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

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

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

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

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

Contents

List of Scilab Codes

Chapter 1

Introduction 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;
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;
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;
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;
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 i

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

clear;
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;
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;
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;
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;
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;
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`

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

```
//Chapter 2
//First Law of Thermodynamics
//Example 4


clear;
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;
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 energ`

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


clear;
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 c`

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


clear;
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;
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;
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;
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;
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

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


clear;
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;
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;
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;
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;
```

```
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`

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


clear;
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;
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;
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;
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;
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;
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;
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;
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;
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;
```

```
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;
```

```
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;
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 sur`

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


clear;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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`

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


clear;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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
//SO, 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;
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 p`

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


clear;
```

```
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;
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;
```

```
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;
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;
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;
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;
clc;


//Given:
T1= 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;
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`

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


clear;
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;
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;
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;
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;
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 temperatu`

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


clear;
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;
```

```
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 efficienc`

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


clear;
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 s`

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


clear;
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 efficien

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


clear;
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;
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`

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


clear;
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;
gama = Cp/Cv
//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;
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;
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;
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;
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;
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;
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;
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 f`

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


clear;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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 give`

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


clear;
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;
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
```

```
R = 8.314;
//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;
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;
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;
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 dil

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


clear;
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;
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 dil`

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


clear;
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;
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;
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;
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;
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 determ

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


clear;
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;
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 constan

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


clear;
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;
```

```
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;
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;
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;
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;
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;
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;
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;
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 solutio`

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


clear;
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;
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;
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;
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;
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;
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;
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;
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;
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 p`

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


clear;
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;
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;
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;
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;
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 1`

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


clear;
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 cont`

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

```

```

clear;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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 consisten`

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 8
//Phase Equilibria
//Example 23


clear;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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;
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`

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


clear;
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;
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;
```

```
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;
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;
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;
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;
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;
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;
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;
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;
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;
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`

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 21


clear;
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 admitt`

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
```

```
//Example 22


clear;
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 be`

```
//A Textbook of Chemical Engineering Thermodynamics
//Chapter 9
//Chemical Reaction Equilibria
//Example 23


clear;
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;
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
```