K
    ^-1)
V = 0.1; //molar volume of organic liquid (m^3/kmol)
P2 = 20; //final pressure (bar)
P1 = 1; //initial pressure (bar)

//To determine the change in entropy of system
//betta = (1/V)*(del V/del T)p
```

```
//Let k = (del V/del T)p
k = betta*V;

//Considering Maxwell's relation Eq. 6.24 (Page no. 193)
//dS = -k*(dP)
S = -k*(P2-P1)*10^5; //entropy change (J/kmol K)
mprintf('Change in entropy is %f J/kmol K',S);
mprintf('\n It is assumed that (del V/del T)p is constant in the pressure range 1 to 20 bar');

//end
```

---

**Scilab code Exa 6.2** To calculate vapour pressure of water at 363 K

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 2


clear all;
clc;


//Given:
T1 = 363; //temperature (K)
T2 = 373; //temperature (K)
P2 = 101.3; //vapour pressure at 373 K (kPa)
H = 2275*18; //mean heat of vaporisation (kJ/kmol)
R =8.314; //ideal gas constant (kJ/kmol K)

//To calculate vapour pressure of water at 363 K
//Using eq. 6.28 (Page no. 196)
P1 = P2/(%e^((H/R)*((1/T1)-(1/T2))));
```

```
mprintf(' Vapour pressure of water at 363 K is %f
   kPa',P1);

//end
```

---

**Scilab code Exa 6.3** To determine the melting point of mercury at 10 bar

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 3


clear all;
clc;


//Given:
d_l = 13.69*10^3; //density of mercury in liquid
   state (kg/m^3)
d_s = 14.193*10^3; //density of mercury in solid
   state (kg/m^3)
T1 = 234.33; //temperature in K
P1 = 1; //initial pressure in bar
P2 = 10; //final pressure in bar
Hf = 9.7876; //heat of fusion of mercury (kJ/kg)

//To determine the melting point of mercury at 10
   bar
//Using Clapeyron equation [Eq. 6.25 Page no. 195]
//Assuming del_V/del_H remains constant, log(T2/T1)
   = (del_V/del_H)*(P2-P1)

del_V = (1/d_l)-(1/d_s);
T2 = T1*(%e^((del_V/Hf)*(P2-P1)));
```

```
mprintf('The melting point of mercury at 10 bar is %f K',T2);

//end
```

---

**Scilab code Exa 6.4** To calculate increase in entropy of solid magnesium

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 4


clear all;
clc;


//Given:
T1 = 300; //initial temperature (K)
T2 = 800; //final temperature (K)

//Heat capacity (J/mol K)
//Cp = 26.04+(5.586*10^-3*T)+(28.476*10^4*T^-2)

//To determine the increase in entropy of solid magnesium
//Integrating Eq 6.31 (Page no. 198), we get
//S = intg(Cp*(dT/T))
S = 26.04*log(T2/T1)+5.586*10^-3*(T2-T1)+28.476*10^4/(-2)*(T2^-2-T1^-2);
mprintf('The increase in entropy of solid magnesium is %f J/mol K',S);

//end
```

---

**Scilab code Exa 6.5** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 5


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 6.6** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 6


clear all;
clc;


//Given:
```

```

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 6.7** To calculate internal energy enthalpy entropy and fre energy for 1 mole of nitrogen

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 7


clear all;
clc;


//Given:
T = 773; //temperature (K)
P = 100; //pressure (bar)
Ho = 0; //enthalpy of nitrogen at 273 K and 1 bar
So = 192.4; //entropy of nitrogen at 298 K and 1 bar
To = 273; //(K)
Po = 1; //(bar)
R = 8.314; //ideal gas constant (kJ/kmol K)
//Cp = 27.3+(4.2*10^-3*T) molal heat capacity at 1
   bar

//To calculate internal energy enthalpy entropy and
   free energyfor one mole of nitrogen
//Step 1:
//Assuming that nitrogen is initially at 273 K and 1
    bar
```

```
//del_H1 = intg(CpdT)
del_H1 = 27.3*(T-To)+4.2*10^-3*(T^2-To^2)/2;

//Assuming that nitrogen is initially at 298 K and 1 bar
//del_S1 = intg(Cp*(dT/T))
del_S1 = 27.3*log(T/To)+4.2*10^-3*(T-To);
H1 = Ho + del_H1;
S1 = So + del_S1;

//Step 2:
//del_H2 = [V - T*(del_V/del_T)p]dP
//Since nitrogen behaves as ideal gas
//(del_V/del_T)p = R/P, V-(R*T)/P = 0
del_H2 = 0;
del_S2 = -R*log(P/Po);
H = H1 + del_H2;
S = S1 + del_S2;

//Internal energy: U = H-PV = H-RT (J/mol)
U = H - (R*T);

//Gibbs free energy (J/mol)
G = H-(T*S);

mprintf('Enthalpy is %5.3e J/mol',H);
mprintf('\n Entropy is %f J/mol K',S);
mprintf('\n Internal energy is %4.3e J/mol',U);
mprintf('\n Gibbs free energy is %4.3e J/mol',G);

//end
```

---

**Scilab code Exa 6.8** To calculate entropy change and mean heat capacity

```
//A Textbook of Chemical Engineering Thermodynamics
```

```
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 8


clear all;
clc;


//Given:
//Equation of state: P(V-B) = RT + (A*P^2)/T
Cp = 33.6; //mean specific heat at atmosheric pressure (J/mol K)
A = 1*10^-3; //m^3 K/(bar)mol
B = 8.0*10^-5; //m^3/mol
R = 8.314*10^-5; //ideal gas constant (m^3 (bar)/mol K)

//To calculate entropy change and mean heat capacity

//(a). The entropy change when the state of gas is changed from state 1 (4 bar, 300 K) to state 2 (12 bar, 400 K)
//The proposed changed is assumed to take place in 3 steps in series as illustrated in Fig. 6.4 (Page no. 206)
//Step 1: Process AC, isothermal at 300 K
//Step 2: Process CD, isobaric at 1 bar
//Step 3: Process DB, isothermal at 400 K
//(del_V/del_T)p = R/P - AP/T^2

//For step 1:
Po = 4; //pressure at A (bar)
P1 = 1; //pressure at C (bar)
T = 300; //temperature (K)
//del_S1 = intg[(del_V/del_T)pdP]
del_S1 = (R*log(Po/P1) - (A/T^2)*(Po^2-P1^2)/2)*10^5; //(J/mol K)
```

```

//For step 2:
T1 = 300; //temperature at C (K)
T2 = 400; //temperature at D (K)
del_S2 = Cp*log(T2/T1); //(J/mol K)

//For step 3:
P2 = 1; //pressure at D (bar)
P3 = 12; //pressure at B (bar)
T = 400; //temperature (K)
del_S3 = (R*log(P2/P3) - (A/T^2)*(P2^2-P3^2)/2)*10^5; //(J/mol K)
S = del_S1+del_S2+del_S3; //total entropy change
mprintf('(a). Total entropy change is %f J/mol K',S);

//(b). The mean heat capacity at 12 bar
//If the change is brouhgt along ACo and CoB
//For ACo
P1 = 4; //pressure at A (bar)
P2 = 12; //pressure at Co (bar)
T = 300; //temperature (K)
del_S1 = R*log(P1/P2) - (A/T^2)*(P1^2-P2^2)/2;

//For CoB
T2 = 400; //temperature at B (K)
T1 = 300; //temperature at Co (K)
del_S2 = S-del_S1;
Cpm = del_S2/(log(T2/T1));
mprintf('\n (b). The mean heat capacity at 12 bar is %f J/mol K',Cpm);

//end
```

**Scilab code Exa 6.9** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 9


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 6.10** To calculate Cv for mercury

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 10


clear all;
clc;


//Given:
betta = 1.8*10^-4; //coeffecient of volume expansion
    (K^-1)
k = 3.9*10^-6; //coeffecient of compressibility (bar
   ^-1)
T = 273; //temperature in K
```

```
d = 13.596*10^3; //density (kg/m^3)
Cp = 0.14*10^3; //(J/kg K)

//To calculate Cv for mercury
//Using equation 6.55 (Page no. 208)
Cv = Cp - (betta^2*T*10^5)/(k*d);

mprintf('Cv for mercury is %f J/kg K',Cv);

//end
```

---

**Scilab code Exa 6.11** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 11


clear all;
clc;


//Given:

//The given example is theoretical and does not involve any numerical computation

//end
```

---

**Scilab code Exa 6.12** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
```

```
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 12


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 6.13** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 13


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 6.14** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 14


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 6.15** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 15


clear all;
clc;


//Given:
```

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

//end
```

**Scilab code Exa 6.16** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 16


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 6.17** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 17


```

```
clear all;
clc;


//Given:

//The give example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 6.18** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 18


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numeriacl computation

//end
```

**Scilab code Exa 6.19** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
```

```
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 19


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 6.20** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 20


clear all;
clc;


//Given:

//The given example is theoretical and does not
   invove any numerical computation

//end
```

---

**Scilab code Exa 6.21** To estimate the fugacity of ammonia

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 21


clear all;
clc;


//Given:
//Eqution of state: P(V-b) = RT
P = 10; //pressure (bar)
T = 298; //temperature (K)
b = 3.707*10^-5; //Vander Waal's constant (m^3/mol)
R = 8.314; //ideal gas constant

//To estimate the fugacity of ammonia
//Since PV = RT + Pb, Z = 1 + (Pb/RT)
//Using equation 6.127 (Page no. 228)
f = P*(%e^((b*P*10^5)/(R*T)));
mprintf('Fugacity f = %f bar',f);

//end
```

**Scilab code Exa 6.22** To determine the fugacity of gas

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
```

```
//Example 22


clear all;
clc;


//Given:
//intg(alphadP) = -556.61 J/mol
P = 50; //pressure in bar
T = 300; //temperature in K
R = 8.314; //ideal gas constant

//To determine the fugacity of gas
//Using equation 6.130 (Page no. 230)
f = P*%e^(-556.61/(R*T));
mprintf('Fugacity of gas at 50 bar and 300 K is %i bar',f);

//end
```

---

**Scilab code Exa 6.23** To determine the fugacity coeffeceint at given pressure

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 23


clear all;
clc;


//Given:
```

```
//Equation of state: PV = RT(1-0.00513P)
P = [1 5 10]; //pressures in bar

//To determine fugacity coefficient at given pressures
//According to Eq. 6.118 (Page no. 228)
//RTd(ln f) = VdP = RT(d ln P - 0.00513dP)
//phi = %e^(-0.00513*P)

for i = 1:3
    phi(i) = %e^(-0.00513*P(i));
    mprintf('\n Fugacity coeffecient at %i bar is %f',P(i),phi(i));
end

//end
```

---

**Scilab code Exa 6.24** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 24


clear all;
clc;


//Given:

//The given example is theoretical and does not involve any numerical computation

//end
```

**Scilab code Exa 6.25** To determine the fugacity of pure ethylene

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 25


clear all;
clc;


//Given:
P = 100; //pressure in bar
T = 373; //temperature in K
a = 0.453; //Vander Waal's constant (J m^3/mol^2)
b = 0.571*10^-4; //Vander Waal's constant (m^3/mol)
V = 2.072*10^-4; //molar volume (m^3/mol)
R = 8.314; //ideal gas constant

//To determine the fugacity of pure ethylene
//Using eq. 6.139 (Page no. 233)
ln_f = (b/(V-b)) - ((2*a)/(R*T*V)) + log((R*T*10^-5)
   /(V-b));
f = %e^ln_f;
mprintf('Fugacity is %f bar',f);

//end
```

**Scilab code Exa 6.26** To determine fugacity and fugacity coeffecient of steam

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 26


clear all;
clc;


//Given:
T = 623; //temperature in K

//Data from steam tables:
H = 3159; //enthalpy at 1000 kPa and 623 K (kJ/kg)
S = 7.3; //entropy at 1000 kPa and 623 K (kJ/kg K)
Ho = 3176; //enthalpy at 101.3 kPa and 623 K (kJ/kg)
So = 8.38; //entropy at 101.3 kPa and 623 K (kJ/kg K
    )
fo = 101.3; //fugacity at 101.3 kPa (kPa)
R = 8.314/18; //ideal gas consatnt (kJ/kg K)

//To determine fugacity and fugacity coeffecient of
    steam
ln_phi = (1/(R*T))*((H-Ho)-T*(S-So));
f = fo*%e^ln_phi;
phi = f/fo;
mprintf('Fugacity of steam is %f bar',f/100);
mprintf('\n Fugacity coeffecient is %f',phi);

//end
```

**Scilab code Exa 6.27** To estimate fugacity of ammonia

```
//A Textbook of Chemical Engineering Thermodynamics
```

```
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 27


clear all;
clc;


//Given:
T = 473; //temperature in K
P = 50*10^5; //pressure in Pa
d = 24.3; //density of ammonia (kg/m^3)
m = 17; //molecular wt of ammonia
R = 8.314; //ideal gas constant

//To estimate the fugacity of ammonia
V = m/(d*1000); //molar volume of ammonia (m^3/kmol)
//Using eq. 6.142 (Page no. 234)
f = (V*(P^2))/(R*T);
mprintf('The fugacity of ammonia is %f bar',f/10^5);

//end
```

**Scilab code Exa 6.28** To calculate the fugacity of liquid water

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 28


clear all;
clc;

```

```

//Given:
T = 303; //temperature in K
P = 10; //pressure in bar
Ps = 4.241/100; //saturation pressure (bar)
sp_vol = 1.004 *10^-3; //specific volume at 303 K (m
    ^3/kg)
R = 8.314; //ideal gas constant

//To calculate the fugacity of liquid water
V = sp_vol*10^-3*18; //molar volume (m^3/mol)

//Assuming vapour behaves as an ideal gas
f_sat = Ps;
//Using Eq. 6.144 (Page no. 235)
ln_phi = (V/(R*T))*(P-Ps)*10^5;
f = f_sat*%e^ln_phi;
mprintf('Fugacity of liquid water at given
    conditions is %f bar',f);

//end
```

---

**Scilab code Exa 6.29** To determine the fugacity of n butane in liquid state at given conditions

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 29


clear all;
clc;


```

```
//Given:
T = 350; //temperature in K
P = 60; //pressure in bar
Ps = 9.35; //vapour pressure at 350 K (bar)
V = 0.1072*10^-3; //molar volume (m^3/mol
phi = 0.834; //fugacity coeffecient
R = 8.314; //ideal gas constant

//To determine fugaity of n butane in liquid state
   at given conditions
f_sat = phi*Ps;
//Using eq. 6.144 (Page no. 235)
ln_phi = (V/(R*T))*(P-Ps)*10^5;
f = f_sat*%e^ln_phi;
mprintf('Fugacity of n-butane in liquid state at
   given conditions is %f bar',f);

//end
```

**Scilab code Exa 6.30** To determine the activity of solid magnesium

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 6
//Thermodynamic Properties of Pure Fluids
//Example 30


clear all;
clc;


//Given:
M = 24.32; //molecular wt of solid magnesium
T = 300; //temperature in K
P = 10; //pressure in bar
```

```
Po = 1; //reference state pressure (bar)
d = 1.745*10^3; //density of Mg at 300 K in kg/m^3

//To determine the ativity of solid magnesiun
//Using eq. 6.149 (Page no. 237)
ln_a = (M/(d*10^3*R*T))*(P-Po)*10^5;
a = %e^ln_a;
mprintf('Acivity of solid magnesium at 300 K and 10 bar is %f',a);

//end
```

# Chapter 7

# Properties of Solutions

**Scilab code Exa 7.1** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 1


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 7.2** To find the volume of mixture

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 2


clear all;
clc;


//Given:
V = 0.1; //volume of mixture required (m^3)
Ve = 0.03; //volume of alcohol
Vw = 0.07; //volume of water
de = 789; //density of ethanol (kg/m^3)
dw = 997; //density of water (kg/m^3)
pe = 53.6*10^-6; //partial molar volume of ethanol (m^3/mol)
pw = 18*10^-6; //partial molar volume of water (m^3/mol)
Me = 46; //molecular wt of ethanol
Mw = 18; //molecular wt of water

//To find the volume of mixture
ne = (Ve*de*10^3)/Me; //number of moles of ethanol
nw = (Vw*dw*10^3)/Mw; //number of moles of water
xe = ne/(ne+nw); //mole fraction of ethanol
xw = 1-ne; //mole fraction of water
act_V = (ne*pe)+(nw*pw);
if (V==act_V)
    then mprintf ('It is possible to prepare the required solution');
else
    Ve_act = (Ve/act_V)*V;
    Vw_act = (Vw/act_V)*V;
    mprintf('\n For the given volumes of ethanol and water, it is not possible to prepare 0.1 cubic m of mixture');
```

```
    mprintf('\n Required volume of ethanol is %f cubic m',Ve_act);
    mprintf('\n Required volume of water is %f cubic m',Vw_act);
end

//end
```

---

**Scilab code Exa 7.3** To find the required volume of methanol and water

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 3


clear all;
clc;


//Given:
V = 2; //volume of desired solution (m^3)
x1 = 0.3; //moles fraction of methanol
x2 = 0.7; //moles fraction of water
V1 = 38.632*10^-6; //partial molar volume of methanol (m^3/mol)
V2 = 17.765*10^-6; //partial molar volume of water (m^3/mol)
mol_V1 = 40.727*10^-6; //molar volume of ethanol (m^3/mol)
mol_V2 = 18.068*10^-6; //molar volume of water (m^3/mol)

//To find the required volume of methanol and water
V_mol = (x1*V1)+(x2*V2); //molar volume of desired
```

```
solution
n = V/V_mol; //no. of moles in the desired solution
n1 = x1*n; //moles of methanol
n2 = x2*n; //moles of water
V_m = n1*mol_V1;
V_w = n2*mol_V2;
mprintf('Volume of methanol to be taken is %f cubic m',V_m);
mprintf('\n Volume of water to be taken is %f cubic m',V_w);

//end
```

---

**Scilab code Exa 7.4** To calculate the volume of water to be added and volume of dilute alcohol solution

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 4


clear all;
clc;


//Given:
V1_w = 0.816*10^-3; //partial molar volume of water in 96% alcohol solution
V1_e = 1.273*10^-3; //partial molar volume of ethanol in 96% alcohol solution
V2_w = 0.953*10^-3; //partial molar volume of water in 56% alcohol solution
V2_e = 1.243*10^-3; //partial molar volume of ethanol in 56% alcohol solution
```

```
d = 0.997*10^3; //density of water (kg/m^3)

//To calculate the volume of water to be added and
   volume of dilute alcohol solution
//Basis:
V = 2*10^-3; //volume of alcohol solution (m^3)
V_sp = (0.96*V1_e)+(0.04*V1_w); //volume of 1 kg of
   laboratory alcohol
m_e = V/V_sp; //mass of 2*10^-3 m^3 alcohol

//(a).
//Let mass of water added be m kg
//Taking an alcohol balance
m = (m_e*0.96)/0.56 - m_e;
v = m/d;
mprintf('\n (a).');
mprintf('\n Mass of water added is %f kg',m);
mprintf('\n Volume of water added is %4.3e cubic m',
   v);

//(b)
m_sol = m_e + m; //mass of alcohol solution obtained
sp_vol = (0.56*V2_e)+(0.44*V2_w); //specific volume
   of 56% alcohol
V_dil = sp_vol*m_sol; //volume of dilute alcohol
   solution
mprintf('\n\n (b)');
mprintf('\n Volume of dilute alcohol solution is %5
   .4e cubic m',V_dil);

//end
```

**Scilab code Exa 7.5** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
```

```
//Chapter 7
//Properties of Solutions
//Example 5


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 7.6** To determine enthalpies of pure components and at infinite dilution

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 6


clear all;
clc;


//Given:
//Function for enthalpy:
H = 400*x1 + 600*x2 + x1*x2*(40*x1+20*x2)

//To determine enthalpies for pure component and at
   infinite dlution
```

```

//(a).
//The given subpart is theoretical and does not
   involve numerical computation

//(b).
//Using eq. 7.27 (Page no. 264)
//H = H1_bar as x1 = 1
H1 = 420-60+40;
//Using eq. 7.28 (Page no. 264)
//H = H2_bar as x2 = 1
H2 = 600;
mprintf('\n (b).');
mprintf('\n Pure state enthalpies are:');
mprintf('\n H1 = %i J/mol',H1);
mprintf('\n H2 = %i J/mol',H2);

//(c).
//H1_inf = H1_bar as x1 = 0, so from eq. 7.27
H1_inf = 420;
//H2_inf = H2_bar as x2 = 0. so from eq 7.28
H2_inf = 640;
mprintf('\n\n (c).');
mprintf('\n At infinite dilution:');
mprintf('\n H1 = %i J/mol',H1_inf);
mprintf('\n H2 = %i J/mol',H2_inf);

//end
```

**Scilab code Exa 7.7** To calculate the partial molar volume of the components

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
```

```
//Example 7


clear all;
clc;


//Given:
//Volume as a function of molality:
function [y] = V(m)
    y = 1.003*10^-3 + 0.1662*10^-4*m + 0.177*10^-5*m^1.5 + 0.12*10^-6*m^2
endfunction

m = 0.1; //molality of solution (mol/kg)

//To calculate the partial molar volume of the components
//Differentiating Eq. 7.29 with reference to m, we get
V1_bar = 0.1662*10^-4 + 0.177*1.5*10^-5*m^0.5 + 0.12*2*10^-6*m;

V_sol = V(m); //volume of aqueous soluttion
n1 = m;
n2 = 1000/18;
V2_bar = (V_sol - n1*V1_bar)/n2;
mprintf('Partial molar volume of water = %4.3e cubic m/mol',V2_bar);
mprintf('\n Partial molar volume of NaCl = %4.3e cubic m/mol',V1_bar);

//end
```

**Scilab code Exa 7.8** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 8


clear all;
clc;


//Given:

//The given example is theoretical and does not any
   numerical computation

//end
```

---

**Scilab code Exa 7.9** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 9


clear all;
clc;


//Given:

//The given example is theoretical and does not any
   numerical computation

//end
```

**Scilab code Exa 7.10** To estimate the solubility of oxygen in water at 298 K

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 10


clear all;
clc;


//Given:
K = 4.4*10^4; //Henry's law constant (bar)
pp = 0.25; //partial pressure of oxygen in bar
M_O2 = 32; //molecular wt of oxygen
M_water = 18; //molecular wt of water

//To estimate the solubility of oxygen in water at 298 K
//Using eq. 7.72 (Page no. 275)
x_O2 = pp/K; //mole fraction of O2
mprintf('Solubility of oxygen is %5.4e moles per mole of water',x_O2);

//In mass units
sol_O2 = (x_O2*M_O2)/M_water;
mprintf('\n Solubility of oxygen in mass units is %4.3e kg oxygen per kg water',sol_O2);

//end
```

**Scilab code Exa 7.11** To confirm that mixture conforms to Raoults Law and to determine Henrys Law constant

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 11


clear all;
clc;


//Given:
xb = [0 0.2 0.4 0.6 0.8 1.0];
pa_bar = [0.457 0.355 0.243 0.134 0.049 0];
pb_bar = [0 0.046 0.108 0.187 0.288 0.386];

//To confirm mixture conforms to Raoult's Law and to
    determine Henry's law constant
clf
xa = 1-xb;
plot(xa,pa_bar);
plot(xa,pb_bar);
xtitle(" ","Mole fraction of A","Partial Pressure");

//For Raoult's Law plotting
x = linspace(0,1,6);
y1 = linspace(0,0.457,6);
y2 = linspace(0.386,0,6);
plot2d(x,y1,style=3);
plot2d(x,y2,style=3);

//For Henry's law plotting
```

```
x = [0 0.2 0.4 0.6 0.8 1.0];
//Form the partial presures plot of component A and B
yh1(1) = 0; yh1(2) = 0.049; //For component A
for i = 3:6
    yh1(i) = yh1(i-1)+(x(i)-x(i-1))*((yh1(2)-yh1(1))/(x(2)-x(1)));
end

yh_2(6) = 0; yh_2(5) = 0.046; //For component B
i = 4;
while (i~=0)
    yh_2(i) = yh_2(i+1) + (x(i)-x(i+1))*((yh_2(6)-yh_2(5))/(x(6)-x(5)));
    i = i-1;
end
plot2d(x,yh1,style=6);
plot2d(x,yh_2,style=6);
legend("Partial pressure "," ","Raoults law"," ","Henrys Law");

//(a)
mprintf('From the graph it can be inferred that, in the region where Raoults law is obeyed by A, the Henrys law is obeyed by B, and vice versa');

//(b)
//Slope of Henry's law
mprintf('\n For component A, Ka = %f bar',yh1(6));
mprintf('\n For component B, Kb = %f bar',yh_2(1));

//end
```

**Scilab code Exa 7.12** To calculate activity and activity coeffecient of chloroform

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 12


clear all;
clc;


//Given:
xa = [0 0.2 0.4 0.6 0.8 1.0];
Pa_bar = [0 0.049 0.134 0.243 0.355 0.457];
Pb_bar = [0.386 0.288 0.187 0.108 0.046 0];

//To calculate activity and activity coeffecient of chloroform
xb = 1-xa;
Pbo = 0.386; //vapour pressure of pure chloroform
//(a). Based on standard state as per Lewis-Randall rule

mprintf('Based on Lewis Randall Rule');
mprintf('\n    Activity           Activity coeffecient ');
for i = 1:6
    a(i) = Pb_bar(i)/Pbo;
    mprintf('\n    %f',a(i));
    if(xb(i)==0)
        mprintf('         Not defined');
    else ac(i) = a(i)/xb(i);
        mprintf('          %f',ac(i));
    end
end

```

```
//(b). Based on Henry's Law
Kb = 0.217; //bar (From Example 7.11 Page no. 276)

mprintf('\n\n\n Based on Henrys Law');
mprintf('\n    Activity           Activity coeffecient');
for i = 1:6
    a(i) = Pb_bar(i)/Kb;
    mprintf('\n    %f',a(i));
    if(xb(i)==0)
        mprintf('         Not defined');
    else
        ac(i) = a(i)/xb(i);
        mprintf('            %f',ac(i));
    end
end

//end
```

---

**Scilab code Exa 7.13** To determine fugacity fugacity coeffecient Henrys Law constant and activity coeffecient

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 13


clear all;
clc;


//Given:
P = 20; //pressure in bar
//Function for fugacity of component 1
```

```
function [y] = f1(x1);
    y = (50*x1)-(80*x1^2)+(40*x1^3)
endfunction

//To determine fugacity fugacity coeffecient Henry's Law constant and activity coeffecient

//(a)
//Fugacity of component in solution becomes fugacity of pure component when mole fraction approaches 1 i.e.
x1 = 1;
f1_pure = f1(x1);
mprintf('(a). Fugacity f1 of pure component 1 is %i bar',f1_pure);

//(b)
phi = f1_pure/P;
mprintf('\n (b). Fugacity coeffecient is %f',phi);

//(c)
//Henry's Law constant is lim (f1/x1)and x1 tends to 0
x1 = 0;
K1 = 50 - (80*x1) + (40*x1^2);
mprintf('\n (c). Henrys Law constant is %i bar',K1);

//(d)
mprintf('\n (d). This subpart is theoretical and does not involve any numerical computation');

//end
```

**Scilab code Exa 7.14** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 14


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 7.15** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 15


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 7.16** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 16


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 7.17** To determine enthalpies at infinite dilution

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 17


clear all;
clc;


```

```
//Given:
//Function for enthalpy change of mixture
//H = x1*x2*(40*x1 + 20*x2)
H1_pure = 400; //enthalpy of pure liquid 1 at 298 K and 1 bar (J/mol)
H2_pure = 600; //enthalpy of pure liquid 2 (J/mol)

//To determine enthalpies at infinite dilution
//Using eq. 7.126 and 7.128 (Page no. 294)
//H1_bar = 20*(1-x1)^2 * (2x1+1)
//Using eq. 7.127 and 7.128 (Page no. 294)
//H2_bar = 40*x1^3

//For infinite dilution x1 = 0, delH1_inf = H1_bar
x1 = 0;
delH1_inf = 20*((1-x1)^2)*(2*x1+1);
H1_inf = H1_pure + delH1_inf; //(J/mol)

//For infinite dilution of 2, x1 = 1 and delH2_inf = H2_bar
x1 = 1;
delH2_inf = 40*x1^3;
H2_inf = delH2_inf + H2_pure; //(J/mol)

mprintf('Enthalpy at infinite dilution for component 1 is %i J/mol',H1_inf);
mprintf('\n Enthalpy at infinite dilution for component 2 is %i J/mol',H2_inf);

//end
```

**Scilab code Exa 7.18** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
```

```
//Properties of Solutions
//Example 18


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 7.19** To determine change in entropy for the contents of the vessel

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 19


clear all;
clc;


//Given:
R = 8.314; //ideal gas constant
n1 = 100; //moles of nitrogen
n2 = 100; //moles of oxygen

//To determine the change in entropy of the contents
    of the vessel
```

```
x1 = n1/(n1+n2);
x2 = n2/(n1+n2);

//Using eq. 7.122 (Page no. 292)
S = -R*(x1*log (x1) + x2*log (x2));
S_tot = S*(n1+n2);
mprintf('Change in entropy of components are %f J/K',S_tot);

//end
```

**Scilab code Exa 7.20** To determine heat of formation of LiCl in 12 moles of water

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 20


clear all;
clc;


//Given:
//For reaction 1
//Li + 1/2Cl2 --> LiCl
Hf = -408.610; //heat of formation (kJ)

//For reaction 2
//LiCl + 12H2O --> LiCl(12H2O)
H_sol = -33.614; //heat of solution (kJ)

//To determine heat of formation of LiCl in 12 moles of water
```

```
//Adding reaction 1 and 2, we get

//Li + 1/2Cl2 + 12H2O --> LiCl(12H2O)
H_form = Hf+H_sol;
mprintf('Heat of formation of LiCl in 12 moles of water is %f kJ',H_form);

//end
```

**Scilab code Exa 7.21** To calculate the free energy of mixing

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 21


clear all;
clc;


//Given:
R = 8.314; //ideal gas constant
n1 = 3; //moles of hydrogen
n2 = 1; //moles of nitrogen
T = 298; //temperature in K
P1 = 1; //pressure of hydrogen in bar
P2 = 3; //pressure of nitrogen in bar

//To calculate the free energy of mixing
V1 = (n1*R*T)/(P1*10^5); //volume occupied by hydrogen
V2 = (n2*R*T)/(P2*10^5); //volume occupied by nitrogen
V = V1+V2; //total volume occupied
```

```
P = ((n1+n2)*R*T)/(V*10^5); //final pressure
   attained by mixture (bar)

//It is assumed that process is taking in two steps
//Step 1: Individual gases are separately brought to
    final pressure at constant temperature
//Step 2: The gases are mixed at constant
   temperature and pressure

//For step 1
G1 = R*T*(n1*log(P/P1) + n2*log(P/P2));

//For step 2, using eq. 7.121 (Page no. 292)
x1 = n1/(n1+n2);
x2 = n2/(n1+n2);
G2 = (n1+n2)*R*T*(x1*log (x1) + x2*log (x2));

G = G1+G2; //free energy in J
mprintf('The free energy of mixing when partition is
    removed is %f kJ',G/1000);

//end
```

**Scilab code Exa 7.22** To calculate the mean heat capacity of 20 mol percent solution

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 22


clear all;
clc;

```

```

//Given:
C_water = 4.18*10^3; //heat capacity of water (J/kg K)
C_ethanol = 2.58*10^3; //heat capacity of ethanol (J/kg K)
G1 = -758; //heat of mixing 20 mol percent ethanol water at 298 K(J/mol)
G2 = -415; //heat of mixing 20 mol percent ethanol water at 323 K (J/mol)
n_wat = 0.8; //moles of water
n_eth = 0.2; //moles of ethanol
T1 = 323; //initial temperature in K
T2 = 298; //final temperature in K

//To calculate the mean heat capacity of 20 mol percent solution
//The whole process is divided in 4 steps

//Step 1: Water is cooled from 323 K t0 298 K
H1 = n_wat*18*C_water*(T2-T1)/1000; //(J)

//Step 2: Ethanol is cooled from 323 to 298 K
H2 = n_eth*46*C_ethanol*(T2-T1)/1000; //(J)

//Step 3: 0.8 mol water and 0.2 mol ethanol are mixed at 298 K
H3 = G1; //(J)

//Step 4:
//Mixture is heated to 323 K
//H = Cpm*(T1-T2)
H = G2;
Cpm = (H-H1-H2-H3)/(T1-T2);

mprintf('Mean heat capacity of solution is %f J/mol K',Cpm);

```

```
//end
```

**Scilab code Exa 7.23** To find the final temperature attained

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 23


clear all;
clc;


//Given:
To = 298; //initial temperature (K)
Cpm = 97.65; //Mean heat capacity of solution (J/mol K)
Hs = -758; //heat of mixing (J/mol)

//To find the final temperature attained
//Since the process is adiabatic
H = 0;
T = (H-Hs)/Cpm + To;
mprintf('The final temperature attained by the mixing is %f K',T);

//end
```

**Scilab code Exa 7.24** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 7
//Properties of Solutions
//Example 24


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

# Chapter 8

# Phase equilibria

**Scilab code Exa 8.1** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 1


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 8.2** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 2


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 8.3** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 3


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 8.4** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 4


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 8.5** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 5


clear all;
clc;


```

```
//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 8.6** To determine composition of vapour and liquid in equilibrium

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 6


clear all;
clc;


//Given:
P1 = 106; //vapour pressure of n-heptane (kPa)
P2 = 74; //vapour pressure of toluene (kPa)
P = 101.3; //total pressure (kPa)

//To determine the composition of the liquid and
   vapour in equilibrium
//Referring eq. 8.51 (Page no. 332)

//Let x be mol fraction of heptane in liquid
x = (P-P2)/(P1-P2);
//Using eq. 8.54 (Page no. 333)
y = x*(P1/P);

mprintf('Composition of liquid heptane is %f mol
```

```
percent',x*100);
mprintf('\n Composition of heptane in vapour form is %f mol percent',y*100);

//end
```

---

**Scilab code Exa 8.7** To determine pressure at the beginning and at the end of the process

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 7


clear all;
clc;


//Given:
P1 = 135.4; //vapour pressure of benzene (kPa)
P2 = 54; //vapour pressure of toluene (kPa)

//To determine the pressure at the beginning and at the end of process

//At beginning
x =  0.5; //liquid phase composition
//Using eq. 8.51 (Page no. 332)
P_beg = P2 + (P1-P2)*x;

//At the end
y = 0.5; //vapour phase composition
//Using eq. 8.54 (Page no. 333) and rearranging
P_end = (P1*P2)/(P1-y*(P1-P2));
```

```

mprintf('Pressure at the beginning of the process is
    %f kPa',P_beg);
mprintf('\n Pressure at the end of the process is %f
    kPa',P_end);

//end
```

---

**Scilab code Exa 8.8** To determine temperature pressure and compositions

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 8


clear all;
clc;


//Given:
//Antoine Equations:

function [y1] = P1(T)
    y1 = %e^(14.5463 - 2940.46/(T-35.93))  //vapour
       pressure of acetone
endfunction

function [y2] = P2(T)
    y2 = %e^(14.2724 - 2945.47/(T-49.15))  //vapour
       pressure of acetonitrile
endfunction

//To determine temperature pressure and compositions
//(a). To calculate x1 and y1
```

```
T = 327; //temperature in K
P = 65; //pressure in kPa

P1_s = P1(T);
P2_s = P2(T);
//Using eq. 8.51 (Page no. 332)
x1 = (P-P2_s)/(P1_s-P2_s);
//Using eq. 8.54 (Page no. 333)
y1 = x1*(P1_s/P);
mprintf('(a)');
mprintf('\n x1 = %f',x1);
mprintf('\n y1 = %f',y1);

//(b). To calculate T and y1
P = 65; //pressure in kPa
x1 = 0.4;

flag = 1;
T2 = 340; //temperatue (assumed)
while(flag==1)
    P1_s = P1(T2);
    P2_s = P2(T2);
    P_calc = P2_s + x1*(P1_s-P2_s)
    if((P_calc-P)<=1)
        flag = 0;
    else
        T2 = T2-0.8;
    end
end
y1 = x1*(P1_s/P);
mprintf('\n\n (b)');
mprintf('\n Temperature is %f K',T2);
mprintf('\n y1 = %f',y1);

//(c). To calculate P and y1
T3 = 327; //temperature in K
x1 = 0.4;

```

```
P1_s = P1(T3);
P2_s = P2(T3);
P = P2_s + x1*(P1_s-P2_s);
y1 = x1*(P1_s/P);
mprintf('\n\n (c)');
mprintf('\n Pressure is %f kPa',P);
mprintf('\n y1 = %f',y1);

//(d). To calculate T and x1
P = 65; //pressure in kPa
y1 = 0.4;

flag = 1;
T = 340; //assumed temperature (K)
while(flag==1)
    P1_s = P1(T);
    P2_s = P2(T);
    y1_calc = (P1_s*(P-P2_s))/(P*(P1_s-P2_s));
    if((y1_calc-y1)>=0.001)
        flag = 0;
    else
        T = T-2;
    end
end
x1 = y1*(P/P1_s);
mprintf('\n\n (d)');
mprintf('\n Temperature = %f K',T);
mprintf('\n x1 = %f',x1);

//(e). To calculate P and x1
T = 327; //temperature (K)
y1 = 0.4;

P1_s = P1(T);
P2_s = P2(T);
//Using eq. 8.54 and 8.51
x1 = (y1*P2_s)/(P1_s-y1*(P1_s-P2_s));
P = x1*(P1_s/y1);
```

```
mprintf('\n\n (e)');
mprintf('\n Pressure = %f kPa',P);
mprintf('\n x1 = %f',x1);

//(f). To calculate fraction of the system is liquid
    and vapour in equilibrium
T = 327; //temperature (K)
P = 65; //pressure (kPa)
y1 = 0.7344;

P1_s = P1(T);
P2_s = P2(T);
x1 = (P-P2_s)/(P1_s-P2_s);
//Let f be the fraction of the mixture that is
   liquid
//Applying acetone balance
f = (0.7-y1)/(x1-y1);
mprintf('\n\n (f)');
mprintf('\n Fraction of mixture that is liquid is %f
    percent',f*100);

//end
```

---

**Scilab code Exa 8.9** To construct boiling point and equilibrium point diagram

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 9


clear all;
clc;

```

```

//Given:
P = 101.3; //total pressure over the system (kPa)
T = [371.4 378 383 388 393 398.6];
Pa = [101.3 125.3 140.0 160.0 179.9 205.3];
Pb = [44.4 55.6 64.5 74.8 86.6 101.3];

//To construct boiling point and equilibrium point diagram
for i = 1:6
    xa(i) = (P-Pb(i))/(Pa(i)-Pb(i)); //Using eq. 8.51
    ya(i) = xa(i)*(Pa(i)/P); //Using eq. 8.54
end

//(a).
//To construct boiling point diagram
clf
plot(xa,T);
plot(ya,T);
xtitle("Boiling Point diagram","xa and ya","Temperature");

//(b).
//To construct the equilibrium diagram
xset("window',1);
clf
plot(ya,xa);
xtitle("Equilibrium Diagram","xa","ya");

//(c).
mprintf('(c). The given subpart is theoretical and does not involve any numerical computation');

//end
```

**Scilab code Exa 8.10** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 10


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 8.11** To calculate van Laar constants

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 11


clear all;
clc;


//Given:
```

```
x1 = 46.1/100; //mole percent of A
P = 101.3; //total pressure of system (kPa)
P1_s = 84.8; //vapour pressure of component A (kPa)
P2_s = 78.2; //vapour pressure of component B (kPa)

//To calculate van Laar constants
gama1 = P/P1_s;
gama2 = P/P2_s;
x2 = 1-x1;

//van Laar constants:
//Using eq. 8.69 (Page no. 348)
A = log (gama1)*(1 + (x2*log(gama2))/(x1*log(gama1))
   )^2;
B = log (gama2)*(1 + (x1*log(gama1))/(x2*log(gama2))
   )^2;

mprintf('van Laar constants are:');
mprintf('\n A = %f',A);
mprintf('\n B = %f',B);

//end
```

---

**Scilab code Exa 8.12** To calculate activity coeffecients in a solution containing 10 percent alcohol

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 12


clear all;
clc;

```

```

//Given:
x2 = 0.448; //mole fraction of ethanol
P = 101.3; //total pressure (kPa)
P1_s = 68.9; //Vapour pressure of benzene (kPa)
P2_s = 67.4; //vapour pressure of ethanol (kPa)

//To calculate activity coeffecients in a solution containing 10% alcohol
x1 = 1-x2;
gama1 = P/P1_s;
gama2 = P/P2_s;

//Using eq. 8.69 (Page no. 348)
//van Laar constants:
A = log (gama1)*(1 + (x2*log(gama2))/(x1*log(gama1)))^2;
B = log (gama2)*(1 + (x1*log(gama1))/(x2*log(gama2)))^2;

//For solution containing 10% alcohol
x2 = 0.1;
x1 = 1-x2;
ln_g1 = (A*x2^2)/(((A/B)*x1+x2)^2);
ln_g2 = (B*x1^2)/((x1+(B/A)*x2)^2);
gama1 = %e^ln_g1;
gama2 = %e^ln_g2;

mprintf('Activity coeffecients:');
mprintf('\n For component 1: %f',gama1);
mprintf('\n For component 2: %f',gama2);

//end
```

**Scilab code Exa 8.13** To calculate equilibrium vapour composition for solution containing 20 mole percent hydrazine

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 13


clear all;
clc;


//Given:
x2 = 0.585; //mol fraction of hydrazine
P = 101.3; //total pressure of system (kPa)
P2_s = 124.76; //vapour pressure of hydrazine (kPa)

//To calculate equilibrium vapour composition for solution containing 20% (mol) hydrazine
x1 = 1-x2;
P1_s = 1.6*P2_s; //vapour pressure of water (kPa)
gama1 = P/P1_s;
gama2 = P/P2_s;

//Using eq. 8.69 (Page no. 348)
//van Laar constants:
A = log (gama1)*(1 + (x2*log(gama2))/(x1*log(gama1)))^2;
B = log (gama2)*(1 + (x1*log(gama1))/(x2*log(gama2)))^2;

//For solution containing 20% hydrazine
x2 = 0.2;
x1 = 1-x2;
ln_g1 = (A*x2^2)/(((A/B)*x1+x2)^2);
ln_g2 = (B*x1^2)/((x1+(B/A)*x2)^2);
gama1 = %e^ln_g1;
```

```
gama2 = %e^ln_g2;

//Using eq. 8.47 (Page no. 325) for components 1 and 2 and rearranging
alpha = 1.6; //alpha = P1_s/P2_s
y1 = 1/(1 + (gama2*x2)/(gama1*x1*alpha));
y2 = 1-y1;

mprintf('Equilibrium vapour composition for solution containing 20 mol percent hydrazine');
mprintf('\n Hydrazine is %f percent',y2*100);
mprintf('\n Water is %f percent',y1*100);

//end
```

**Scilab code Exa 8.14** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 14


clear all;
clc;


//Given:

//The given example is theoretical and does not involve any numerical computation

//end
```

**Scilab code Exa 8.15** To determine the total pressure

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 15


clear all;
clc;


//Given:
x1 = 0.047; //mol fraction of isopropanol
P1 = 91.11; //vapour pessure of pure propanol (kPa)
P = 91.2; //toatl pressure of system (kPa)
P2 = 47.36; //vapour pressure of water (kPa)

//van Laar consatnts:
A = 2.470;
B = 1.094;

//To determine the total pressure:
x2 = 1-x1;
//Using eq. 8.68 (Page no. 348)
ln_g1 = (A*x2^2)/(((A/B)*x1 + x2)^2);
ln_g2 = (B*x1^2)/((x1 + (B/A)*x2)^2);
gama1 = %e^ln_g1;
gama2 = %e^ln_g2;

//Total pressure:
P_tot = (gama1*x1*P1) + (gama2*x2*P2);
if(P==P_tot)
    mprintf('This is equal to total pressure');
```

```
else
    mprintf('This is less than the total pressure.
       This error must have been caused by air leak'
       );
end


//end
```

---

**Scilab code Exa 8.16** To construct the Pxy diagram

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 16


clear all;
clc;


//Given:
P1 = 24.62; //vapour pressure of cyclohexane (kPa)
P2 = 24.41; //vapour pressure of benzene (kPa)

//Activity coeffecients are given by:
//ln_g1 = 0.458*x2^2;
//ln_g2 = 0.458*x1^2;

//To construct the P-x-y diagram
x1 = [0 0.2 0.4 0.6 0.8 1.0]
x2 = 1-x1;

for i = 1:6
    g1(i) = %e^(0.458*x2(i)^2); //activity
```

```
        coeffecient for component 1
    g2(i) = %e^(0.458*x1(i)^2); //activity coeffecient for component 2
    P(i) = (g1(i)*x1(i)*P1) + (g2(i)*x2(i)*P2); //total pressure (kPa)
    y1(i) = (g1(i)*x1(i)*P1)/P(i);
end
disp(P);
disp(y1);

//To construct P–x–y diagram
clf
plot(x1,P);
plot(y1,P);
xtitle(”P–x–y Diagram”,”x1 and y1”,”Pressure”);

//end
```

---

**Scilab code Exa 8.17** To determine the composition and total pressure of azeotrope

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 17


clear all;
clc;


//Given:
P = 40.25; //total pressure (kPa)
y1 = 0.566; //mol fraction of benzene in vapour phase
```

```
x1 = 0.384; //mol fraction of benzene in liquid state
P1 = 29.6; //vapour pressure of benzene (kPa)
P2 = 22.9; //vapour pressure of ethanol (kPa)

//To determine the composition and total pressure of azeotrope
x2 = 1-x1;
y2 = 1-y1;

//Using eq. 8.47 (Page no. 325)
//Activity coeffecients:
g1 = (y1*P)/(x1*P1);
g2 = (y2*P)/(x2*P2);

//Using eq. 8.69 (Page no. 348)
//van Laar constants:
A = log(g1)*((1 + (x2*log(g2))/(x1*log(g1)))^2);
B = log(g2)*((1 + (x1*log(g1))/(x2*log(g2)))^2);

//Assuming azeotropic comp. (for hit and trial method)
x1 = 0.4;
flag = 1;
while(flag==1)
    x2 =1-x1;
    ln_g1 = (A*x2^2)/(((A/B)*x1 + x2)^2);
    ln_g2 = (B*x1^2)/((x1 + (B/A)*x2)^2);
    g1 = %e^ln_g1;
    g2 = %e^ln_g2;
    P_1 = g1*P1;
    P_2 = g2*P2;
    if((P_1-P_2)<=1) and ((P_1-P_2)>=-1)
        flag = 0;
    else
        x1 = x1+0.1;
    end
end
```

```
mprintf('Azeotropic compositon of benzene is %i
    percent',x1*100);
mprintf('\n Total pressure of azeotrope is %f kPa',(
    P_1+P_2)/2);

//end
```

---

**Scilab code Exa 8.18** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 18


clear all;
clc;


//Given:

//The given example is theoretical and does not
    involve any numerical computation

//end
```

---

**Scilab code Exa 8.19** To calculate equilibrium pressure and composition

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 19
```

```


clear all;
clc;


//Given:
//Wilson constants:
a12 = 1225.31; //(J/mol)
a21 = 6051.01; //(J/mol)
V1 = 74.05*10^-6; //(m^3/mol)
V2 = 18.07*10^-6; //(m^3/mol)

R = 8.314; //ideal gas constant
T = 349; //temperature in K

//Antoine Equation:
//Vapour pressure of 1st element
function [y1] = P1(T)
    y1 = %e^(14.39155-(2795.817/(T-43.198)))
endfunction

//Vapour pressure of 2nd element
function [y2] = P2(T)
    y2 = %e^(16.26205-(3799.887/(T-46.854)))
endfunction

//To calculate equilibrium pressure and composition
//Using eq. 8.73 (Page no. 350)
//Wilson Parameters:
W12 = (V2/V1)*%e^(-a12/(R*T));
W21 = (V1/V2)*%e^(-a21/(R*T));

//Using Antoine equation
P1_s = P1(T);
P2_s = P2(T);

//(a). Composition of vapour in equilibrium
```

```
x1 = 0.43;
x2 = 1-x1;

//Using eq. 8.72 (Page no. 350)
//Wilson equations:
//Activity coeffecient of 1st component
function [y3] = g_1(n1,n2) //n1 is mol fraction of 1 and n2 is for 2
    y3 = %e^(-log(n1 + W12*n2) + n2*((W12/(n1+W12*n2))-(W21/(W21*n1+n2))));
endfunction

//Activity coeffecint of 2nd component
function [y4] = g_2(n1,n2)
    y4 = %e^(-log(n2 + W21*n1) - n1*((W12/(n1+W12*n2))-(W21/(W21*n1+n2))));
endfunction

//Activity coeffecients:
g1 = g_1(x1,x2);
g2 = g_2(x1,x2);

P = (g1*x1*P1_s) + (g2*x2*P2_s);
y1 = (g1*x1*P1_s)/P;

mprintf('(a).');
mprintf('\n Equilibrium pressure is %f kPa',P);
mprintf('\n Composition of acetone vapour in equilibrium is %f',y1);


//(b). Composition of liquid in equilibrium
y1 = 0.8;
y2 = 1-y1;
g1 = 1; g2 = 1; //assumed activity coeffecients
P_as = 1/((y1/(g1*P1_s)) + (y2/(g2*P2_s)));

//Hit and trial method:
```

```
flag = 1;
while(flag==1)
    x1 = (y1*P_as)/(g1*P1_s);
    x2 = 1-x1;
    g1 = g_1(x1,x2);
    g2 = g_2(x1,x2);
    P_calc = 1/((y1/(g1*P1_s)) + (y2/(g2*P2_s)));
    if((P_calc-P_as)<=1) and ((P_calc-P_as)>=-1)
        flag = 0;
    else
        P_as = P_calc;
    end
end

mprintf('\n\n (b).');
mprintf('\n Equilibrium Pressure is %f kPa',P_calc);
mprintf('\n Composition of acetone in liquid in
   equilibrium is %f',x1);

//end
```

---

**Scilab code Exa 8.20** To determine parameters in Wilsons equation

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 20


clear all;
clc;


//Given:
P = 101.3; //total pressure of system (kPa)
```

```
T = 337.5; //temperature in K
x1 = 0.842;

//Antoine constants
//For methanol(1)
A1 = 16.12609;
B1 = 3394.286;
C1 = 43.2;

//For methyl ethyl ketone (2)
A2 = 14.04357;
B2 = 2785.225;
C2 = 57.2;

//To determine parameters in Wilson's equation
P1_s = %e^(A1-(B1/(T-C1)));
P2_s = %e^(A2-(B2/(T-C2)));
x2 = 1-x1;
g1 = P/P1_s;
g2 = P/P2_s;

//Using eq. 8.72 and rearranging:
function [y1] = Wils(n) //n is the Wilson's parameter W12
    y1 = (((g1*x2)/(1-(n*x1/(x1+n*x2))+(x1/x2)*log(g1*(x1+n*x2))))^(x2/x1))*(g1*(x1+n*x2));
endfunction

flag = 1;
W12 = 0.5; //assumed value
while(flag==1)
    res = Wils(W12);
    if ((res-1)>=-0.09)
        flag = 0;
    else
        W12 = W12+0.087;
    end

```

```
end

//For 2nd Wilson parameter:
//Using eq. 8.72 and rearranging:
k = log(g1*(x1+W12*x2))/x2 - (W12/(x1+W12*x2));
W21 = (-k*x2)/(1+k*x1);

mprintf("wilson parameters are: %f, %f',W12,W21);

//end
```

**Scilab code Exa 8.21** To alculate bubble and dew point and the composition

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 21


clear all;
clc;


//Given:
P = 101.3; //total pressure in kPa
T = [333 343 353 363]; //temperatures(K)
Pa = [81.97 133.29 186.61 266.58]; //Partial
    pressure of component A (kPa)
Pb = [49.32 73.31 106.63 166.61]; //Partial pressure
     of component B (kPa)
Pc = [39.32 62.65 93.30 133.29]; //Partial pressure
    of component C (kPa)
xa = 0.45; //mole fraction of methanol
xb = 0.3; //mole fraction of ethanol
```

```
xc = 1-xa-xb; //mole fraction of propanol

//To calculate bubble and dew point and the composition

//(a). To calculate bubble point and vapour composition
clf
plot2d(T,Pa);
plot2d(T,Pb,style=3);
plot2d(T,Pc,style=6);
xtitle(” ”,”Temperature”,”Vapour pressures”);
legend(”Pa”,”Pb”,”Pc”);

//Using eq. 8.84 (Page no. 362)
//At bubble temperature, sum(yi) = sum((xi∗Pi)/P) = 1
for i = 1:4
    sum_y(i) = (xa*Pa(i))/P + (xb*Pb(i))/P + (xc*Pc(i))/P;
end

Tb = interpln([sum_y’;T],1); //obtaining temperature at which sum (yi) = 1

//Obtaining vapour pressures at bubble temperature
Pb1 = interpln([T;Pa],Tb);
Pb2 = interpln([T;Pb],Tb);
Pb3 = interpln([T;Pc],Tb);

//Calculating equilibrium vapour composition
ya = (xa*Pb1*100)/P;
yb = (xb*Pb2*100)/P;
yc = (xc*Pb3*100)/P;

mprintf(’(a).’);
mprintf(’\n The bubble temperature is %f K’,Tb);
mprintf(’\n The equilibrium vapour contains %f
```

```
methanol, %f ethanol and %f propanol',ya,yb,yc);

//(b). The dew point and liquid composition
//Vapour phase compositions at dew point
ya = 0.45; //methanol
yb = 0.30; //ethanol
yc = 0.25; //propanol

//At dew point, sum(xi) = sum ((yi*P)/Pi) = 1
for i = 1:4
    sum_x(i) = (ya*P)/Pa(i) + (yb*P)/Pb(i) + (yc*P)/Pc(i);
end

Td = interpln([sum_x';T],1); //obtaining temperature at which sum (xi) = 1

//Obtaining vapour pressures at dew temperature
Pd1 = interpln([T;Pa],Td);
Pd2 = interpln([T;Pb],Td);
Pd3 = interpln([T;Pc],Td);

//Calculating liquid composition
xa = (ya*P*100)/Pd1;
xb = (yb*P*100)/Pd2;
xc = (yc*P*100)/Pd3;

mprintf('\n\n (c).');
mprintf('\n The dew point is %f K',Td);
mprintf('\n At dew point liquid contains %f methanol, %f ethanol and %f propanol',xa,xb,xc);

//end
```

**Scilab code Exa 8.22** To calculate bubble and dew point temperatures

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 22


clear all;
clc;


//Given:
//All Ki values are obtained from Fig. 13.6 0f Chemical Engineer's Handbook, 5th ed.
P = 1447.14; //pressure of the system (kPa)
x = [0.25 0.4 0.35]; //composition of the components
T = [355.4 366.5]; //assumed temperatures (K)
K1 = [2.00 0.78 0.33]; //value of Ki at 355.4 K
K2 = [2.30 0.90 0.40]; //value of Ki at 366.5 K

//To calculate bubble and dew point temperatures
//(a). The bubble point temperature and composition of the vapour

//At bubble point temperature, sum(K*x) = 1
Kx = [0 0];
for i =1:3
    Kx(1) = Kx(1)+K1(i)*x(i);
    Kx(2) = Kx(2)+K2(i)*x(i);
end
Tb = interpln([Kx;T],1);

//At Tb K, from Fig. 13.6 of Chemical Engineer's Handbook
Kb = [2.12 0.85 0.37]

//Calculation of vapour composition
```

```
y1 = Kb(1)*x(1)*100;
y2 = Kb(2)*x(2)*100;
y3 = Kb(3)*x(3)*100;

mprintf('(a).');
mprintf('\n The bubble point temperature is %f K',Tb);
mprintf('\n At bubble point vapour contains %f percent propane, %f percent butane and %f percent pentane',y1,y2,y3);

//(b). The dew point temperature and composition of the liquid
T = [377.6 388.8]; //assumed temperatures (K)
y = [0.25 0.40 0.35]; //vapour composition at dew point
K1 = [2.6 1.1 0.5]; //at 377.6 K
K2 = [2.9 1.3 0.61]; //at 388.8 K

//At dew point, sum(yi/Ki) = 1
Ky = [0 0];
for i = 1:3
    Ky(1) = Ky(1) + y(i)/K1(i);
    Ky(2) = Ky(2) + y(i)/K2(i);
end
Td = interpln([Ky;T],1);

//At Td K,
Kd = [2.85 1.25 0.59];

//Calculation of liquid composition
x1 = y(1)*100/Kd(1);
x2 = y(2)*100/Kd(2);
x3 = y(3)*100/Kd(3);

mprintf('\n\n (b).');
mprintf('\n The dew point temperature is %f K',Td);
mprintf('\n Liquid at dew point contains %f percent
```

```
propane, %f percent butane and %f percent pentane',x1,x2,x3);

//(c). Temperature and composition when 45% of initial mixture is vaporised
//Basis:
F = 100; V = 45; L = 55;

//For the given condition eq. 8.91 (Page no. 364) is to be satisfied
//sum(zi/(1+ L/(VKi))) = 0.45

z = [0.25 0.4 0.35];
T = [366.5 377.6]; //assumed temperatures
K1 = [2.3 0.9 0.4]; //at 366.5 K
K2 = [2.6 1.1 0.5]; //at 377.6 K

Kz = [0 0];
for i =1:3
    Kz(1) = Kz(1) + z(i)/(1 + L/(V*K1(i)));
    Kz(2) = Kz(2) + z(i)/(1 + L/(V*K2(i)));
end

//The required temperature is T3
T3 = interpln([Kz;T],0.45);

//At T3 K
K3 = [2.5 1.08 0.48];

//Calculating liquid and vapour compositions
for i = 1:3
    y(i) = (z(i)/(1 + L/(V*K3(i))))/0.45;
    x(i) = ((F*z(i)) - (V*y(i)))/L;
    disp(x(i));
end

mprintf('\n\n (c).');
mprintf('\n The equilibrium temperature is %f K',T3)
```

```
;
mprintf('\n Liquid composition in equilibrium is %f percent propane, %f percent butane and %f percent pentane',x(1)*100,x(2)*100,x(3)*100);
mprintf('\n Vapour composition in equilibrium is %f percent propane, %f percent butane and %f percent pentane',y(1)*100,y(2)*100,y(3)*100);

//end
```

---

**Scilab code Exa 8.23** To test whetherthe given data are thermodynamically consistent or not

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 23


clear all;
clc;


//Given:
P = 101.3; //total pressure (kPa)
x1 = [0.003 0.449 0.700 0.900];
y1 = [0.432 0.449 0.520 0.719];
P1 = [65.31 63.98 66.64 81.31]; //(kPa)
P2 = [68.64 68.64 69.31 72.24]; //(kPa)

//To test whether the given data are thermodynamically consistent or not
x2 = 1-x1;
y2 = 1-y1;
for i = 1:4
```

```
    g1(i) = (y1(i)*P)/(x1(i)*P1(i));
    g2(i) = (y2(i)*P)/(x2(i)*P2(i));
    c(i) = log(g1(i)/g2(i)); //k = ln (g1/g2)
end

clf
plot(x1,c)
a = get("current_axes");
set(a,"x_location","origin");

//As seen from the graph net area is not zero
mprintf('The given experimental data do not satisfy
   the Redlich-Kistern criterion');

//end
```

**Scilab code Exa 8.24** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 24


clear all;
clc;



//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 8.25** To estimate the constants in Margules equation

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 25


clear all;
clc;


//Given:
x1 = [0.0331 0.9652]; //composition of chloroform
P = [40.84 84.88]; //total pressure for system (kPa)
P1 = 82.35; //vapour pressure of chloroform at 328 K (kPa)
P2 = 37.30; //vapour pressure of acetone at 328 K (kPa)

//To estimate the constants in Margules equation
//Using eq. 8.103 and 8.104 (Page no. 375)
g1_inf = (P(1)-(1-x1(1))*P2)/(x1(1)*P1);
g2_inf = (P(2)-(x1(2)*P1))/((1-x1(2))*P2);

//Margules equation:
//ln_g1 = x2^2*[A + 2*(B-A)*x1]
//ln_g2 = x1^2*[B + 2*(A-B)*x2]
//A = ln_g1_inf when x1 tends to 0, same for B

A = log(g1_inf);
B = log(g2_inf);

mprintf('Margules constants are:');
```

```
mprintf('\n A = %f',A);
mprintf('\n B = %f',B);

//end
```

---

**Scilab code Exa 8.26** To calculate the partial pressure of water in vapour phase

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 26


clear all;
clc;


//Given:
//At 333 K
x1 = [0 0.033 0.117 0.318 0.554 0.736 1.000]; //
   liquid composition of acetone
pp1 = [0 25.33 59.05 78.37 89.58 94.77 114.63]; //
   partial pressure of acetone (kPa)
Pw = 19.91; //vapour pressure of water at 333 K (kPa
   )

//To calculate the partial pressure of water in
   vapour phase

//Using eq. 8.100 (Page no. 372) [Gibbs-Duhem
   Equation] and rearranging

//dp2/p2 = -x1/(1-x1)*intg(dp1/p1)

```

```
//ln p2/Pw = -x1/(1-x1)*intg(dp1/p1)
//Let k = x1/((1-x1)*p1)
for i = 2:6
    k(i) = x1(i)/((1-x1(i))*pp1(i));
end
k(1) = 0; k(7) = 0.1; //k(7) should tend to infinity

clf
plot(pp1,k)

//From graph, area gives the integration and hence partiaal pressure of water is calculated
pp2 = [19.91 19.31 18.27 16.99 15.42 13.90 0];

mprintf("The results are:");
mprintf('\n  Acetone composition       Partial pressure of water');
for i = 1:7
    mprintf('\n       %f                          %f', x1(i),pp2(i));
end

//end
```

**Scilab code Exa 8.27** to calculate under three phase equilibrium

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 27


clear all;
clc;

```

```

//Given:
P = 93.30; //total pressure in kPa
T1 = 353; //(K)
T2 = 373; //(K)
Pa1 = 47.98; //Vapour pressure of water at 353 K (kPa)
Pb1 = 2.67; //Vapour pressure of liquid at 353 K (kPa)
Pa2 = 101.3; //Vapour pressure of water at 373 K (kPa)
Pb2 = 5.33; //Vapour pressure of liquid at 373 K (kPa)

//To calculate under three phase equilibrium:
//(a). The equilibrium temperature
P1 = Pa1+Pb1; //sum of vapour pressures at 353 K
P2 = Pa2+Pb2; //at 373 K

//Since vapour pressure vary linearly with temperature, so T at which P = 93.30 kPa
T = T1 + ((T2-T1)/(P2-P1))*(P-P1);
mprintf('(a). The equilibrium temperature is %f K',T);

//(b). The composition of resulting vapour
//At equilibrium temp:
Pa = 88.5; //vapour pressure of water (kPa)
Pb = 4.80; //vapour pressure of liquid (kPa)

//At 3-phase equilibrium, ratio of mol fractions of components is same as the ratio of vapour pressures
P = Pa+Pb; //sum of vapour pressures
y = Pa/P; //mole fraction of water
mprintf('\n The vapour contains %f mol percent water vapour',y*100);

```

```
//end
```

---

**Scilab code Exa 8.28** To prepare temperature composition diagram

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 30


clear all;
clc;


//Given:
T = [323 333 343 348 353 363 373]; //temperatures (K)
P2 = [12.40 19.86 31.06 37.99 47.32 70.11 101.3]; //vapour pressure for benzene (kPa)
P1 = [35.85 51.85 72.91 85.31 100.50 135.42 179.14]; //vapour pressure for water (kPa)
Tb = 353.1; //boiling temperature (K)
Pb = 101.3; //boiling pressure (kPa)

//To prepare temperature composition diagram

//To find three phase temperature
clf
for i =1:7
    P(i) = P1(i) + P2(i);
end
plot(P,T);
//From graph, at P = 101.3 kPa..
T_ = 340; //three phase temperature

```

```
//At three phase temperature
P1_ = 71.18; //(kPa)
P2_ = 30.12; //(kPa)
xb_ = P1_/Pb; //mol fraction of benzene at triple point

//For the dew point curve
//For curve BE in temp range from 342 to 373 K
for i = 3:7
    y1(i) = 1-(P2(i)/Pb);
end

clf
xset('window',1);
T1(1) = 342; y1_(1) = 0.7;
for i= 2:6
    T1(i) = T(i+1);
    y1_(i) = y1(i+1);
end
plot(y1_,T1);

//For the curve Ae in the temp range of 342 K to 353.1 K
for i = 3:5
    y2(i) = P1(i)/Pb;
end

T2(1) = 342; y2_(1) = 0.7;
for i = 2:4
    T2(i) = T(i+1);
    y2_(i) = y2(i+1);
end
plot(y2_,T2);
xrect(0,342,1,342);
xtitle(”Temperature Composition diagram”,”xa,ya”,”Temperature”);

//end
```

# Chapter 9

# Chemical Reaction Equilibria

**Scilab code Exa 9.1** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 1


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 9.2** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 2


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 9.3** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 3


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 9.4** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 4


clear all;
clc;


//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

**Scilab code Exa 9.5** Theoretical problem

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 5


clear all;
clc;


```

```
//Given:

//The given example is theoretical and does not
   involve any numerical computation

//end
```

---

**Scilab code Exa 9.6** To calculate equilibrium constant

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 6


clear all;
clc;


//Given:
Go_reac = 97540; //standard free energy of formation
    of reactant (J/mol)
Go_pdt = 51310; //standard free energy of formation
   of product (J/mol)
R = 8.314; //ideal gas constant
T = 298; //temperature (K)
//Reaction: N2O4(g) —> 2NO2(g)

//To calculate equilibrium constant
//Using eq. 9.50 (Page no.413)
Go = 2*Go_pdt - Go_reac;

//Using eq. 9.31 (Page no. 406)
K = %e^(-Go/(R*T));
mprintf('The equilbrium constant %f',K);
```

```

//end
```

---

**Scilab code Exa 9.7** To calculate equilibrium constant at 500 K

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 6


clear all;
clc;


//Given:
T1 = 298; //temperature in K
Hf = -46100; //standard heat of formation (J/mol)
Go = -16500; //standard free energy change (J/mol)
R = 8.314; //ideal gas constant
T = 500;
//Reaction: N2(g) + 3H2(g) --> 2NH3(g)

//To calculate the equilibrium constant at 500 K
//Using eq. 9.50 (Page no. 413)
del_Go = 2*Go;

//Using eq. 9.31 (Page no. 406)
K1 = %e^(-del_Go/(R*T1)); //equilibrium const at 298
    K
Ho = 2*Hf; //standard heat of reaction

//Using eq. 9.37 (Page no. 411)
K = K1*(%e^((-Ho/R)*(1/T - 1/T1)));
mprintf('The equilibrium constant at 500 K is %f',K)
```

```
;

//end
```

---

**Scilab code Exa 9.8** To alculate standard free energy change and heat of formation

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 8


clear all;
clc;


//Given:
R = 8.314; //ideal gas constant
T2 = 317; //temperature in K
T1 = 391; //(K)
x2 = 0.31; //mol fraction of n-butane at 317 K
x1 = 0.43; //mol fraction of iso-butane at 391 K

//To calculate standard free energy change and heat of reaction
//At 317 K
K2 = (1-x2)/x2; //equilibrium constant at 317 K
K1 = (1-x1)/x1; //equilibrium constant at 391 K

//Using eq. 9.31 (Page no. 406)
//Standard free energy change
G2 = -R*T2*log(K2); //at 317 K (J/mol)
G1 = -R*T1*log(K1); //at 391 K (J/mol)

```

```
//Using eq. 9.37 (Page no. 411)
Ho = -log(K2/K1)*R/(1/T2 - 1/T1);

mprintf('Standard free energy change of the reaction');
mprintf('\n At 317 K is %f J/mol',G2);
mprintf('\n At 391 K is %f J/mol',G1);
mprintf('\n Average value of heat of reaction is %f J/mol',Ho);

//end
```

**Scilab code Exa 9.9** To estimate free energy change and equilibrium constant at 700 K

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 9


clear all;
clc;


//Given:
//Reaction: N2(g) + 3H2(g) --> 2NH3(g)
To = 298; //temperature in K
T = 700; //(K)
R = 8.314; //ideal gas constant
Hf = -46100; //standard heat of formation (J/mol)
Gf = -16500; //standard free energy of formtion of ammonia (J/mol)

//Specific heat data
```

```
//Cp = 27.27 + 4.93*10^-3T (for N2)
//Cp = 27.01 + 3.51*10^-3T (for H2)
//Cp = 29.75 + 25.11*10^-3T (for NH3)

//To estimate free energy change and equilirium constant at 700 K
Ho = 2*Hf;
Go = 2*Gf;
alpha = 2*29.75 - 27.27 - 3*27.01;
betta = (2*25.11 - 4.93 - 3*3.51)*10^-3;

//Using eq. 9.46 (Page no. 412)
del_H = Ho - alpha*To - (betta/2)*To^2;
//Using eq. 9.48 (Page no. 413)
A = -(Go - del_H + alpha*To*log(To) + (betta/2)*To^2)/(R*To);

//Using eq. 9.47 and 9.48 (Page no. 412)
K = %e^((-del_H/(R*T)) + (alpha/R)*log(T) + (betta/(2*R))*T + A);
G = del_H - alpha*T*log(T) -(betta/2)*T^2 - A*R*T;

mprintf('At 700 K');
mprintf('\n Equilibrium constant is %3.2e',K);
mprintf('\n Standard free energy change is %f J/mol',G);

//end
```

---

**Scilab code Exa 9.10** to calculate equilibrium constant at 600 K

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 10
```

```


clear all;
clc;


//Given:
//Reaction: CO(g) + 2H2(g) --> CH3OH(g)
T = 600; //temperature in K
R = 8.314; //ideal gas constant

//Gibbs free energy at 600 K (J/mol K)
Gc = -203.81; //for CO
Gh = -136.39; //for hydrogen
Gm = -249.83; //for methanol

//Heats of formation at 298 K (J/mol)
Hc = -110500; //for CO
Hm = -200700; //for methanol

//To calculate equilibrium constant at 600 K
Go = T*((Gm-Gc-(2*Gh)) + (1/T)*(Hm-Hc));
//Using eq. 9.31 (Page no. 406)
K = %e^(-Go/(R*T));
mprintf('Equilibrium constant is %4.3e',K);

//end
```

**Scilab code Exa 9.11** To calculate equilibrium constant at 500K

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 11

```

```

clear all;
clc;


//Given:
//Reaction: N2(g) + 3H2(g) --> 2NH3(g)
T = 500; //temperature in K
R = 8.314; //ideal gas constant

//Free energy at 500 K (J/mol K)
Fn = -177.5; //for nitrogen
Fh = -116.9; //for hydrogen
Fa = -176.9; //for ammonia

//The function (Ho at 298 K - Ho at 0 K) [J/mol]
Hn = 8669; //for nitrogen
Hh = 8468; //for hydrogen
Ha = 9920; //for methanol

//Free energy of formation at 298 K (J/mol)
Hf = -46100;

//To calculate equilibrium constant at 500 K
//Using eq. 9.53 (Page no. 414)
sum_F = (2*Fa - Fn - 3*Fh) - (2*Ha - Hn - 3*Hh)/T; //(J/mol K)
//Using eq. 9.57 (Page no.415)
Go = T*(sum_F + 2*Hf/T);
K = %e^(-Go/(R*T));

mprintf('Equilibrium constant is %f',K);

//end
```

**Scilab code Exa 9.12** To find the value of n

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 12


clear all;
clc;


//Given:
//M polymerises to Mn, n>1
P1 = 1; //pressure (bar)
P2 = 2; //(bar)
x1 = 0.15; //mol fraction of polymer at 1 bar
x2 = 0.367; //mol fraction of polymer at 2 bar

//To find the value of n

//(a)
//The given subpart is theoreical and does not
   involve any numerical computation

//(b)
//K1 = x1/(1-x1)^n = K*P1^n-1
//K2 = x2/(1-x2)^n = K*P2^n-1
//Dividing the above equations and taking log on
   both sides
//(n-1)log 2 = log(x2/x1)+nlog(1-x1/1-x2)

n = round((log(x2/x1)+log(2))/(log(2)-log((1-x1)/(1-
   x2))));
mprintf('The value of n is %i',n);

//end
```

**Scilab code Exa 9.13** To determine the percent conversion

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 13


clear all;
clc;


//Given:
//Reaction: N2 + 3H2 --> 2NH3
K = 2*10^-4; //equilibrium constant of reaction

//To determine the percent conversion:

//Basis:
//1 mole nitrogen and 3 moles of hydrogen in the reactant mixture
//Let e be the extent of reaction
//Using eq. 9.3 (Page no. 400)
//mol fraction of nitrogen is (1-e)/(4-2e)
//mol fraction of hydrogen is (3-3e)/(4-2e)
//mol fraction of ammonia is 2e/(4-2e)
//so, ([2e/(4-2e)]^2)/[(1-e)/(4-2e)][3(1-e)/(4-2e)]^3 = K*P^2

//(a)
P = 20; //(bar)
//e(4-2e)/(1-e)^2 = 0.73485
e = poly(0,'e');
f = 2.73845*e^2 - 5.4697*e + 0.73485;
```

```
x = roots(f);
mprintf('(a) Percentage conversion is %f percent',x
   (2)*100);


//(b)
P = 200; //(bar)
//e(4-2e)/(1-e)^2 = 7.3485
e = poly(0,'e');
f = 9.3485*e^2 - 18.697*e + 7.3485;
x = roots(f);
mprintf('\n\n (b) Percentage conversion is %f
   percent',x(2)*100);

//end
```

---

**Scilab code Exa 9.14** To calculate fractional dissociation of steam

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 14


clear all;
clc;


//Given:
//Reaction: CO(g) + H2O(g) --> CO2(g) + H2(g)
K = 1; //equilibrium constant for reaction

//Mole fraction of components:
//CO: (1-e)/2
//H2O: (1-e)/2
```

```
//CO2: e/2
//H2: e/2

//To calculate fractional dissociation of steam

//(a).
//(e/2)(e/2)/[(1-e)/2][(1-e)/2] = K
//Solving we get:
e = 1/2;
mprintf('(a) Fractional dissociation of steam is %i percent',e*100);

//(b). If reactant stream is diluted with 2 mol nitrogen
//Mole fraction of components
//CO: (1-e)/4
//H20: (1-e)/4
//CO2: e/4
//H2: e/4

//so, K = (e/4)(e/4)/[(1-e)/4][(1-e)/4]
//On solving we get
e = 1/2;
mprintf('\n\n (b) After dilution fractional distillation of steam is %i percent',e*100);

//end
```

---

**Scilab code Exa 9.15** To determine conversion of nitrogen affected by argon

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 15
```

```


clear all;
clc;


//Given:
//Reaction: N2 + 3H2 --> 2NH3
K = 2*10^-4; //equilibrium constant of reaction
P = 20; //pressure in bar

//To determine conversion of nitrogen affected by
   argon

//Mole fraction of components
//Nitrogen: (1-e)/(6-2e)
//Hydrogen: 3(1-e)/(6-2e)
//Ammonia: 2e/(6-2e)

//[2e/(6-2e)]^2/[(1 - e)/(6-2e)][3(1 - e)/(6-2e)]^3 = K*
   P^2
//e(3-e)/(1-e)^2 = 0.3674

e = poly(0,'e');
f = 1.3674*e^2 - 3.7348*e + 0.3674;
x = roots(f);
mprintf('Percentage coversion in presence of argon
   is %f percent',x(2)*100);
mprintf('\n while in absence of argon is 14.48
   percent'); //From example 9.13

//end
```

**Scilab code Exa 9.16** To calculate the fractional dissociation of steam

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 16


clear all;
clc;


//Given:
//Reaction: CO(g) + H2O(g) --> CO2(g) + H2(g)
P = 1; //pressure in bar
K = 1; //equilibrium constant of reaction

//To calculate the fractional dissociation of steam
//Basis: 1 mole water vapour present in reactant
   stream
//Let e be the extent of reaction

//(a). CO supplied is 100% in excess of the
   stoichiometric requirement
//Mole fraction of components:
//CO: (2-e)/3
//H20: (1-e)/3
//CO2: e/3
//H2: e/3

//e^2/{(1-e)(2-e)] = K = 1, so
//3e-2 = 0;
e = 2/3;
mprintf('(a). The conversion of steam is %f percent'
   ,e*100);

//(b). CO supplied is only 50% of the theoretical
   requirement
//Mole fraction of components
//CO: (0.5-e)/1.5
```

```
//H20: (1-e)/1.5
//CO2: e/1.5
//H2: e/1.5

//e^2/[(0.5-e)(1-e)] = K = 1
//1.5e-0.5 = 1
e = 0.5/1.5;
mprintf('\n\n (b). Percentage conversion of steam is %f percent',e*100);

//end
```

---

**Scilab code Exa 9.17** To calculate the fractional distillation of steam

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 17


clear all;
clc;


//Given:
//Reaction: CO(g) + H2O(g) --> CO2(g) + H2(g)
//Mixture contains 1 mol CO, 1 mol H20 and 1 mol CO2 initially
K = 1; //equilibrium constant of reaction

//To calculate the fractional distillation of steam

//Mole fraction of components at equilibrium
//CO: (1-e)/3
//H2O: (1-e)/3
```

```
//CO2: (1+e)/3
//H2: e/3

//[e(1+e)]/[(1-e)^2] = K = 1
//3e-1 = 0
e = 1/3;
mprintf('Percentage conversion of steam is %f percent',e*100);

//end
```

---

**Scilab code Exa 9.18** To evaluate the percent conversion of CO

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 18


clear all;
clc;


//Given:
//Reaction: CO(g) + 2H2(g) --> CH3OH(g)
Kf = 4.9*10^-5;
Kfi = 0.35;
P = 300; //pressure in bar

//To evaluate the percent conversion of CO
//Basis: 100 moles of initial gas mixture
n_CO = 25;
n_H2 = 55;
n_inert = 20;
v = -1-2+1; //change in number of moles in reaction
```

```

//Mole fractions in the equilibrium mixture
//CO = (25-e)/(100-2e)
//H2 = (55-2e)/(100-2e)
//CH3OH = e/(100-2e)

Ky = (Kf/Kfi)*P^(-v);
//[e/(100-2e)]/[(25-e)/(100-2e)][(55-2e)/(100-2e)]^2 = Ky, so

e = poly(0,'e');
f = (4+4*Ky)*e^3 - (400+320*Ky)*e^2 + (10000+8525*Ky)*e - 75625*Ky
x = roots(f);

conv = x(3)/n_CO; //first two roots are complex
mprintf('Percentage conversion of CO is %f percent',conv*100);

//end
```

**Scilab code Exa 9.19** To determine the composition of gases leaving the reactor

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 19


clear all;
clc;


//Given:
```

```
//Reaction: 1/2N2 + 3/2H2 --> NH3
Kp = 1.25*10^-2 ;//equilibrium constant
P = 50; //pressure in bar
v = 1-(3/2)-(1/2); //change in number of moles in reaction

//Initial composition of gas mixture
n_h = 60;
n_n = 20;
n_inert = 100-n_h-n_n;

//To determine the composition of gases leaving the reactor
//Mole fractions in the equilibrium mixture
//N2: [20-(e/2)]/(100-e)
//H2: [60-(3e/2)]/(100-e)
//NH3: e/(100-e)

Ky = Kp*(P^-v);
//e/(100-e)/[(20-(e/2)]^1/2[{60-(3e/2)}/(100-e)]^3/2 = Ky

e = poly(0,'e');
f = (1.6875*Ky^2-1)*e^4 - (270*Ky^2+200)*e^3 + (16200*Ky^2-10000)*e^2 - (334800*Ky^2)*e + 4320000*Ky^2;
x = roots(f);
e = x(4);

//x(4) being the only positive root is the percentage conversion
//Mole fractions in equilibrium mixture
x_n = (20-(e/2))/(100-e);
x_h = (60-3*(e/2))/(100-e);
x_a = e/(100-e);
x_inert = 1 - x_n - x_h - x_a;

mprintf('Composition of gas leaving the reactor is')
```

```
;
mprintf('\n Nitrogen  : %f percent',x_n*100);
mprintf('\n Hydrogen  : %f percent',x_h*100);
mprintf('\n Ammonia   : %f percent',x_a*100);
mprintf('\n Inert gas : %f percent',x_inert*100);

//end
```

---

**Scilab code Exa 9.20** To evaluate the equilibrium constant

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 20


clear all;
clc;


//Given:
//Reaction: C2H4(g) + H2O(l) --> C2H5OH(aq)
P = 85; //pressure in bar
n_e = 0.015; //mol percent of ethanol
n_w = 0.95; //mole percent of water
n_a = 0.48; //mol percent of ethylene in vapour phase
M = 18; //molecular mass of water
fc = 0.9; //fugacity coeffecient for ethylene

//To evaluate the equilibrium constant
//K = a_c/(a_a*a_b)

m_e = n_e/(n_w*M*10^-3); //mol/kg water
a_c = m_e;
```

```
fa = fc*n_a*P; //bar
a_a = fa;

//Since mol fraction of water is close to unity, so fugacity coeffecient of water is assumed to be 1
a_b = n_w;
K = a_c/(a_a*a_b);
mprintf('The equilibrium constant is %5.4e (mol C2H4)/(kg water bar)',K);

//end
```

---

**Scilab code Exa 9.21** To calculate the decomposition pressure and temperature at 1 bar

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 21


clear all;
clc;


//Given:
//Reaction: CaCO3(s) --> CaO(s) + CO2(g)
T = 1000; //temperature of reaction in K
P = 1; //pressure in bar
R = 8.314; //ideal gas constant

//Function for standard free energy of the reaction
function [y] = G(T)
    y = 1.8856*10^5 - 243.42*T + 11.8478*T*log(T) - 3.1045*10^-3*T^2 + 1.7271*10^-6*T^3 -
```

```
    (4.1784*10^5)/T
endfunction

//To calculate the decomposition pressure and temperaure at 1 bar
Go = G(T);
K = %e^(-Go/(R*T));
//Using eq. 9.75 (Page no. 432)
p_CO2 = K; //decomposition pressure
mprintf('Decomposition pressure of limestone at 1000 K s %f bar',p_CO2);

//At pressure = 1 bar
K = 1;
Go = 0; //since K = 1

T = 1160; //assumed temperature (K)
flag = 1;
while(flag==1)
    res = round(G(T));
    if(res<=0)
        flag = 0;
    else
        T = T+1;
    end
end
mprintf('\nDecomposition temperature at 1 bar is %i K',T);

//end
```

---

**Scilab code Exa 9.22** To evaluate wt of iron produced per 100 cubic m of gas admitted

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 22


clear all;
clc;


//Given:
//Reaction: FeO(s) + CO(g) --> Fe(s) + CO2(g)
K = 0.403; //equilibrium constant of reaction
T = 1200; //temperature of reaction (K)
To = 273; //standard temperature (K)
Vo = 22.4*10^-3; //molar volume at STP
M = 55.8; //molecular mass of iron

//To calculate wt of iron produced per 100 m^3 of gas admitted
//Basis: 100 mol of gas entering
n = 100; //moles of gas entering
n_C = 20; //moles of carbon mono oxide
n_N = 80; //moles of nitrogen

//Let e be the extent of reaction
//Mole fractions in equilibrium mixture
//CO = (20-e)/100
//CO2 = e/100
//e/(20-e) = K
e = (20*K)/(1+K);
n_CO2 = e; //moles of CO2 at equilibrium
n_Fe = n_CO2; //by stoichiometry
V = (n*Vo*T)/To; //volume of 100 mol of gas at 1200 K and 1 bar

//Let m be iron produced per 100 m^3 gas
m = (n_Fe*100*M)/V;
```

```
mprintf('Iron produced per 100 cubic m of gas is %f kg',m/1000);

//end
```

---

**Scilab code Exa 9.23** To calculate the composition at equilibrium assuming ideal behaviour

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 23


clear all;
clc;


//Given:
P = 1; //pressure in bar
K1 = 0.574; //equilibrium constant for eq. 9.88 (Page no. 437)
K2 = 2.21; //equilibrium constant for eq. 9.89 (Page no. 437)

//To calculate the composition at equilibrium assuming ideal behaviour
//Let e1 and e2 be the extent of first and second reactions

v1 = 1+3-1-1;
v2 = 1+1-1-1;
Ky1 = K1*P^-v1;
Ky2 = K2*P^-v2;

```

```
//mole fractions in equilibrium mixture are:
//CH4: (1-e1)/(6+2e1)
//H2O: (5-e1-e2)/(6+2e1)
//CO: (e1-e2)/(6+2e1)
//H2: (3e1+e2)/(6+2e1)
//CO2: e2/(6+2e1)

//For 1st reaction:
//Ky1 = [(e1-e2)(3e1+e2)^3]/[(1 - e1)(5-e1-e2)(6+2e1)^2]
//For 2nd reaction:
//Ky2 = [e2(3e1+e2)]/[(e1-e2)(5-e1-e2)]
//on solving, we get:
deff('[y] = f2(e)',['f_1 = [(e(1)-e(2))*(3*e(1)+e(2))^3]/[(1 - e(1))*(5-e(1)-e(2))*(6+2*e(1))^2]-Ky1','f_2 = [e(2)*(3*e(1)+e(2))]/[(e(1)-e(2))*(5-e(1)-e(2))]-Ky2','y = [f_1;f_2]'])
eo = [0.9 0.6]; //initial guesses
[e,fes,m] = fsolve(eo',f2);

//Mole fraction of components:
n_m = (1-e(1))/(6+2*e(1));
n_w = (5-e(1)-e(2))/(6+2*e(1));
n_CO = (e(1)-e(2))/(6+2*e(1));
n_h = (3*e(1)+e(2))/(6+2*e(1));
n_c = e(2)/(6+2*e(1));

mprintf('Mole fraction of the components are:');
mprintf('\n Methane = %f',n_m);
mprintf('\n Water = %f',n_w);
mprintf('\n Carbon monoxide = %f', n_CO);
mprintf('\n Hydrogen = %f',n_h);
mprintf('\n Carbon dioxide = %f',n_c);

//end
```

**Scilab code Exa 9.24** To determine the number of degrees of freedom

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 24


clear all;
clc;


//Given:
//A system consisting of CO, CO2, H2, H2O, CH4

//To determine the number of degrees of freedom

//Formation reactions for each of compounds is
    written
//a. C + 1/2O2 --> CO
//b. C + O2 --> CO2
//c. H2 + 1/2O2 --> H2O
//d. C + 2H2 --> CH4

//Elements C and O2 are not present, so they are to
    be eliminated
//Combining a and b
//e. CO2 --> CO + 1/2O2

//Combining a and d
//f. CH4 + 1/2O2 --> CO + 2H2

//Combining c and e
//g. CO2 + H2 --> CO + H2O
```

```

//Combining c and f
//h. 3H2 + CO --> CH4 + H2O

//Equations g and h represent independent chemical
   reactions, so
r = 2;
C = 5; //no. of components
pi = 1; //no. of phases

//From eq. 9.90 (Page no. 438)
F = C-pi-r+2;
mprintf('The number of degrees of freedom are %i',F)
   ;

//end
```