Scilab Textbook Companion for Stoichiometry And Process Calculations by K. V. Narayanan And B. Lakshmikutty[1]

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Book Description

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

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

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

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

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Chapter 2

Units and Dimensions

Scilab code Exa 2.1 Mass flow rate

```
clc()
funcprot(0)
V1 = 15;//ft^3/min
ft = 0.3048;//m
min = 60;//secs
V = V1*ft^3/min;
disp("m^3/s",V,"Volumetric flowrate = ")
D = 1000;//kg/m^3
M = V * D;
disp("kg/s",M,"mass flowrate = ")
```

Scilab code Exa 2.2 Poundal to Newton

```
clc()
funcprot(0)
ft = 0.3048;//m
lb = 0.4536;//kg
P = ft*lb;
disp("N",P,"1 poundal is 1 ft*lb/s^2 = ")
```

Scilab code Exa 2.3 Conversion of N per m2

```
clc()
funcprot(0)
kgf = 9.80665;//N
cm = 10^-2;//m
P = kgf/cm^2;
disp("N/m^2",P,"1 kgf/cm^2 = ")
lbf = 32.174;//lb*ft//s^2
lb = 0.4535924;//kg
ft = 0.3048;//m
in = 0.0254;//m
P1 = lbf*lb*ft/in^2;
disp("N/m^2",P1,"1 lbf/in^2 = ")
```

Scilab code Exa 2.4 Thermal conductivity

```
clc()
Q1 = 10000;//kJ/hr
kJ = 1000;//J
hr = 3600;//s
Q = Q1*kJ/hr;//J/s
disp("J/s",Q,"Q = ")
x = 0.1;//m
A = 1//m^2
T = 800;//K
k = x*Q/(A*T);
disp("W/(m*K)",k,"thermal conductivity = ")
J = 1/4.1868;//cal
k1 = k*J*hr/1000;
disp("kcal/(h*m*C)",k1,"thermal conductivity = ")
```

Scilab code Exa 2.5 Mass and FPS system

```
clc()
F = 300;//N
a = 9.81;//m/s^2
m = F/a;//kg
disp("kg",m,"mass in kg = ")
lb = 4.535924/10;//kg
m1 = m/lb;
disp("lb",m1,"mass in pounds = ")
```

Scilab code Exa 2.6 Kinetic energy calculation

```
clc()
z = 15;//m
PE = 2000;//J
g = 9.8067;//m/s^2
m = PE/(z*g);
disp("kg",m,"mass = ")
v = 50;//m/s
KE = 1/2*m*(v^2)/1000;
disp("kJ",KE,"kinetic energy = ")
```

Scilab code Exa 2.7 Force and pressure for piston cylinder

```
clc()
g = 9.81;//m/s^2
m = 100 * 0.4536;//kg
P = 101325;//N/m^2
```

```
D1 = 4;//inch
D = D1 * 2.54 * 10^-2;//m
A = 3.1415 * (D^2)/4;//m^2
F1 = P * A;//N
F2 = m * g;//N
F = F1 + F2;
disp("N",F,"Total force acting on the gas = ")
P1 = F / A;//N/m^2
P2 = P1/100000;//bar
P3 = P1/(6.894757 * 10^3);//psi
disp("N/m^2",P1,"Pressure in N/m^2 = ")
disp("bar",P2,"Pressure in bar = ")
disp("psi",P3,"Pressure in psi = ")
d = 0.4;//m
W = F * d;
disp("J",W,"Work done = ")
PE = m * g * d;
disp("J",PE,"Change in potential energy = ")
```

Scilab code Exa 2.8 units conversion

```
clc()
//kG = (6.7 * 10^-4) * (( G * (ds + dt) / ds)^0.8) /
    ((ds^0.4)*(dG^0.2))
//kG - lbmol/(h ft^2 atm), G - lb/(ft^2 h), ds, dG,
   dt - feet
//kG1 - kmol/(m^2 h atm), G1 - kg/(m^2 h), ds1, dG1,
    dt1 - m
G = 0.2048;//G1 * lb/(ft^2 h)
d = 3.2808;//d1 * ft
ds = d;
dt = d;
dG = d;
kG = 4.885;//kG1 (lbmol/(h ft^2 atm) = 4.885 * kmol
   /(m^2 h atm))
```

```
C = (6.7 * 10^-4) * (( G * d / ds)^0.8) / ((ds^0.4)*(dG^0.2))* kG;
disp(C,"Co-efficient = ")
// this is the constant for the equation
// the equation thus becomes,
// kG1 = C * (( G1 * (ds1 + dt1) / ds1)^0.8) / ((ds1^0.4)*(dG1^0.2))
```

Scilab code Exa 2.9 units conversion

```
clc()
//Cp = 7.13 + 0.577 * (10^-3) * t + 0.0248 * (10^-6) * t^2
//Cp - Btu/lb-mol F, t - F
//Cp1 - kJ/kmol K , t1 - K
a = 7.13;
b = 0.577 * 10^-3;
c = 0.0248 * 10^-6;
//t = 1.8 * t1 - 459.67
Cp = 4.1868;//Cp1 (Btu/lb-mol F = 4.1868 * (kJ/kmol K) )
//substituting the above, we get,
//Cp1 = 28.763 + 4.763 * (10^-3) * t1 + 0.3366 * (10^-6) * t^2
a1 = 28.763;
b1 = 4.763 * (10^-3);
c1 = 0.3366 * (10^-6);
disp(a1,"a1 = ")
disp(b1,"b1 = ")
disp(c1,"c1 = ")
// this are the co efficents for the following equation;
// Cp1 = a1 + b1 * t1 + c1 * (t1)^2
```

Chapter 3

Fundamental concepts of stoichiometry

Scilab code Exa 3.1 pounds per minute to kmol per hour

```
clc()
m = 1000 * 0.4536;//kg/min
M = 30.24;//gm/mol
m1 = m * 60 / M;
disp("kmol/hr",m1,"molar folw rate = ")
```

Scilab code Exa 3.2 Number of molecules

```
clc()
MK = 39.1;
MC = 12.0;
MO = 16;
MK2CO3 = MK * 2 + MC + MO * 3;
m = 691;
N = m / MK2CO3;
A = 6.023 * 10^23;
```

```
molecules = N * A;
disp("molecules",molecules,"Total no. of molecules =
   ")
```

Scilab code Exa 3.3 Moles of sodium sulphate

```
clc()
Na = 23;//gm/mol
MNa = 100;//kg
N = MNa * 1000 / Na ;//g-atoms
NNa2SO4 = N / 2;
disp("kmol",NNa2SO4,"(a) moles of sodium sulphate =
   ")
MNa2SO4 = 142.06;
m = NNa2SO4 * MNa2SO4/1000;
disp("kg",m,"(b)kilograms of sodium sulphate = ")
```

Scilab code Exa 3.4 Pyrites and oxygen moles

```
clc()
MFe = 55.85;
MO = 16;
MS = 32;
MFeS2 = MFe + MS * 2;
MFe2O3 = MFe * 2 + MO * 3;
MSO3 = MS + MO * 3;
m1SO3 = 100;//kg
N1 = m1SO3 / (MSO3);//kmol
NFeS2 = N1 / 2;
mFeS2 = NFeS2 * MFeS2;
disp("kg",mFeS2,"mass of pyrites to obtain 100kg of
   SO3 =")
m2SO3 = 50;//kg
```

```
N2 = m2SO3 / (MSO3);//kmol
NO2 = N2 * 15/8;
mO2 = NO2 * MO * 2;
disp("kg",mO2,"mass of Oxygen consumed to produce 50
   kg of SO3 =")
```

Scilab code Exa 3.5 Volume of oxygen

```
clc()
MKClO3 = 122.55
mKClO3 = 100;//kg
NKClO3 = mKClO3 / MKClO3;
NO2 = 3 * NKClO3 / 2;
V1 = 22.4143;//m^3/kmol;
V = V1 * NO2;
disp("m^3",V,"volume of oxygen produced = ")
```

Scilab code Exa 3.6 Reaction of iron and steel

```
clc()
mH2 = 100;//kg
NH2 = mH2/2.016;
NFe = 3 * NH2 / 4;
mFe = NFe * 55.85;
disp("kg",mFe,"(a)mass of iron required = ")
NH2O = NH2 ;
mH2O = NH2O * 18;
disp("kg",mH2O,"mass of steam required =")
V1 = 22.4143;//m^3/kmol;
V = V1 * NH2;
disp("m^3",V,"Volume of hydrogen = ")
```

Scilab code Exa 3.7 Equivalent weight

```
clc()
MCaCO3 = 100.08;
GE = MCaCO3 / 2;
disp("g",GE,"Gram equivalent wt. of CaCO3 =")
```

Scilab code Exa 3.8 Specific gravity calculation

```
clc()
m1 = 1;//kg (mass in air)
m2 = 0.9;//kg (mass in water)
m3 = 0.82;//kg (mass in liquid)
L1 = m2 - m1;//kg (loss of mass in water)
L2 = m3 - m1;//kg (loss of mass in liquid)
sp.g = L2 /L1;
disp(sp.g,"specific gravity of liquid = ")
```

Scilab code Exa 3.9 Specific gravity of mixture

```
clc()
m1 = 10;//kg
m2 = 5;//kg
sp.g1 = 1.17;
sp.g2 = 0.83;
Dwater = 1000;//kg/m^3
DA = Dwater * sp.g1;
DB = Dwater * sp.g2;
V1 = m1 / DA;
```

```
V2 = m2 / DB;
V = V1 + V2;
Dmix = (m1 + m2)/ V ;
sp.g3 = Dmix / Dwater;
disp(sp.g3,"specific gravity of mixture =")
```

Scilab code Exa 3.10 Baume scale

```
clc()
Tw = 100;//Tw
sp.g = Tw/200 + 1;
Be = 145 - 145/sp.g;
disp("Be",Be,"specific gravity on beume scale =")
```

Scilab code Exa 3.11 Density using API scale

```
clc()
API1 = 30;//API
sp.g1 = 141.5/(131.5 + API1);// (since, API = 141.5/sp.g -131.5)
Dwater = 999;//kg/m^3;
Doil1 = sp.g1 * Dwater;
V1 = 250;//m^3
m1 = V1 * Doil1;
API2 = 15;//API
sp.g2 = 141.5/(131.5 + API2);// (since, API = 141.5/sp.g -131.5)
Dwater = 999;//kg/m^3;
Doil2 = sp.g2 * Dwater;
V2 = 1000;//m^3
m2 = V2 * Doil2;
Dmix = (m1 + m2)/(V1 + V2);
disp("kg/m^3",Dmix,"density of the mixture =")
```

Scilab code Exa 3.12 Drying Ammonium sulphate

```
clc()
m1 = 250;//kg
mwater1 = 50;//kg
mdrysolid1 = m1 - mwater1;
wfe1 = mwater1 / m1;
wr1 = mwater1 / mdrysolid1;
wtpercentw1 = mwater1 * 100 / m1;
wtpercentd1 = mwater1 * 100 / mdrysolid1;
a = 90;//%
mwater2 = mwater1 * (1 - a/100);
m2 = mdrysolid1 + mwater2;
wfe2 = mwater2 / m2;
wr2 = mwater2 / mdrysolid1;
wtpercentw2 = mwater2 * 100 / m2;
wtpercentd2 = mwater2 * 100 / mdrysolid1;
disp(wfe1,"(a)weight fraction of water at entrance =
    ")
disp(wfe2,"weight fraction of water at exit = ")
disp(wr1,"(b)weight ratio of water at entrance = ")
disp(wr2,"weight ratio of water at exit = ")
disp(wtpercentw1,"(c)weight percent of moisture on
    wet basis at entrance = ")
disp(wtpercentw2,"weight percent of moisture on wet
    basis at exit = ")
disp(wtpercentd1,"(d)weight percent of moisture on
    dry basis at entrance = ")
disp(wtpercentd2,"weight percent of moisture on dry
    basis at exit = ")
```

Scilab code Exa 3.13 Percentage of water removed

```
clc()
mdrysolid = 100;//kg
percentin = 25;
mwaterin = mdrysolid * percentin / 100;
percentout = 2.5;
mwaterout = mdrysolid * percentout / 100;
mremoved = mwaterin - mwaterout;
percentremoved = mremoved *100 / mwaterin ;
disp(percentremoved,"percentage of water removed = "
    )
```

Scilab code Exa 3.14 Amount and percentage water removed

```
clc()
m = 1;//kg
percent1 = 20;//%
mwaterin = m * percent1 / 100;
mdrysolid = m - mwaterin;
percent2 = 2.44;//%
mout = mdrysolid / (1 - percent2/100);
mwaterout = mout - mdrysolid;
mremoved = mwaterin - mwaterout;
percentremoved = mremoved * 100 / mwaterin ;
disp("kg",mremoved,"weight of water removed = ")
disp("%",percentremoved,"percentage of water removed
     = ")
```

Scilab code Exa 3.15 NaCl solution

```
clc()
mwater = 100;//kg
mNaCl = 35.8;//kg
msolu = mwater + mNaCl;
```

```
mfr = mNaCl / msolu;
mpr = mfr * 100;
MNaCl = 58.45;//kg/kmol
NNaCl = mNaCl / MNaCl;
MH2O = 18;//kg/kmol
NH2O = mwater / MH2O;
Mfr = NNaCl / (NNaCl + NH2O);
Mpr = Mfr * 100;
N = NNaCl *1000 / mwater;
disp(mfr,"(a)mass fraction of NaCl =")
disp(mpr,"mass percent of NaCl= ")
disp(Mfr,"(b)mole fraction of NaCl =")
disp(Mpr,"mole percent of NaCl = ")
disp(N,"kmol NaCl per 1000 kg of water =")
```

Scilab code Exa 3.16 Molal absolute humidity

```
clc()
Y = 0.015;//kg water vapour/kg dry air
Mair = 29;//kg/kmol
Mwater = 18.016;//kg/kmol
Nwater = Y / Mwater;//kmol
Nair = 1 / Mair;//kmol
Mpr = Nwater *100 / (Nwater + Nair);
Mr = Nwater / Nair;
disp(Mpr,"(a)mole percent of water vapour = ")
disp("kmol water/kmol dry air",Mr,"(b) molal
    absolute humidity =")
```

Scilab code Exa 3.17 K2CO3 solution

```
clc()
msolu = 100;//g
```

```
MK2CO3 = 138.20;//g/mol
percent1 = 50;//%
mK2CO3 = percent1 *msolu / 100;
NK2CO3 = mK2CO3 / MK2CO3;
mwater = msolu - mK2CO3;
Nwater = mwater / 18.06;
Mpr = NK2CO3 * 100 / (NK2CO3 + Nwater);
sp.gr  =1.53;
Vsolu = msolu/sp.gr;//mL
Vwater = mwater / 1;//mL
Vpr = Vwater * 100/ Vsolu;
Molality = NK2CO3 / (mwater * 10^-3);
Molarity = NK2CO3 / (Vsolu * 10^-3);
Eq.wt = MK2CO3 / 2;
No = mK2CO3/Eq.wt;
N = No / (Vsolu * 10^-3);
disp("%",Mpr,"(a)Mole prcent of salt = ")
disp("%",Vpr,"(b)Volume percent of water = ")
disp("mol/kg",Molality,"(c)Molality = ")
disp("mol/L",Molarity,"(d)Molarity = ")
disp("N",N,"(e)Normality")
```

Scilab code Exa 3.18 Molarity and Molality of Alcohol solution

```
clc()
msolu = 100;//kg
percent1 = 60;//%
Dwater = 998;//kg/m^3
Dalco = 798;//kg/m^3
Dsolu = 895;//kg/m^3
Vsolu = msolu/Dsolu;
malco = msolu * percent1 / 100;
Valco = malco / Dalco;
Vpr = Valco * 100 / Vsolu;
Malco = 46.048;//kg/kmol
```

```
N = malco/Malco;
Molarity = N/(Vsolu );
mwater = msolu - malco;
Molality = N * 1000 /mwater;
disp("%",Vpr,"(a)Volume percent of ethanol in
   solution = ")
disp("mol/L",Molarity,"(b)Molarity = ")
disp("mol/(kg of water)",Molality,"(c)Molality = ")
```

Scilab code Exa 3.19 CO to phosgene

```
clc()
//CO + CL2 = COCl2
Np = 12;//moles
NCl2 = 3;//moles
NCO = 8;//moles
N1Cl2 = NCl2 + Np;
N1CO = NCO + Np;
pr.ex = (N1CO - N1Cl2)* 100/N1Cl2;
pr.co = (N1Cl2-NCl2) * 100/ N1Cl2;
T = Np + NCl2 + NCO;
T1 = N1Cl2 + N1CO;
N = T / T1;
disp("%",pr.ex,"(a)percent excess of CO = ")
disp("%",pr.co,"(b)percent conversion = ")
disp(N,"(c)Moles of total products per mole of total
    reactants = ")
```

Scilab code Exa 3.20 Extent of reaction

```
clc()
Nn2 = 2;//moles
Nh2 = 7;//moles
```

```
Nnh3 = 1;//mole
n0 = Nn2 + Nh2 + Nnh3;
v = 2 - 1- 3;
//YN2 = (2 - E)/(10 - 2*E)
//Yh2 = (7-3*E)/(10 - 2*E)
//Ynh3 = (1 + 2*E)/(10 - 2*E)
disp("mole fraction of N2 = (2 - E)/(10 - 2*E)")
disp("mole fraction of H2 = (7-3*E)/(10 - 2*E)")
disp("mole fraction of NH3 = (1 + 2*E)/(10 - 2*E)")
```

Scilab code Exa 3.21 ethylene to ethanol

```
clc()
msolu = 100;//g
MK2CO3 = 138.20;//g/mol
percent1 = 50;//%
mK2CO3 = percent1 *msolu / 100;
NK2CO3 = mK2CO3 / MK2CO3;
mwater = msolu - mK2CO3;
Nwater = mwater / 18.06;
Mpr = NK2CO3 * 100 / (NK2CO3 + Nwater);
sp.gr  =1.53;
Vsolu = msolu/sp.gr;//mL
Vwater = mwater / 1;//mL
Vpr = Vwater * 100/ Vsolu;
Molality = NK2CO3 / (mwater * 10^-3);
Molarity = NK2CO3 / (Vsolu * 10^-3);
Eq.wt = MK2CO3 / 2;
No = mK2CO3/Eq.wt;
N = No / (Vsolu * 10^-3);
disp("%",Mpr,"(a)Mole prcent of salt = ")
disp("%",Vpr,"(b)Volume percent of water = ")
disp("mol/kg",Molality,"(c)Molality = ")
disp("mol/L",Molarity,"(d)Molarity = ")
disp("N",N,"(e)Normality")
```

Chapter 4

Ideal Gases and Gas Mixtures

Scilab code Exa 4.1 gas constant R

```
clc()
P1 = 760; //mmHg
T1 = 273.15; //K
V1 = 22.4143 * 10^-3; //m^3/mol
R1 = P1 * V1 / T1;
disp("m^3 mmHg / (molK)",R1,"Gas constant R =")
P2 = 101325; //N/m^2
T2 = 273.15; //K
V2 = 22.4143 * 10^-3; //m^3/mol
R2 = P2 * V2 / T2; //J/molK
R3 = R2 / 4.184; //cal/molK
disp("cal/molK",R3,"Gas constant R in MKS system =")
```

Scilab code Exa 4.2 Molar volume of air

```
clc()
T = 350; //K
P = 1; //bar
```

```
V1 = 22.4143 * 10^-3;//m^3 (suffix 1 represents at
    STD)
P1 = 1.01325;//bar
T1 = 273.15;//K
V = P1 * V1 * T/(T1 * P);
disp("m^3/mol",V,"Molar volume =")
```

Scilab code Exa 4.3 Ideal gas equation

```
clc()
P = 10;//bar
T = 300;//K
V = 150;//L
P1 = 1.01325;//bar ( \suffix 1 represents at STD)
T1 = 273.15;//K
V2 = T1 * P * V /(T * P1);//m^3
V1 = 22.4143;//m^3/mol
N = V2 / V1;//mol
MO2 = 32;
m = N * MO2/1000;
disp("kg",m,"Mass of oxygen in the cylinder = ")
```

Scilab code Exa 4.4 Maximum allowable temperature of tyre

```
clc()
P = 195;//kPa
T = 273;//K
P1 = 250;//kPa
T1 = P1 * T / P;
disp("K",T1,"Maximum temperature to which tyre may
    be heated = ")
```

Scilab code Exa 4.5 Pressure calculation

```
clc()
V = 250;//L
T = 300;//K
V1 = 1000;//L
P1 = 100;//kPa
T1 = 310;//K
P = T * P1 * V1 /(T1 * V);
disp("kPa",P,"Original pressure in the cylinder = ")
```

Scilab code Exa 4.6 weight composition and density calculation

```
clc()
Vper1 = 70;//% ( 1 = HCl)
Vper2 = 20;//% ( 2 = Cl2)
Vper3 = 10;//% ( 3 = CCl4)
M1 = 36.45;
M2 = 70.90;
M3 = 153.8;
m1 = Vper1 * M1;
m2 = Vper2 * M2;
m3 = Vper3 * M3;
mper1 = m1 * 100/(m1+ m2 + m3);
mper2 = m2 * 100/(m1+ m2 + m3);
mper3 = m3 * 100/(m1+ m2 + m3);
disp(mper1," (a) weight percent of HCl= ")
disp(mper2,"weight percent of Cl2= ")
disp(mper3,"weight percent of CCl4= ")
m = (m1 + m2 + m3)/(Vper1 + Vper2 + Vper3);
disp("kg",m,"(b)average molecular weight = ")
v = 22.4143;//m^3/kmol
```

```
Vtotal = v * (Vper1 + Vper2 + Vper3);
D = (m1 + m2 + m3)/Vtotal;
disp("kg/m^3",D,"(c)Density at standard condiions =
  ")
```

Scilab code Exa 4.7 calculations for natural gas

```
clc()
per1 = 93;//% ( 1 = methane)
per2 = 4.5;//% (2 = ethane)
per3 = 100 - (per1 + per2);//% ( 3 = N2);
T = 300;//K
p = 400;//kPa
P3 = p * per3 / 100;
v = 10;//m^3
V2 = per2 * v / 100;
M1 = 16.032;
M2 = 30.048;
M3 = 28;
N1 = per1;
N2 = per2;
N3 = per3;
m1 = M1 * N1;
m2 = M2 * N2;
m3 = M3 * N3;
m = m1 + m2 + m3;
Vstp = 100 * 22.4143 * 10^-3;//m3 at STP
D = m /(1000 * Vstp);
Pstp = 101.325;//kPa
T1 = 273.15;//K
V = T * Pstp * Vstp / ( T1 * p);
D1 = m /(1000 * V);
Mavg = m /100;
mper1 = m1 * 100 / (m1 + m2 + m3);
mper2 = m2 * 100 / (m1 + m2 + m3);
```

```
mper3 = m3 * 100 / (m1 + m2 + m3);
disp("kPa",P3,"(a) Partial pressure of nitrogen = ")
disp("m^3",V2,"(b) pure-component volume of ethane = ")
disp("kg/m^3",D,"(c) Density at standard conditions = ")
disp("kg/m^3",D1,"(d) Density at given condition = ")
disp(Mavg,"(e) Average molecular weight = ")
disp("%",mper1,"(f) weight percent of Methane = ")
disp("%",mper2,"weight percent of Ethane = ")
disp("%",mper3,"weight percent of Nitrogen = ")
```

Scilab code Exa 4.8 Volume of gas from absorption columnn

```
clc()
per1 = 20;//% ( 1 = ammonia)
Vstp = 22.4143;//m^3/kmol
Pstp = 101.325;//kPa
Tstp = 273.15;//K
V1 = 100;//m^3
P1 = 120;//kPa
T1 = 300;//K
P2 = 100;//kPa
T2 = 280;//K
per2 = 90;//% (absorbed)
N = V1 * P1 * Tstp / (Vstp * Pstp * T1);//kmol
Nair = (1 - per1 / 100) * N;
N1 = per1 * N/100;
Nabs = per2 * N1 / 100;
N2 = N1 - Nabs;//leaving
Ntotal = Nair + N2;
Vstp1 = Ntotal * Vstp;//m^3
V2 = Vstp1 * Pstp * T2 / (Tstp * P2);
disp("m^3",V2,"Volume of gas leaving = " )
```

Scilab code Exa 4.9 dehumidification

```
clc()
V = 100;//m^3
Ptotal = 100;//kPa
Pwater = 4;//kPa
Pair = Ptotal - Pwater;
T = 300;//K
T1 = 275;//K
Vstp = 22.4143;//m^3/kmol
Tstp = 273.15;//K
Pstp = 101.325;//kPa
Pwater1 = 1.8;//kPa
Pair1 = Ptotal - Pwater1;
V1 = V * Pair * T1 / ( T * Pair1);
Nwater = V * Pwater * Tstp/ (Vstp * Pstp * T);
Nwater1 = V1 * Pwater1 * Tstp/ (Vstp * Pstp * T1);
m = (Nwater - Nwater1) * 18.02;
disp("m^3",V1,"(a) volume of air after
    dehumidification = ")
disp("kg",m,"(b) Mass of water vapour removed = ")
```

Scilab code Exa 4.10 Absorption column for H2S

```
clc()
V = 100;//m^3
P = 600;//kPa
T = 310;//K
per1 = 20;//% ( H2S entering )
per2 = 2;//% ( H2S leaving )
Pstp = 101.325;//kPa
```

```
Tstp = 273.15;//K
Vstp = 22.414;//m^3/kmol
Vstp1 = V * P * Tstp / ( T * Pstp)
N = Vstp1 / Vstp;
N1 = N * per1 / 100;
N2 = N - N1;// ( 2 = inerts)
Nleaving = N2 / ( 1 - per2 / 100);
N1leaving = per2 * Nleaving / 100;
mabsorbed = (N1 - N1leaving) * 34.08;//( molecular
    wt. = 34.08)
mgiven = 100;//kg/h
Vactual = mgiven * V / mabsorbed;
Nactual = Nleaving * Vactual / V;// actual moles
    leaving
Vstpl = Nactual * Vstp;// volume leaving at STP
P2 = 500;//kPa
T2 = 290;//K
V2 = Vstpl * Pstp * T2 / ( P2 * Tstp);
Precovery = (N1 - N1leaving)*100 / N1;
disp("m^3/h",Vactual,"(a)Volume of gas entering per
    hour")
disp("m^3/h",V2,"(b)Volume of gas leaving per hour")
disp("%",Precovery,"(c)Percentage recovery of H2S")
```

Scilab code Exa 4.11 Reaction stoichiometry for preparation of ammonia

```
clc()
//N2 + 3H2 = 2NH3
V1 = 100;//m^3 ( 1 = N2)
V2 = V1 * 3;// ( According to Avagadros principle ,
    equal volumes of all gases under similar
    condition contains same no. of moles)
disp("m^3",V2,"(a)Volume of hydrogen required at
    same condition = ")
P1 = 20;//bar
```

```
T1 = 350;//K
P2 = 5;//bar
T2 = 290;//K
V3 = 3 * V1 * P1 * T2 / ( P2 * T1);
disp("m^3",V3,"(b)Volume required at 50 bar and 290K = ")
m = 1000;//kg ( ammonia )
N = m / 17.03;//kmol
N1 = N/2;// ( nitrogen)
N2 = N * 3 / 2;//(hydrogen)
P3 = 50;//bar
T3 = 600;//K
Pstp = 1.01325;//bar
Tstp = 273.15;//K
Vstp = 22.414;//m^3/kmol
V1stp = N1 * Vstp;
V4 = V1stp * Pstp * T3 / (P3 * Tstp);// ( nitrogen at 50 bar and 600K)
V5 = V4 * 2 ;// ( ammonia at 50 bar and 600K)
V6 = V4 * 3 ;// ( hydrogen at 50 bar and 600K)
disp("m^3",V4,"(c)Volume of nitrogen at 50 bar and 600K")
disp("m^3",V6,"   Volume of hydrogen at 50 bar and 600K")
disp("m^3",V5,"   Volume of ammonia at 50 bar and 600K")
```

Scilab code Exa 4.12 Reaction stoichiometry for preparation of producer gas

```
clc()
N = 100;//kmol producer gas
P1 = 25;//% ( Carbon monoxide )
P2 = 4;//% ( Carbon Dioxide )
P3 = 3;//% ( Oxygen )
```

```
P4 = 68;//% ( Nitrogen )
N1 = N * P1/100;
N2 = N * P2/100;
N3 = N * P3/100;
N4 = N * P4/100;
NC = N1 + N2;
m = NC * 12;
Ngas = N / m;//moles of gas for 1 kg of Carbon
Vstp = 22.4143;//m^3/kmol
Vstp1 = Vstp * Ngas;
P = 1;//bar
T = 290;//k
Pstp = 1.01325;//bar
Tstp = 273.15;//K
V = T * Vstp1 * Pstp / (Tstp * P );
disp("m^3",V,"(a)Volume of gas at 1 bar and 290 K
    per kg Carbon = ")
//CO + 1/2 * O2 = CO2
Nrequired  = N1/2 - N3;//(oxygen required)
Nsupplied = Nrequired * 1.2;
PO1 = 21;//% ( Oxygen percent in air)
Nair = Nsupplied * 100/PO1;
V1 = 100;//m^3;
Vair = V1 * Nair / N;
disp("m^3",Vair,"(b)Volume of air required = ")
NCO2 = N2 + N1;
NO2 = Nsupplied - Nrequired;
NN2 = N4 + (Vair * (1 - PO1/ 100));
Ntotal = NCO2 + NO2 + NN2;
PCO2 = NCO2 * 100 / Ntotal;
PO2 = NO2 * 100 / Ntotal;
PN2 = NN2 * 100 / Ntotal;
disp("%",PCO2,"Percent composition of Carbon Dioxide
    = ")
disp("%",PO2,"Percent composition of Oxygen = ")
disp("%",PN2,"Percent composition of Nitrogen = ")
```

Scilab code Exa 4.13 Reaction stoichiometry for preparation of Chlorine from HCl

```
clc()
//4HCl + O2 = 2Cl2 + 2H2O
n = 1;//mol ( Basis 1 mol of HCl )
NO2 = n / 4;
NO2supp = 1.5 * NO2;
Nair = NO2supp * 100 / 21;
V = 100;//m^3
Vair = V * Nair / n;
disp("m^3",Vair,"(a)Volume of air admitted = ")
P1 = 80;//% ( HCl converted)
Ncon = n * P1 /100;
N2 = Ncon/4;// oxygen required
NH2O = Ncon / 2;
NCl2 = Ncon / 2;
nHCl = n - Ncon;
nO2 = NO2supp - N2;
Nnitro = Nair - NO2supp;
Ntotal = nHCl + nO2 + NH2O + NCl2 + Nnitro;
V1 = V * Ntotal;
P1 = 1;//bar
T1 = 290;//K
P2 = 1.2;//bar
T2 = 400;//K
V2 = V1 * P1 * T2 / ( P2 * T1);
disp("m^3",V2,"(b)Volume of gas leaving = ")
VCl2 = NCl2 * V;
Pstp = 1.01325;//bar
Tstp = 273;//K
Vstp = 22.4143;//m^3/kmol
Vstp1 = Tstp * P1 * VCl2 / (T1 * Pstp);
Nstp = Vstp1/Vstp;
```

```
m = Nstp * 70.90;
disp("kg",m,"(c)Kilograms of Chlorine produced = ")
Ntotaldry = nHCl + nO2 + NCl2 + Nnitro;//dry basis
p1 = nHCl*100/Ntotaldry;
p2 = nO2*100/Ntotaldry;
p3 = NCl2*100/Ntotaldry;
p4 = Nnitro*100/Ntotaldry;
disp("%",p1,"(d)Percent composition of HCl in exit
    stream = ")
disp("%",p2,"   Percent composition of Oxygen in
    exit stream = ")
disp("%",p3,"   Percent composition of Chlorine in
    exit stream = ")
disp("%",p4,"   Percent composition of nitrogen in
    exit stream = ")
```

Scilab code Exa 4.14 Reaction stoichiometry for dissociation of Carbon Dioxide

```
clc()
// CO2 = CO + 1/2 * O2
P1 = 1;//bar
T1 = 3500;//K
P2 = 1;//bar
T2 = 300;//K
V2 = 25;//L
V1 = V2 * P2 * T1 / ( P1 * T2 );
disp("L",V1,"(a)Final volume of gas if no
    dissociation occured = ")
Pstp = 1.01325;//bar
Tstp = 273;//K
Vstp = 22.4143;//m^3
N2 = V2 * P2 * Tstp / ( Vstp * Pstp * T2);
// let x be the fraction dissociated , then after
    dissociation ,
```

```
// CO2 = (1 − x)mol, CO = xmol, O2 = (0.5∗x)mol
//total moles = 1 − x + x + o.5 ∗ x = 1 + 0.5 ∗ x
V = 350;//L
N1 = V * P1 * Tstp / (Vstp * Pstp * T1);
// 1 + 0.5 ∗ x = N1, therefore
x = (N1 - 1) / 0.5 ;
p = x*100;
disp("%",p,"(b)CO2 converted = ")
```

Chapter 5

Properties of Real Gases

Scilab code Exa 5.1 Van der waals equation

```
clc()
V = 0.6;//m^3;
T = 473;//K
N = 1 * 10 ^ 3;//mol
R = 8.314;//Pa * m^3/molK
P = N * R * T / (V * 10^5);
disp("bar",P,"(a)Pressure calculated using ideal gas
    equation = ")
a = 0.4233;//N * m^4 / mol^2
b = 3.73 * 10^-5;//m^3/mol
P1 = (R*T/(V/N - b)-a/(V/N)^2)/10^5;
disp("bar",P1,"(a)Pressure calculated using van der
   waals equation = ")
```

Scilab code Exa 5.2 Van der waals equation for CO2 gas

```
clc()
P = 10^7;//Pa;
```

```
T = 500; //K
R = 8.314; //Pa * L / mol K
V = N * R * T / ( P * 1000);
disp("m^3",V,"(a)Volume of CO2 calculated using ideal gas equation = ")
```

Scilab code Exa 5.3 Redlich Kwong equation for gaseous ammonia

```
clc()
V = 0.6 * 10^-3; //m^3
T = 473; //K
Tc = 405.5; //K
Pc = 112.8 * 10 ^ 5//Pa
R = 8.314;
a = 0.4278 * (R^2) * (Tc ^ 2.5)/Pc;
b = 0.0867 * R * Tc / Pc;
P1 = (R*T/(V - b) - a/((T^0.5)*V*(V + b)))/10^5;
disp("bar",P1,"Pressure developed by gas = ")
```

Scilab code Exa 5.4 Molar Volume calculation for gaseous ammonia

```
clc()
P = 10^6; //Pa
T = 373; //K
Tc = 405.5; //K
Pc = 112.8 * 10 ^ 5//Pa
R = 8.314;
a = 0.4278 * (R^2) * (Tc ^ 2.5)/Pc;
b = 0.0867 * R * Tc / Pc;
//P1 = (R*T/(V - b) - a/((T^0.5)*V*(V + b)))/10^5;
//10^6=((8.314*373)/(V-2.59*10^-5))-8.68/((373^0.5)*V*(V+2.59*10^-5)
//solving this we get ,
```

```
V = 3.0 * 10^-3;//m^3/mol
disp("m^3/mol",V,"molar volume of gas = ")
```

Scilab code Exa 5.5 virial equation of state

```
clc()
B = -2.19 * 10^-4;//m^3/mol
C = -1.73 * 10^-8;//m^6/mol^2
P = 10;//bar
T = 500;//K
//virial equation is given as, Z = PV/RT = 1 + B/V +
    C/V^2
//V = (RT/P)*(1 + B/V + C/V^2)
// now by assuming different values for V on RHS and
    checking for corresponding V on LHS, we have to
    assume such value of V on RHS by which we get the
    same value for LHS V
//by trial and error we get,
V = 3.92 * 10^-3;//m^3
disp("m^3",V,"Molar volume of methanol = ")
```

Scilab code Exa 5.6 Lyderson method for n butane

```
clc()
T = 510;//K
P = 26.6;//bar
Tc = 425.2;//K
Pc = 38;//bar
Zc = 0.274;
R = 8.314;
Pr = P / Pc;
Tr = T / Tc;
disp(Pr,"Pr = ")
```

```
disp(Tr,"Tr = ")
//From fig. 5.4 and 5.5 from the text book
Z = 0.865;
D = 0.15;
Z1 = Z + D * ( Zc - 0.27);
V = R * T * Z1 / (P * 10^5);
disp("m^3/mol",V,"Molar volume of n−butane = ")
```

Scilab code Exa 5.7 Pitzer correlation for n butane

```
clc()
T = 510;//K
P = 26.6;//bar
Tc = 425.2;//K
Pc = 38;//bar
w = 0.193;
R = 8.314;
Pr = P / Pc;
Tr = T / Tc;
disp(Pr,"Pr = ")
disp(Tr,"Tr = ")
//From fig. 5.6 and 5.7 from the text book
Z0 = 0.855;
Z1 = 0.042;
Z = Z0 + w*Z1;
disp(Z,"Z = ")
V = R * T * Z / (P * 10^5);
disp("m^3/mol",V,"Molar volume of n−butane = ")
```

Scilab code Exa 5.8 Molar volume by different methods

```
clc()
P = 6000;//kPa
```

```
T = 325;//K
xn2 = 0.4;
xethane = 0.6;
an2 = 0.1365;//N m^4 / mol^2
bn2 = 3.86 * 10^-5;//m^3/mol
aethane = 0.557;//N m^4 / mol^2
bethane = 6.51 * 10^-5;//m^3/mol
Pcn2 = 3394;//kPa
Tcn2 = 126.2;//K
Pcethane = 4880;//kPa
Tcethane = 305.4;//K
R = 8.314;
V = R * T / (P*1000);
disp("m^3/mol",V,"(a)Molar volume by ideal gas equation =")
a = (xn2 * (an2^0.5) + xethane * (aethane^0.5))^2;
b = (xn2*bn2 + xethane*bethane);
//substituting the above values in van der waals equation, and solving, we get
V1 = 3.680 * 10^-4;//m^3/mol
disp("m^3/mol",V1,"(b)Molar volume by van der waals equation =")
Prin2 = P/Pcn2;
Trin2 = T/Tcn2;
Priethane = P/Pcethane;
Triethane = T/Tcethane;
// using compressibilty chart,
Zn2 = 1;
Zethane = 0.42;
Z = xn2 * Zn2 + xethane * Zethane;
V2 = Z * R * T / P;
disp("m^3/mol",V2,"(c)Molar volume based on compressibilty factor =")
Pri1n2 = xn2*P/Pcn2;
Tri1n2 = T/Tcn2;
Pri1ethane = xethane*P/Pcethane;
Tri1ethane = T/Tcethane;
// using compressibilty chart,
```

```
Zn21 = 1;
Zethane1 = 0.76;
Z1 = xn2 * Zn21 + xethane * Zethane1;
V3 = Z1 * R * T / P;
disp("m^3/mol",V3,"(c)Molar volume based on daltons
   law =")
Tc = xn2 * Tcn2 + xethane * Tcethane;
Pc = xn2 * Pcn2 + xethane * Pcethane;
Zc = 0.83;
V4 = Zc * R *T / P;
disp("m^3/mol",V4,"(d)Molar volume by kays method ="
   )
```

Scilab code Exa 5.9 Van der waals equation and Kays method

```
clc()
P1 = 40;//% ( nitrogen )
P2 = 60;//% ( ethane )
T = 325;//K
V = 4.5 * 10^-4;//m^3/mol
a1 = 0.1365;//N*m^4/mol^2
b1 = 3.86 * 10 ^ -5;//m^3/mol
a2 = 0.557;//N*m^4/mol^2
b2 = 6.51 * 10 ^ -5;//m^3/mol
Pc1 = 3394;//kPa
Tc1 = 126.1;//K
Pc2 = 4880;//kPa
Tc2 = 305.4;//K
R = 8.314;
Pideal = R * T / (V * 1000);//kPa
disp("kPa",Pideal,"(a)Pressure of Gas by the ideal
   gas equation = ")
y1 = P1/100;
y2 = P2/100;
a = (y1 * (a1^(1/2)) + y2 * (a2^(1/2)))^2;
```

```
b = y1 * b1 + y2 * b2;
Pv = ((R * T / (V - b)) - a / (V^2))/1000;
disp("kPa",Pv,"(b)Pressure of Gas by Van der waals
    equation = ")
Tc = y1*Tc1 + y2*Tc2;
Pc = y1*Pc1 + y2*Pc2;
Vc = R * Tc / Pc;//Pseudo critical ideal volume
Vr = V / Vc;//Pseudo reduced ideal volume
Tr = T / Tc;//Pseudo reduced temperature
//From fig 5.3, we get Pr = 1.2
Pr = 1.2;
Pk = Pr * Pc;
disp("kPa",Pk,"(b)Pressure of Gas by the Kays method
    = ")
```

Chapter 6

Vapour Pressure

Scilab code Exa 6.1 Quality of steam

```
clc()
P = 500; //kPa
SV = 0.2813; //m^3/kg
Vsaturatedl = 1.093 * 10^-3; //m^3/kg
Vsaturatedv = 0.3747; //m^3/kg
// let the fraction of vapour be y
//(1-y)*Vsaturatedl + y*Vsaturatedv = SV
//then we get, (1-y)*(1.093*10^-3) + y*(0.3747) = 0.2813
y = (SV - Vsaturatedl)/(Vsaturatedv - Vsaturatedl);
P1 = y * 100;
P2 = 100 - P1;
disp("%",P1,"Percentage of Vapour = ")
disp("%",P2,"Percentage of Liquid = ")
```

Scilab code Exa 6.2 Calculation of vapour pressure

```
clc()
```

```
T1 = 363;//K
T2 = 373;//K
P2s = 101.3;//kPa
J = 2275 * 18;//kJ/kmol
R = 8.314;//kJ/kmolK
//ln (P2s/P1s) = J * (1/T1 - 1/T2) / R
P1s = P2s/exp(J * (1/T1 - 1/T2) / R);
disp("kPa",P1s,"Vapour pressure of water at 363 K =
   ")
```

Scilab code Exa 6.3 Clausius Clapeyron equation for acetone

```
clc()
P1s = 194.9;//kPa
P2s = 8.52;//kPa
T1 = 353;//K
T2 = 273;//K
T3 = 300;//K
Pair = 101.3;//kPa
//log (P2s/P1s) = J * (1/T1 - 1/T2) / R
//let J / R = L
L = log (P2s/P1s)/(1/T1 - 1/T2);
P3s = P1s * exp(L * (1/T1 - 1/T3)) ;
Ptotal = P3s + Pair;//at saturation vapour pressure
   = partial pressure
disp("kPa",Ptotal,"(a)Final pressure of the mixture
   = ")
MP = P3s * 100 / Ptotal;
// mole percent = moles of acetone * 100 / total
   moles
//= Partial pressure of acetone * 100 / total
   Pressure
disp("%",MP,"(b)Mole percent of acetone in the final
    mixture = ")
```

Scilab code Exa 6.4 Antoine equation for n heptane

```
clc()
A = 13.8587;
B = 2911.32;
C = 56.56;
T1 = 325;//K
//Pressure at normal condition = 101.3kPa
P2 = 101.3;//kPa
//Antoine equation - lnP = A - B / (T - C)
lnP = A - (B / (T - C));
P1 = exp(lnP);
disp("kPa",P1,"(a)Vapour pressure of n-heptane at
   325K = ")
T2 = B/(A - log(P2)) + C;
disp("K",T2,"(b)Normal boiling point of n-heptane =
   ")
```

Scilab code Exa 6.5 Cox chart

```
clc()
T = [273 293 313 323 333 353 373];
Ps = [0.61 2.33 7.37 12.34 19.90 47.35 101.3];
plot2d('ll',T,Ps,rect=[250,0.1,380,195]);
P = get("hdl");
xtitle('Construction of cox chart','Temperature, K',
   'Pressure, kPa');
T1 = [273 353]
Ps1 = [8.52 194.9]
plot2d('ll',T1,Ps1);
```

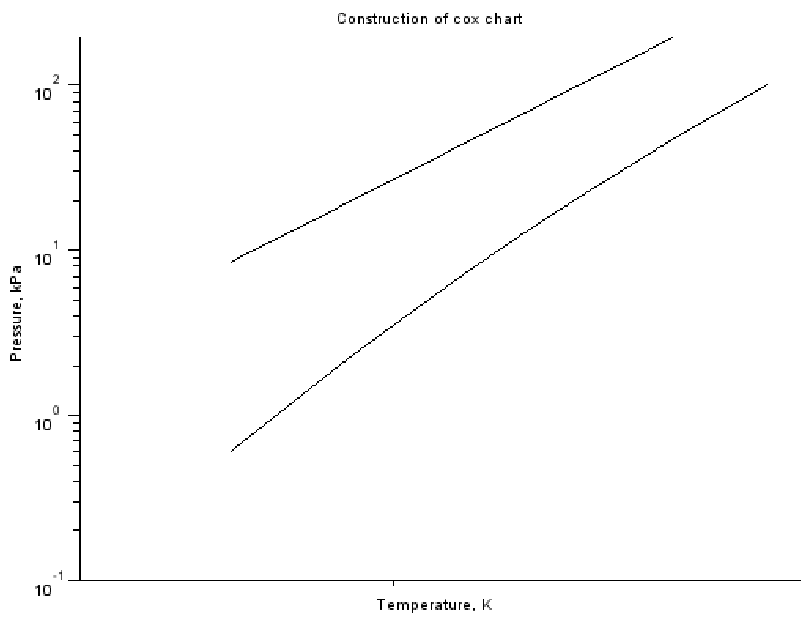

Figure 6.1: Cox chart

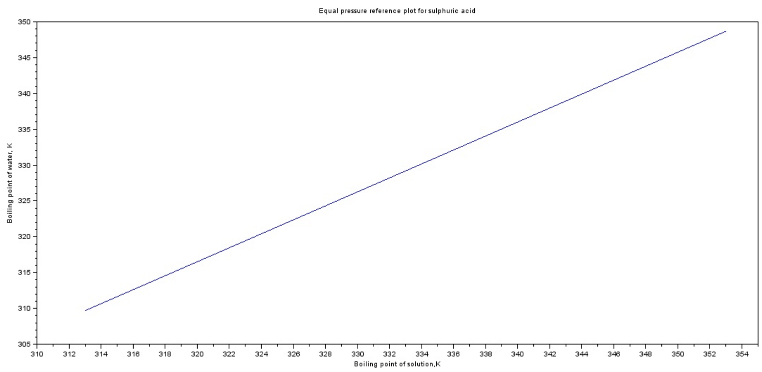

Figure 6.2: Duhring line

Scilab code Exa 6.6 Duhring line

```
clc()
Pswater1 = 6.08;//kPa
T1 = 313;//K
//lnPs = 16.26205 - 3799.887/(T - 46.854)
Tb1 =3799.887/(16.26205 - log(Pswater1)) + 46.854;
disp("K",Tb1,"boiling point of water at 6.08kPa
    vapour pressure = ")
Pswater2 = 39.33;//kPa
T2 = 353;//K
Tb2 =3799.887/(16.26205 - log(Pswater2)) + 46.854;
disp("K",Tb2,"boiling point of water at 39.33 kPa
    vapour pressure = ")
Tb = [Tb1 Tb2];
T = [T1 T2];
plot(T,Tb);
```

```
xtitle('Equal pressure reference plot for sulphuric
   acid','Boiling point of solution ,K','Boiling
   point of water, K');
T3 = 333;//K
//corresponding to T3 on x axis, on y we get
Tb3 = 329;//K
Pswater3 = exp(16.26205 - 3799.887/(Tb3 - 46.854));
disp("kPa",Pswater3,"Vapour pressure of solution at
   333K")
```

Chapter 7

Solutions and Phase Behaviour

Scilab code Exa 7.1 composition calculation of Liquid and vapour at equilibrium

```
clc()
Pas = 71.2;//kPa
Pbs = 48.9;//kPa
P = 65;//kPa
//P=(Pas-Pbs)*xa+Pbs,xa=mole fraction of n-heptane,
   liq. condition,therefore
xa = (P - Pbs)/(Pas - Pbs);
//ya = Pa / P , Vapour condition
ya = Pas * xa / P;
P1 = xa * 100;
P2 = ya * 100;
disp("%",P1,"Percentage of hepatne in liquid = ")
disp("%",P2,"Percentage of hepatne in vapour = ")
```

Scilab code Exa 7.2 Composition and total pressure calculation

```
clc()
```

```
P1 = 100;//kPa ( Vapour pressure of liq A )
P2 = 60;//kPa ( Vapour pressure of liq B )
T = 320;//K
//Pa = xa * P1 = 100 * xa
//Pa = xb * P2 = 60 * xb
//P = xa * P1 + ( 1 - xa )* P2
// = 100xa + ( 1 - xa )* 60
// = 60 + 40*xa
//ya = Pa / P
//0.5 = 100*xa / ( 60 + 40 * xa)
xa = 60 * 0.5 / (100 - 20);
Per1 = xa * 100;
disp("%",Per1,"(a)Percentage of A in liquid = ")
Ptotal = 60 + 40 * xa;
disp("kPa",Ptotal,"(b)Total pressure of the vapour =
    ")
```

Scilab code Exa 7.3 Mole fraction calculation for particular component in liquid vapour mixture

```
clc()
xa = 0.25;
xb = 0.30;
xc = 1 - xa - xb;
Ptotal = 200;//kPa
Pcs = 50;//kPa(Vapour pressure of c)
Pc = xc * Pcs;//(partial pressure of c)
yc = Pc / Ptotal;
yb = 0.5;
ya = 1 - yb - yc;
per1 = ya * 100;
disp("%",per1,"Percentage of A in vapour = ")
```

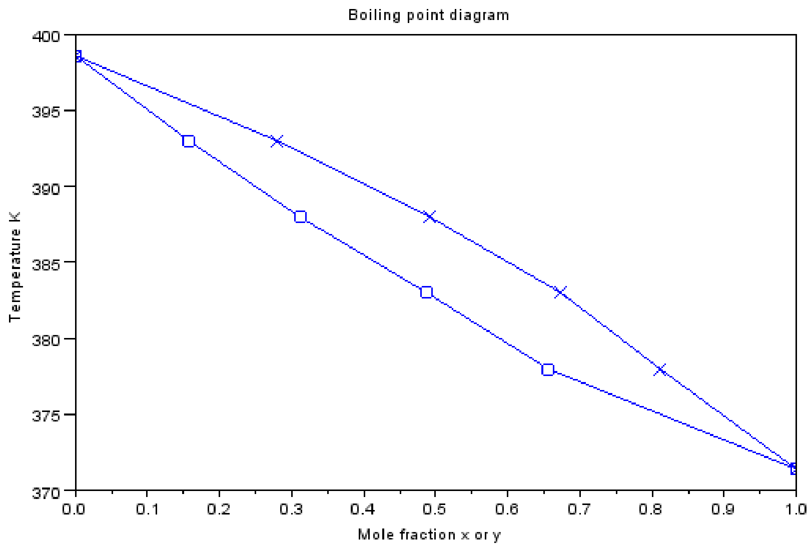

Figure 7.1: Boiling point diagram

Scilab code Exa 7.4 Flash vapourization of benzene toluene mixture

```
clc()
P = 101.3;//kPa
Pbs = 54.21;//kPa
Pas = 136.09;//kPa
xf = 0.65;
xw = (P - Pbs)/(Pas - Pbs);
yd = xw * Pas / P ;
// f = ( xf - xw ) / ( yd - xw )
f = ( xf - xw ) / ( yd - xw );
per1 = f * 100;
disp("%",per1,"mole percent of the feed that is
    vapourised = ")
```

Scilab code Exa 7.5.a Boiling point diagram

```
clc()
T = [371.4 378 383 388 393 398.6]
Pas = [101.3 125.3 140 160 179.9 205.3]
Pbs = [44.4 55.6 64.5 74.8 86.6 101.3]
Ptotal = 101.3; //kPa
for i = 1:6
    x(i) = (Ptotal - Pbs(i))/(Pas(i) - Pbs(i));
end
for i = 1:6
    y(i) = x(i) * Pas(i) / Ptotal;
end
plot(x,T,'-o');
plot(y,T,'-x');
xtitle('Boiling point diagram','Mole fraction x or y
    ','Temperature K')
```

Scilab code Exa 7.5.b Equilibrium Diagram

```
clc()
T = [371.4 378 383 388 393 398.6]
Pas = [101.3 125.3 140 160 179.9 205.3]
Pbs = [44.4 55.6 64.5 74.8 86.6 101.3]
Ptotal = 101.3; //kPa
for i = 1:6
    x(i) = (Ptotal - Pbs(i))/(Pas(i) - Pbs(i));
end
for i = 1:6
    y(i) = x(i) * Pas(i) / Ptotal;
end
w = x;
plot(x,w);
```

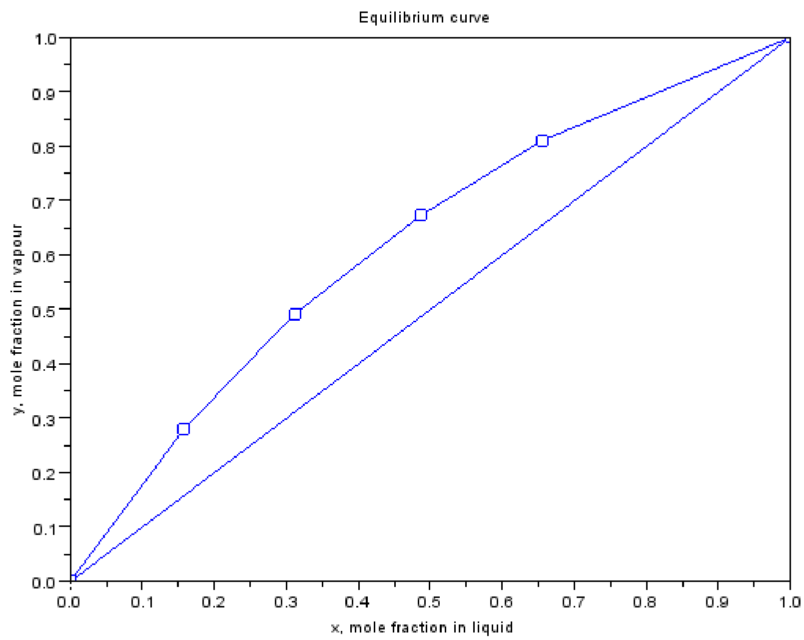

Figure 7.2: Equilibrium Diagram

```
plot(x,y,'-o');
xtitle('Equilibrium curve','x, mole fraction in
    liquid','y, mole fraction in vapour');
```

Scilab code Exa 7.6 Bubble point temperature and vapour composition

```
clc()
Ps = 100;//kPa
A1 = 13.8587;//(1 = n-heptane)
A2 = 13.8216;//(2 = n-hexane)
B1 = 2911.32;
B2 = 2697.55;
C1 = 56.51;
C2 = 48.78;
//lnPs = A - B / ( T - C)
T1 = B1 / (-log(Ps)+A1) + C1;
T2 = B2 / (-log(Ps)+A2) + C2;
x2 = 0.25;
```

Scilab code Exa 7.7 Dew point temperature pressure and concentration

```
clc()
//lnPas = 14.5463 - 2940.46/(T - 35.93)
//lnPbs = 14.2724 - 2945.47 / (T - 49.15)
//xa = (P - Pbs)/(Pas - Pbs)
//Ya = Pas * (P - Pbs)/(P * (Pas - Pbs))
Ya = 0.4;
P = 65;//kPa
//various temperature value are assumed and tried
    till LHS = RHS, we get
T = 334.15;//K
Pas = exp(14.5463 - 2940.46/(T - 35.93));
Pbs = exp(14.2724 - 2945.47 / (T - 49.15));
```

```
xa = (P - Pbs)/(Pas - Pbs);
disp("K",T,"(a)The Dew point temperature at 65 kPa =
    ")
disp(xa,"    Concentration of the first drop of
    liquid = ")
T1 = 327;//K
Pas1 = exp(14.5463 - 2940.46/(T1 - 35.93));
Pbs1 = exp(14.2724 - 2945.47 / (T1 - 49.15));
xa1 = Ya * Pbs1 / (Pas1 - Ya*(Pas1 - Pbs1));
P1 = xa1 * Pas1 / Ya;
disp("kPa",P1,"(b)The dew point pressure at 327 K =
    ")
disp(xa1,"    Concentration at 327K = ")
```

Scilab code Exa 7.8 Partial pressure of acetaldehyde

```
clc()
MW = 44.032;
Mwater = 18.016;
x = 2;//%
Pa = 41.4;//kPa
Mfr = (x/MW)/(x/MW + (100-x)/Mwater);
//henry's law gives Pa = Ha * xa
Ha = Pa / Mfr;
Molality = 0.1;
Mfr1 = Molality / (1000/Mwater + Molality);
Pa1 = Ha * Mfr1;
disp("kPa",Pa1,"Partial Pressure = ")
```

Scilab code Exa 7.9 Raults law application

```
clc()
//1 - pentane, 2 - hexane, 3 - heptane
```

```
x1 = 0.6;
x2 = 0.25;
x3 = 0.15;
A1 = 13.8183;
A2 = 13.8216;
A3 = 13.8587;
B1 = 2477.07;
B2 = 2697.55;
B3 = 2911.32;
C1 = 39.94;
C2 = 48.78;
C3 = 56.51;
//As raoults law is applicable , Ki = yi/xi = Pis/P
//yi = xi*Pis/P
//ln P = A- B/(T-C)
//Assuming ,
P = 400;//kPa
T = 369.75;//K
Pas1 =exp(A1 - B1 / (T - C1));
Pas2 =exp(A2 - B2 / (T - C2));
Pas3 =exp(A3 - B3 / (T - C3));
Yi = (x1*Pas1 + x2*Pas2 + x3*Pas3)/P;
disp("K",T,"(a)bubble point temperature of the mixture = ")
y1 = x1*Pas1/P;
y2 = x2*Pas2/P;
y3 = x3*Pas3/P;
disp("%",y1*100,"(b)composition of n-pentane in vapour = ")
disp("%",y2*100,"composition of n-hexane in vapour = ")
disp("%",y3*100,"composition of n-heptane in vapour = ")
T1 = 300;//K
Ps1 =exp(A1 - B1 / (T1 - C1));
Ps2 =exp(A2 - B2 / (T1 - C2));
Ps3 =exp(A3 - B3 / (T1 - C3));
P1 = x1*Ps1 + x2*Ps2 + x3*Ps3;
```

```
disp("kPa",P1,"(c)Bubble point pressure =")
```

Scilab code Exa 7.10 Dew point temperature and pressure

```
clc()
//1 − pentane , 2 − hexane , 3 − heptane
y1 = 0.6;
y2 = 0.25;
y3 = 0.15;
A1 = 13.8183;
A2 = 13.8216;
A3 = 13.8587;
B1 = 2477.07;
B2 = 2697.55;
B3 = 2911.32;
C1 = 39.94;
C2 = 48.78;
C3 = 56.51;
P = 400;//kPa
T = 300;//K
//As raoults law is applicable , Ki = yi/xi = Pis/P
//xi = yi*P/Pis
//ln P = A− B/(T−C)
//Assuming ,
T1 = 385.94;//K
Pas1 =exp(A1 - B1 / (T1 - C1));
Pas2 =exp(A2 - B2 / (T1 - C2));
Pas3 =exp(A3 - B3 / (T1 - C3));
disp("K",T,"(a)Dew point temperature of the mixture
   = ")
Ps1 =exp(A1 - B1 / (T - C1));
Ps2 =exp(A2 - B2 / (T - C2));
Ps3 =exp(A3 - B3 / (T - C3));
P1 = 1/(y1/Ps1 + y2/Ps2 + y3/Ps3);
disp("kPa",P1,"(b)Dew point pressure = ")
```

Scilab code Exa 7.11 bubble point and dew point

```
clc()
//1 − methanol , 2 − ethanol , 3 − propanol
x1 = 0.45;
x2 = 0.3;
x3 = 1 - (x1 + x2);
P = 101.3;//kPa
// by drawing the temperature vs vapour pressure
   graph and interpolation ,assuming ,
T = 344.6;//K
Ps1 = 137.3;
Ps2 = 76.2;
Ps3 = 65.4;
y1 = x1 * Ps1 / P;
y2 = x2 * Ps2 / P;
y3 = x3 * Ps3 / P;
disp("K",T,"(a)Bubble point temperature = ")
disp("%",y1*100,"Composition of methanol in vapour =
   ")
disp("%",y2*100,"Composition of ethanol in vapour =
   ")
disp("%",y3*100,"Composition of propanol in vapour =
   ")
//again , for xi = 1
T1 = 347.5;//K
P1 = 153.28;
P2 = 85.25;
P3 = 73.31;
xa = x1 * P / P1;
xb = x2 * P / P2;
xc = x3 * P / P3;
disp("K",T1,"(b)Dew point temperature = ")
disp("%",xa*100,"Composition of methanol in liquid =
```

```
")
disp("%",xb*100,"Composition of ethanol in liquid = ")
disp("%",xc*100,"Composition of propanol in liquid = ")
```

Scilab code Exa 7.12 component calculations

```
clc()
xp = 0.25;
xnb = 0.4;
xnp = 0.35;
P = 1447.14;//kPa
//assuming temperatures 355.4 K and 366.5 K , corresponding Ki values are found from nomograph and total Ki value are 0.928 and 1.075 resp, thus bubble point temperature lies between, using interpolation bubble point temperature is found to be,
Tb = 361;//K
disp("K",Tb,"(a) The buuble point temperature = ")
//At 361,
Kip = 2.12;
Kinb = 0.85;
Kinp = 0.37;
xp1 = Kip * xp;
xnb1 = Kinb * xnb;
xnp1 = Kinp * xnp;
disp(xp1,"concentration of propane at bubble point = ")
disp(xnb1,"concentration of n-butane at bubble point = ")
disp(xnp1,"concentration of n-pentane at bubble point = ")
//At dew point Yi/Ki = 1, at 377.6K this is 1.1598
```

```
and at 388.8K it is 0.9677, by interpolation dew point is found to be
Td = 387;//K
Kip1 = 2.85;
Kinb1 = 1.25;
Kinp1 = 0.59;
yp1 = xp/Kip1;
ynb1 = xnb/Kinb1;
ynp1 = xnp/Kinp1;
disp("K",Td,"(b) The dew point temperature = ")
disp(yp1,"concentration of propane at dew point = ")
disp(ynb1,"concentration of n-butane at dew point = ")
disp(ynp1,"concentration of n-pentane at dew point = ")
//summation zi / (1 + L/VKi)= 0.45, using trial and error, we find
T = 374.6;//K
L = 0.55;
V = 0.45;
Kip2 = 2.5;
Kinb2 = 1.08;
Kinp2 = 0.48;
t = (xp/(1+L/(V*Kip2)))+(xnb/(1+L/(V*Kinb2))) + (xnp/(1+L/(V*Kinp2)));
yp2 = (xp/(1+L/(V*Kip2)))/t;
ynb2 = (xnb/(1+L/(V*Kinb2)))/t;
ynp2 = (xnp/(1+L/(V*Kinp2)))/t;
xp2 = (xp - V * yp2)/L;
xnb2 = (xnb - V * ynb2)/L;
xnp2 = (xnp - V * ynp2)/L;
disp("K",T,"(c)Temperature of the mixture = ")
disp(yp2,"vapour phase concentration of propane = ")
disp(ynb2,"vapour phase concentration of n-butane = ")
disp(ynp2,"vapour phase concentration of n-pentane = ")
disp(xp2,"liquid phase concentration of propane = ")
```

```
disp(xnb2,"liquid phase concentration of n-butane = ")
disp(xnp2,"liquid phase concentration of n-pentane = ")
```

Scilab code Exa 7.13 equilibrium temperature and composition

```
clc()
P = 93.30;//kPa
T1 = 353;//K
T2 = 373;//K
Pwater1 = 47.98;//kPa
Pwater2 = 101.3;//kPa
Pliq1 = 2.67;//kPa
Pliq2 = 5.33;//kPa
T = T1 + (T2 - T1)*(P - (Pwater1 + Pliq1))/(Pwater2 + Pliq2 - (Pwater1 + Pliq1));
disp("K",T,"(a)The equilibrium temperature = ")
Pwater = 88.50;
y = Pwater * 100 /P;
disp("%",y,"(b)Water vapour in vapour mixture = ")
```

Scilab code Exa 7.14 Temperature composition diagram

```
clc()
//the three phase temperature is first find out, which comes to be 342K, the corresponding Ps1 = 71.18, Ps2 = 30.12
T = [342 343 348 353 363 373];
Ps2 = [30.12 31.06 37.99 47.32 70.11 101.3];
Ps1 = [71.18 72.91 85.31 100.5 135.42 179.14];
```

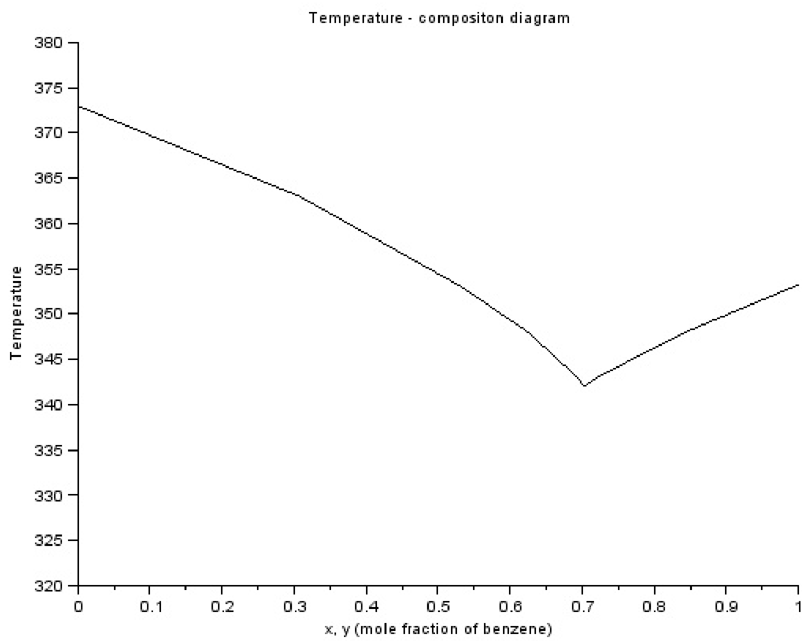

Figure 7.3: Temperature composition diagram

```
P = 101.3;//kPa
for i = 1:4
    y1(i) = 1 - (Ps1(i))/P;
end
for i = 1:6
    y2(i) = 1 - (Ps2(i))/P;
end
plot2d(y2,T);
plot2d(1-y1,T,rect = [0,320,1,380]);
xtitle('Temperature − compositon diagram','x, y (
   mole fraction of benzene)','Temperature')
```

Scilab code Exa 7.15 Boiling point calculation

```
clc()
T = 379.2;//K
P = 101.3;//kPa
Ps = 70;//kPa
Molality = 5;
Pws = exp(16.26205 - 3799.887/(T - 46.854));
k = P / Pws;
Pws1 = Ps / k;
T1 = 3799.887 / (16.26205 - log( Pws1)) + 46.854;
disp("K",T1,"Boiling point of the solution = ")
```

Chapter 8

Humidity and Humidity chart

Scilab code Exa 8.1 Nitrogen and ammonia gas mixture

```
clc()
T = 280; //K
P = 105; //kPa
Pas = 13.25; //kPa ( Vpaour pressure of acetone )
Pa = Pas; // ( As gas is saturated , partial pressure
   = vapour pressure )
Mfr = Pa / P; //(Mole fraction)
Mpr = Mfr * 100;
disp("%",Mpr,"(a)The mole percent of acetone in the
   mixture = ")
Ma = 58.048; //(molecular weight of acetone)
Mn = 28; //(molecular weight of nitrogen)
N = 1; //mole
Na = Mfr * N;
Nn = N - Na;
ma = Na * Ma ;
mn = Nn * Mn;
mtotal = ma + mn;
maper = ma *100 / mtotal;
mnper = mn *100/ mtotal;
disp("%",maper,"(b)Weight percent of acetone = ")
```

```
disp("%",mnper,"Weight percent of nitrogen = ")
Vstp = 22.4;//m^3/kmol
Pstp = 101.3;//kPa
Tstp = 273.15;//K
V = Vstp * Pstp * T / ( Tstp * P );
C = ma/V;
disp("kg/m^3",C,"(c)Concentration of vapour = ")
```

Scilab code Exa 8.2 Benzene vapour air mixture

```
clc()
P = 101.3;//kPa
Per1 = 10;//%
Pa = P * Per1 / 100;// ( a - benzene )
Ps = Pa;//( saturation )
//lnPs = 13.8858 - 2788.51/(T - 52.36)
T = 2788.51 / ( 13.8858 - log(Ps)) + 52.36;
disp("K",T,"Temperature at which saturation occurs =
    ")
```

Scilab code Exa 8.3 Evaporation of acetone using dry air

```
clc()
Pdryair = 101.3;//kPa
Pacetone = 16.82;//kPa
Nratio = Pacetone / (Pdryair - Pacetone);
mratio = Nratio * 58.048 / 29;// ( Macetone =
    58.048, Mair = 29 )
macetone = 5;//kg ( given )
mdryair = macetone / mratio;
disp("kg",mdryair,"Minimum air required = ")
```

Scilab code Exa 8.4 Humidity for acetone vapour and nitrogen gas mixture

```
clc()
Pa = 15;//kPa ( partial pressure of acetone)
Ptotal = 101.3;//kPa
Mfr = Pa / Ptotal;
disp(Mfr,"(a)Mole fraction of acetone = ")
Macetone = 58.048;
Mnitrogen = 28;
mafr = Mfr * Macetone / ( Mfr * Macetone + (1-Mfr)*
    Mnitrogen );
disp(mafr,"(b)Weight fraction of acetone = ")
Y = Mfr / ( 1 - Mfr );
disp("moles of acetone/moles of nitrogen",Y,"(c)
    Molal humidity = ")
Y1 = Y * Macetone / Mnitrogen ;
disp("kg acetone/kg nitrogen",Y1,"(d)Absolute
    humidity = ")
Pas = 26.36;//kPa ( vapour pressure)
Ys = Pas / ( Ptotal - Pas);//saturation humidity
disp("moles of acetone/moles of nitrogen",Ys,"(e)
    Saturation humidity = ")
Y1s = Ys * Macetone / Mnitrogen;
disp("kg acetone/kg nitrogen",Y1s,"(f)Absolute
    saturation humidity = ")
V = 100;//m^3
Vstp =22.4143;//m^3/kmol
Pstp = 101.3;//kPa
Tstp = 273.15;//K
T = 295;//K
N = V * Ptotal * Tstp / (Vstp * Pstp * T );
Nacetone = N * Mfr;
macetone = Nacetone * Macetone;
```

```
disp("kg",macetone,"(g)Mass of acetone in 100m^3 of the total gas = ")
```

Scilab code Exa 8.5 Percent saturation and relative saturation

```
clc();
Pa = 15;//kPa ( Partial pressure )
Pas = 26.36;//kPa ( Vapour pressure )
RS = Pa * 100 / Pas ;
Y = 0.1738;
Ys = 0.3517;
PS = Y * 100 / Ys;
disp("%",RS,"Relative humidity = ")
disp("%",PS,"Percent humidity = ")
```

Scilab code Exa 8.6 Analysis of Moist air

```
clc()
mwater = 0.0109;//kg
V = 1;//m^3
T = 300;//K
P = 101.3;//kPa
Vstp =22.4143;//m^3/kmol
Pstp = 101.3;//kPa
Tstp = 273.15;//K
N = V * P * Tstp / (Vstp * Pstp * T );
Nwater = mwater / 18.016;
Nfr = Nwater / N;
Pwater = Nfr * P;
disp("kPa",Pwater,"(a)Partial pressure of water vapour = ")
Ps = exp(16.26205 - 3799.887/(T - 46.854));
RS = Pwater * 100 / Ps;
```

```
disp("%",RS,"(b)Relative saturation = ")
Y1 = Pwater *18 / ((P - Pwater)*29);
disp("kg water / kg dry air",Y1,"(c)Absolute
    humidity = ")
Y1s = Ps *18 / ((P - Ps)*29);
PS1 = Y1 * 100 / Y1s;
disp("%",PS1,"(d)Percent saturation = ")
PS = 10;//%
Y1S = Y1 * 100/PS ;
//Y1S = Pas/(P - Pas ) * 18 /29
Pas1 = 29 * P * Y1S / (18 + 29*Y1s);
T1 = 3799.887 / (16.26205-log(Pas1)) + 46.854;
disp("K",T1,"(e)Temperature at which 10% saturation
    occurs = ")
```

Scilab code Exa 8.7 Heating value calculation for a fuel gas

```
clc()
T = 300;//K
P = 100;//kPa
S = 25000//kJ/m^3
T1= 295;//K
P1 = 105;//kPa
RS = 50;//%
Ps = 3.5;//kPa
Ps1 = 2.6;//kPa
Vstp = 22.4143;//m^3/kmol
Pstp = 101.3;//kPa
Tstp = 273.15;//K
V = 1;//m^3
N = V * P * Tstp/(Vstp * Pstp * T);
Nfuel = N * (P - Ps)/P;
Smol = S / Nfuel;//kJ/kmol
N1 = V * P1 * Tstp/(Vstp * Pstp * T1);
Pwater = Ps1 * RS /100;
```

```
Nfuel1 = N1 * (P1 - Pwater )/P1;
S1 = Smol * Nfuel1;
disp("kJ/m^3",S1,"Heating value of gas at 295K and
    105kPa = ")
```

Scilab code Exa 8.8 Analysis of nitrogen benzene mixture

```
clc()
T = 300;//K
T1 = 335;//K
P = 150;//kPa
//lnPs = 13.8858 - 2788.51 / ( T - 52.36)
Ps = exp(13.8858 - 2788.51 / ( T - 52.36));
Ps1 = exp(13.8858 - 2788.51 / ( T1 - 52.36));
Pa = Ps;//(Vapour pressure at dew point is equal to
    the partial pressure of the vapour)
Y = Pa / (P - Pa);
Ys = Ps1 / (P - Ps1);
PS = Y * 100 / Ys;
disp("%",PS,"(a)Percent saturation = ")
Ma = 78.048;
Mb = 28;
Q = Y * Ma / Mb ;
disp("kg benzene/kg nitrogen",Q,"(b)Quantity of
    benzene per kilgram of nitrogen = ")
V = 1;//m^3 ( basis )
Vstp = 22.4143;//m^3/kmol
Pstp = 101.3;//kPa
Tstp = 273.15;//K
N = V * P * Tstp/(Vstp * Pstp * T1);
y = Y / ( 1 + Y );
Nbenzene = N * y;
C = Nbenzene * Ma;
disp("kg/m^3",C,"(c)Kilogram of benzene per m^3 of
    nitrogen = ")
```

```
P1 = 100;//kPa
Pbenzene = y * P1;
T1 = 2788.51 / ( 13.8858 - log (Pbenzene)) + 52.36;
disp("K",T1,"(d)Dew point = ")
Per1 = 60;//%
Y2 = Y * (1- Per1/100);
//Y2 = Pa / (P - Pa)
P = Pa / Y2 + Pa;
disp("kPa",P,"(e)Pressure required = ")
```

Scilab code Exa 8.9 Drying

```
clc()
T = 300;//K
T1 = 285;//K
Pwater = 3.56;//kPa
Pwater1 = 1.4;//kPa
V = 1;//m^3 ( Basis )
Vstp = 22.4143;//m^3/kmol
N = V / Vstp;
Pstp = 101.3;//kPa
Y = Pwater / (Pstp - Pwater);
Y1 = Pwater1 / (Pstp - Pwater1);
Nremoved = Y - Y1;
Ndryair = N * 1 / (1 + Y);
mremoved = Ndryair * Nremoved * 18.016;
disp("kg",mremoved,"(a)amount of water removed = ")
Nremaining = Ndryair * Y1 ;
V1 = (Ndryair + Nremaining) * Vstp ;
disp("m^3",V1,"(b)Volume of gas at stp after drying = ")
```

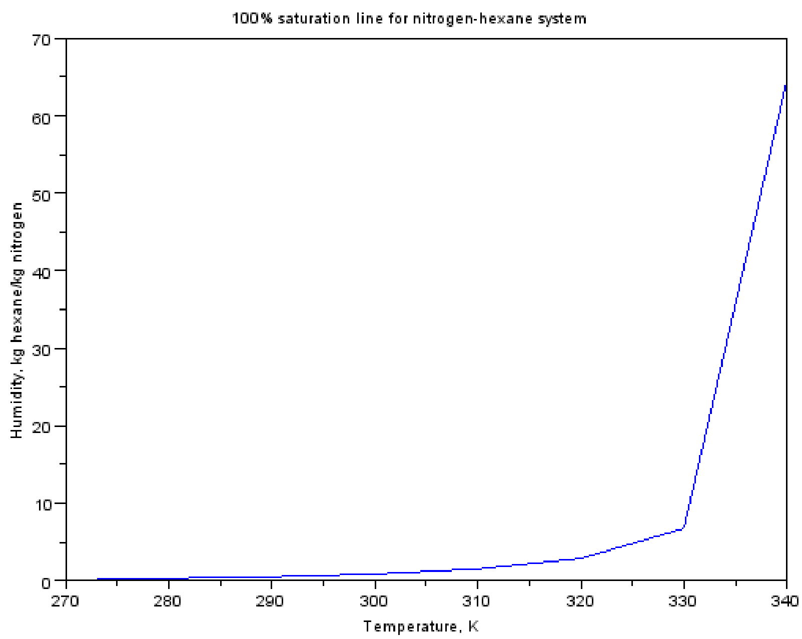

Figure 8.1: Saturation lines for hexane

Scilab code Exa 8.10 Saturation lines for hexane

```
clc()
P = 100;//kPa
T = [273 280 290 300 310 320 330 340];
for i =1:8
    Ps(i) = exp(13.8216 - 2697.55/(T(i)-48.78));
end
disp((Ps))
for j = 1:8
    Ys(j) = Ps(j) * 86.11 / ((P - Ps(j))*28);
end
disp(Ys)
plot(T,Ys,rect=[273,0,333,10]);
xtitle('100% saturation line for nitrogen-hexane
   system','Temperature, K','Humidity, kg hexane/kg
   nitrogen');
```

Scilab code Exa 8.11 Psychometric chart application

```
clc()
Td = 328;//K ( dry bulb )
P = 101.3;//kPa
PS = 10;//%
//refering to the psychometric chart, corresponding
   to 328 K and 10% saturation
Y1 = 0.012;//kg water / kg dry air
disp("kg water / kg dry air",Y1,"(a)Absolute
   humidity = ")
//Y1 = Pa * 18 / ( P - Pa ) * 29
Pa = Y1 * P * 29 /( 18 + Y1 * 29 );
```

```
disp("kPa",Pa,"(b)Partial Pressure of water vapour = ")
//using psychometric chart, saturation humidity at 328 K is given as
Y1s = 0.115;//kg water / kg dry air
disp("kg water / kg dry air",Y1s,"(c)The absolute humidity at 328K = ")
//at saturation partial pressure = vapour pressure
Pas = Y1s * P * 29 /( 18 + Y1s * 29 );
disp("kPa",Pas,"(d)Vapour Pressure of water vapour = ")
RS = Pa * 100 / Pas;
disp("%",RS,"(e)Percent relative saturation = ")
//using psychometric chart, moving horizontally keeping humidity constant to 100% saturation, we get dew point as,
T = 290;//K
disp("K",T,"(f)Dew point = ")
```

Scilab code Exa 8.12 Humid heat calculation for a sample of air

```
clc()
Ca = 1.884;//kJ/kgK
Cb = 1.005;//kJ/kgK
Y1 = 0.012;
//Cs = Cb + Y1 * Ca
Cs = Cb + Y1 * Ca;
disp("kJ/kgK",Cs,"Humid heat of the sample = ")
P = 101.3;//kPa
V = 100;//m^3
R = 8.314;
T = 328;//K
T1 = 373;//K
N = P * V / ( R * T );
Pa = 1.921;//kPa
```

```
Ndryair = N * (P - Pa)/P;
mdryair = Ndryair * 29;
Ht = mdryair * Cs * (T1 - T);
disp("kJ",Ht,"Heat to be supplied = ")
```

Scilab code Exa 8.14 wet bulb temperature and dry bulb temperature

```
clc()
P = 101.3;//kPa
MW = 58;
T1 = 280.8;//K
Ps = 5;//kPa
pr = 2;//kJ/kgK ( Psychometric ratio )
Hvap = 360;//kJ/kg
Tw = T1;
Yw1 = Ps * MW / (( P - Ps) * 29);
// Tw = Tg - Hvap * ( Yw1 - Y1) / (hG / kY), where
   hG/kY is the psychmetric ratio pr
Y1 = 0;
Tg = Tw + Hvap * ( Yw1 - Y1) / pr;
disp("K",Tg,"The air temperature = ")
```

Scilab code Exa 8.15 Humidity calculation

```
clc()
Td = 353.2;//K
Tw = 308;//K
Hvap = 2418.5;//kJ/kg
pr = 0.950;//kJ/kg
Ps = 5.62;//kPa
P = 101.3;//kPa
Yw1 = (Ps * 18)/ (( P - Ps) * 29);
Y1 = Yw1 - pr * ( Td - Tw ) / Hvap;
```

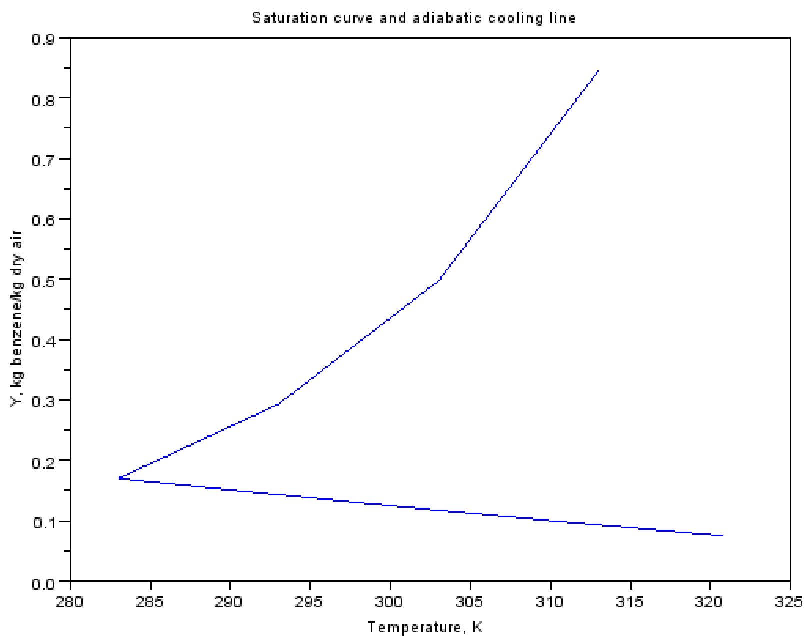

Figure 8.2: SAturation curve and adiabatic cooling line

```
disp("kg water/kg dry air",Y1,"Humidity = ")
//humidity can also be directly obtained from
   psychometric chart , which we get to be 0.018 kg
   water/kg dry air
```

Scilab code Exa 8.16 SAturation curve and adiabatic cooling line

```
clc()
P = 101.3;//kPa
T = [283 293 303 313];
for i=1:4
```

```
    Ps(i) = exp(13.8858 - 2788.51/(T(i)-52.36));
end
for j =1:4
    Ys(j) = Ps(j) * 78.048 / ((P - Ps(j))*29);
end
disp(Ps)
disp(Ys)
plot(T,Ys,rect = [270,0,323,0.9]);
//Tas = Tg - L *(Y1as - Y1) / Cs
//Cs = Cb + Y1 *Ca = 1.005 + Y1 * 1.2,
L = 435.4;//kJ/kgK
//for different value of Tg and Y1 tried, we have the following set of values
Tg = [283 290.4 300 310.1 320.8];
Y1 = [0.1701150 0.15 0.125 0.1 0.075];
plot(Tg,Y1);
xtitle('Saturation curve and adiabatic cooling line','Temperature, K','Y, kg benzene/kg dry air');
```

Scilab code Exa 8.17 Adiabatic drier

```
clc()
Tin = 380.7;//K
Pin = 101.3;//kPa
Tdew = 298;//K
mremoved = 2.25;//kg
V = 100;//m^3
//using humidity chart, humidity of air at dry bulb temperature of 380.7K and dew point = 298K is,
Y = 0.02;// kg water /kg dry air
disp("kg water /kg dry air",Y,"(a)Humidity of air entering the drier = ")
Tstp = 273.15;//K
Vstp = 22.4143;//m^3/kmol
N = V * Tstp / ( Vstp * Tin );
```

```
MY = Y * 29 / 18;//molal humidity
Ndryair = N / ( 1 + MY );
mdryair = Ndryair *29;
mwaterin = mdryair * Y;
mwaterout = mwaterin + mremoved;
Yout = mwaterout / mdryair;
// percent humidity is calculated using the chart,
   and is
PY = 55;//%
disp("kg water /kg dry air",Yout,"(b)exit air
   humidity = ")
disp("%",PY,"Percent humidity = ")
//from the humidity chart
Twet = 313.2;//K
Td = 322.2;//K
disp("K",Twet,"(c)exit air wet bulb temperature = ")
disp("K",Td,"(c)exit air dry bulb temperature = ")
MYout = Yout * 29 / 18;
Nout = Ndryair * ( 1 + MYout ) / 1;
V1 = Nout * Vstp * Td / Tstp;
disp("m^3",V1,"(d)Volume of exit air = ")
```

Scilab code Exa 8.18 Psychometric chart application

```
clc()
P = 101.3;//kPa
Td = 303;//K
Tw = 288;//K
//using psychometric chart,
Y1 = 0.0045;//kg water/ kg dry air
PY = 18;//%
Theated = 356.7;//K
Cb = 1.005;
Ca = 1.884;
Cs = Cb + Y1 * Ca;
```

```
Q = 1 * Cs * (Theated - Td);
disp("kg water/ kg dry air",Y1,"(a)Humidity of the
   initial air = ")
disp("%",PY,"(b)Percent humidity = ")
disp("K",Theated,"(c)Temperature to which the air is
    heated = ")
disp("kJ",Q,"(d)Heat to be suppplied = ")
```

Scilab code Exa 8.19 Psychometric chart application and given wet bulb and dry bulb temperature

```
clc()
Tw = 313;//K
Td = 333;//K
//Using th psychometric chart,
Y = 0.04;//kg water/ kg dry air
PS = 26.5;//%
VS = 1.18;//m^3/kg dry air ( volume of saturated air
    )
VD = 0.94;//m^3/kg dry air ( volume of dry air )
VH = VD + PS * (VS - VD )/100;
HS = 470;//J / kg dry air ( enthalpy of saturated
   air )
HD = 60;//J / kg dry air ( enthalpy of dry air )
H = HD + PS * ( HS - HD )/100;
disp("kg water/ kg dry air",Y,"(a)Absolute Humidity
   of the air = ")
disp("%",PS,"(b)Percent humidity = ")
disp("m^3/kg dry air",VH,"(c)Humid volume = ")
disp("kJ/kg dry air",H,"(d)Enthalpy of wet air = ")
```

Chapter 9

Material Balance in Unit Operations

Scilab code Exa 9.1 Combustion of coal

```
clc()
PC1 = 85;//% ( Percent carbon in coal )
PA1 = 15;//% ( Percent ash in coal )
PA2 = 80;//% ( Percent ash in cinder )
PC2 = 20;//% ( Percent carbon in cinder )
m = 100;//kg (weight of coal )
mash = PA1 * m / 100;
w = mash * 100 / PA2;// weight of cinder
mcarbon = w - mash;
Plost = mcarbon * 100 / ( m - mash );
disp("kg",w,"weight of cinder formed = ")
disp("%",Plost,"Percent fuel lost = ")
```

Scilab code Exa 9.2 Drying of wood

```
clc()
```

```
m = 1;//kg ( mass of completely dry wood )
P1 = 40;//% ( percentage moisture in wet wood )
P2 = 5;//% ( Percentage moisture in dry wood )
mwaterin = P1 * m / ( 100 - P1 );
mwaterout = P2 * m / ( 100 - P2 );
mevaporated = mwaterin - mwaterout;
disp("kg",mevaporated,"mass of water evaporated per
    kg of dry wood = ")
```

Scilab code Exa 9.3 Effluent discharge

```
clc()
F1 = 6*1000;//L/s
BOD1 = 3 * 10^-5;//g/L
BOD2 = 5 * 10^-3;//g/L
V = 16 * 10^3;//m^3/day
v = V * 10^3 / (24 * 3600);//L/s
//Let BOD of the effluent be BODeff,
BODeff = (BOD2 * (F1 + v) - BOD1 * F1) / ( v );
disp("g/L",BODeff,"BOD of the effluent of the plant
    = ")
```

Scilab code Exa 9.4 benzene requirement calculation

```
clc()
D = 100;//kg of overhead product
xfa = 0.956;
xdw = 0.074;
xdb = 0.741;
xda = 0.185;
//water balance gives
F = D * xdw / (1 - xfa) ;
W = F * xfa - xda * D;
```

```
W1 = 100;
B = xdb*D;
Bused = B * W1 / W;
disp("kg",Bused,"Quantity of benzene required = ")
```

Scilab code Exa 9.5 Fortification of waste acid

```
clc()
//let , W - waste acid , S - Sulfuric acid , N - nitric
    acid , M - mixed acid
xsh2so4 = 0.95;
xsh2o = 0.5;
xwh2so4 = 0.3;
xwhno3 = 0.36;
xwh2o = 0.34;
xmh2so4 = 0.4;
xmhno3 = 0.45;
xmh2o = 0.15;
xnhno3 = 0.8;
xnh2o = 0.2;
M = 1000;//kg
// total material balance , W + S + N = 1000;
//H2SO4 balance , xwh2so4 * W + xsh2so4 * S = xmh2so4
    *M
//HNO3 balance , xwhno3 * W + xnhno3 * N = xmhno3*M
//H2O balance , xwh2o*W+xnh2o*N + xsh2o*S = xmh2o*M
//solving the above equations simultaneously , we get
    ,
W = 70.22;//kg
S = 398.88;//kg
N = 530.9;//kg
disp("kg",W,"Waste acid = ")
disp("kg",S,"Concentrated H2SO4 = ")
disp("kg",N,"Concentrated HNO3 = ")
```

Scilab code Exa 9.6 Triple effect evaporator

```
clc()
F = 1000;//kg
Psolute1 = 20;//%
Psolute2 = 80;//%
//taking solute balance
L3 = F * Psolute1 / Psolute2;
//taking total material balance
V = (F -L3) / 3;
//for first effect , total balance gives ,
L1 = F - V;
//solute balance gives ,
Psolute3 = F * Psolute1 / L1;
//For second effect , total balance gives ,
L2 = L1 - V;
//solute balnce gives ,
Psolute4 = L1 * Psolute3 / L2;
disp("%",Psolute3,"solute entering second effect = "
    )
disp("kg",L1,"Weight entering second effect")
disp("%",Psolute4,"solute entering third effect = ")
disp("kg",L2,"Weight entering third effect")
```

Scilab code Exa 9.7 Crystallization operation

```
clc()
F = 100;//kg
xf = 0.25;
x2 = 7/107;
P1 = 10;//%
```

```
W3 = P1 * F * (1-xf)/100;//(W3 - weight of water
    evaporated)
// let W1 and W2 be weight of crystal and weight of
    mother liquor remaining after crystallization
    resp.,
//F = W1 + W2 + W3
//100 = W1 + W2 + 7.5
//solute balance gives, F*xf = W1*x1 + W2*x2
//100*0.25 = W1*1+W2 * 0.0654
W2 = (F - W3 - F*xf)/(1-x2);
W1 = F - W3 - W2;
disp("kg",W1,,,"yeild of the crystals = ")
```

Scilab code Exa 9.8 Evaporation of Na2CO3

```
clc()
F = 100;//kg
xf = 0.15;
P1 = 80;//% ( Carbonate recovered )
M1 = 106;//(Molecular weight of Na2CO3)
M2 = 286;//(Molecular weight of Na2CO3.10H2O)
x1 = M1 / M2;//(Weight fraction of Na2CO3 in
    crystals)
Mrecovered = P1 * F * xf / 100;
Wcrystal = Mrecovered / x1;
disp("kg",Wcrystal,"(a)quantity of crystals formed =
    ")
//Na2CO3 balance gives, F*xf = Wcrystal*x1 + W2*x2
//W2 weight of mother liquor remaining after
    crystallization
//let M = W2 * x2,therefore
M = F * xf - Mrecovered;
x2 = 0.09;
W2 = M/x2;
W3 = F - Wcrystal - W2;//weight of water evaporated
```

```
disp("kg",W3,"(b)Weight of water evaporated = ")
```

Scilab code Exa 9.9 Crystallization

```
clc()
m = 100;//kg (of 60% solution)
//w - water added to the original solution
//w1 - wt. of Na2S2O3.5H2O crystallized
//w2 - wt. of mother liquor obtained
//w3 - solution carried away by the crystals
xf = 0.6;
Mna2s2o3 = 158;
Mna2s2o35h2o = 248;
mcrystals = m * xf * Mna2s2o35h2o / Mna2s2o3;
// free water available = m + w - 1 - mcrystals
//concentration of impurity = 1/(w+4.823)
//total balance, 100 - 1 + w = w1 + w2 + w3
//w1 + w2 + w3 - w = 99
//Na2S2O3 balance, 60 = (w1 + w2 * 1.5/2.5 + w3 * 1.5/2.5)*158/248
//w1 + 0.6 * w2 + 0.6 * w3 = 94.177
//each gram crystals carry 0.05 kg solution,
//w3 = 0.05 * w1
//impurity % = 0.1
//impurity = w3 /(2.5 * (w+4.823))
//solving above equations, we get
w = 14.577;//kg
w1 = 65.08;//kg
w2 = 45.25;//kg
w3 = 0.05 * w1;
disp("kg",w,"(a)amount of water  added = ")
disp("kg",w1,"(b)amount of Na2S2O3.5H2O crystals added = ")
m1 = w1 * Mna2s2o3 / Mna2s2o35h2o + w3 * 1.5 * Mna2s2o3 / (2.5 * Mna2s2o35h2o);
```

```
P = m1*100/(m*xf);
disp("%",P,"(c)Percentage recovery of Na2S2O3 = ")
```

Scilab code Exa 9.10 Extraction

```
clc()
m = 100;//kg
Pin1 = 40;//% ( tannin )
Pin2 = 5;//% ( moisture )
Pin3 = 23;//% ( soluble non tannin material )
Pin4 = 100 - Pin1 - Pin2 - Pin3;//% ( insoluble
    lignin )
// since, lignin is insoluble, all of it will be
    present in the residue
Pout1 = 3;//%
Pout2 = 50;//%
Pout3 = 1;//%
Pout4 = 100 - Pout1 - Pout2 - Pout3;
//let W be the mass of residue, then we get
W = Pin4 * m / Pout4;
Ptannin = W * Pout1 * 100 / (m * Pin1);
disp("%",Ptannin,"Percent of original tannin
    unextracted = ")
```

Scilab code Exa 9.11 Leaching operation

```
clc()
F = 100;//kg
//F - feed, R - overflow, U - underflow, S - solvent
//F + S = U + R ( Total balance )
Poil1 = 49;//% ( 1 - feed )
Ppulp1 = 40;//%
Psalts1 = 3;//%
```

```
Pwater = 100 - Poil1 - Ppulp1 - Psalts1;
Phexane2 = 25;//%(2 - underflow)
Psalts2 = 2.5;//%
Poil2 = 15;//%
Pwater2 = 7.5;//%
Ppulp2 = 100 - Phexane2 -  Poil2 - Pwater2 - Psalts2
    ;
Poil3 = 25;//% ( 3 - extract )
//taking pulp ( inert ) balance
U = Ppulp1 * F / Ppulp2;
//oil balance gives , F * Poil1 = U * Poil2 + R *
    Poil3 ,from these , we get
R = (F * Poil1 - U * Poil2)/Poil3;
S = U + R - F;
disp("kg",S,"(a)The amount of solvent used for
    extraction = ")
Precovered = 95;//%
mhexane2 = Phexane2 * U / 100;
mrecovered = mhexane2 * Precovered / 100;
P = mrecovered * 100 / S ;
disp("%",P,"(b)Percent of hexane used that is
    recovered from the underflow = ")
Poil = Poil3 * R * 100 / (F * Poil1 );
disp("%",Poil,"(c)Percent recovery of oil = ")
```

Scilab code Exa 9.12 Dryer and oven

```
clc()
//F = feed(wet solid), V1 = water evaporated(drier),
     V2 = water evaporated(oven), S1 = Dry solid(
    drier), S2 = Dry solid(oven)
F = 1000;//kg
xf = 0.8;
x1 = 0.15;
x2 = 0.02;
```

```
//moisture free solid balance for drier, F * ( 1 -
    xf) = S1 * ( 1 - x1 )
S1 = F * ( 1 - xf )/(1 - x1);
//total balance for drier , F = S1 + V1
V1 = F - S1;
//For oven, S1 * ( 1 - x1 ) = S2 * ( 1 -x2 )
S2 = S1 * ( 1 - x1 )/(1 - x2);
//Also, S1 = S2 + V2
V2 = S1 - S2;
disp("kg",S1,"(a)Weight of product leaving the drier
    = ")
disp("kg",S2,"   Weight of product leaving the oven
    = ")
P1 = V1 *100/ (F * xf);
P2 = V2 *100/ (F * xf);
disp("%",P1,"(b)Percentage of original water removed
    in drier = ")
disp("%",P2,"   Percentage of original water removed
    in oven = ")
```

Scilab code Exa 9.13 Adiabatic drier

```
clc()
//Ss = solid flow rate,
Pwaterin = 25;//%
Pwaterout = 5;//%
X1 = Pwaterin/(100 - Pwaterin);//kg water/kg dry air
X2 = Pwaterout/(100 - Pwaterout);//kg water/kg dry
    air
//form humidity chart,
Y2 = 0.015;//kg water/kg dry air
Y1 = 0.035;//kg water/kg dry air
m = 1;//kg of dry air
//Ss * X1 + Y2 = Ss * X2 + Y1
Ss = (Y1 - Y2) / ( X1 - X2 );
```

```
T = 87.5 + 273.15;//K
P = 101.3;//kPa
Tstp = 273.15;//K
Pstp = 101.3;//kPa
Vstp = 22.4143;//m^3/mol
V = 100;//m^3
N = V * P * Tstp / ( Vstp * Pstp * T);
Nr2 = Y2 * 29 / 18;//kmol of water / kmol of dry air
Ndryair = N * 1 / (1 + Nr2);
mdryair = Ndryair * 29;
mevaporated = mdryair * ( Y1 - Y2 );
disp("kg",mevaporated,"(a)total moisture evaporated
    per 100m^3 of air entering = ")
Ss1 = mdryair * Ss;
mproduct = Ss1 * ( 1 + X2 );
disp("kg",mproduct,"(b)mass of finished product per
    100m^3 of air entering = ")
```

Scilab code Exa 9.14 Extraction of isopropyl alcohol

```
clc()
//F = feed , E = extract , S = solvent , R = Raffinate
xwaterF = 0.7;//Feed
xalcoholF = 0.3;
xwaterR = 0.71;//raffinate
xalcoholR = 0.281;
xethyR = 0.009;
xwaterE = 0.008;//Extract
xalcoholE = 0.052;
xethyE = 0.94;
//Total balance , R + E = F + S
F = 100;//kg
//R + E = 100 + S                              (1)
//Isopropyl balance , xalcoholR * R + xalcoholE*E =
    xalcoholF * F
```

```
//0.281*R + 0.052 * E = 30                  (2)
//Ethylene tetra chloride balance, xethyR * R +
    xethyE * E = S
//0.009*R + 0.94*E = S                      (3)
//Solving equation 1, 2 and 3 simultaneously, we get
    ,
S = 45.1;
E = 47.04;
R = 98.06;
disp("kg",S,"(a)Amount of solvent used = ")
disp("kg",E,"(b)Amount of extract = ")
disp("kg",R,"   Amount of raffinate = ")
mextracted = E * xalcoholE;
P1 = mextracted * 100 / (F * xalcoholF);
disp("%",P1,"(c)Percent of isopropyl alcohol
    extracted = ")
```

Scilab code Exa 9.15 Absorption of acetone

```
clc()
G1 = 100;//kmol
//G1 and G2 be the molar flow rate of the gas at the
     inlet and the exit of the absorber resp.,y1 and
    y2 mole fraction at entrance and exit resp.,
y1 = 0.25;//%
y2 = 0.05;//%
//air balance gives, G1 * ( 1-y1 ) = G2 * ( 1-y2 )
G2 = G1 * ( 1-y1 ) / (1 - y2);
maleaving = G2 * y2;
maentering = G1 * y1;
Pabsorbed = (maentering - maleaving) * 100 / (
    maentering);
disp("%",Pabsorbed,"Percentage of acetone absorbed =
     ")
```

Scilab code Exa 9.16 Absorption of SO3

```
clc()
F = 5000;//kg/h
P1 = 50;//% (H2O4 in)
MH2SO4 = 98.016;
P1gas = 65;//(nitrogen in gas entering)
P2gas = 35;// ( SO3)
MN2 = 28;
MSO3 = 80;
Mavg = ( MN2 * P1gas + MSO3 * P2gas)/100;//avg
    molecular wt. of entering gas
G = 4500;//kg/h
Ng = G / Mavg;
NN2 = Ng * P1gas / 100;
NSO3 = Ng - NN2;
P2 = 75;//% (H2O4 out)
//W be the mass of 75% H2SO4, x and y be the moles
    of SO3 and water vapour leaving resp.,
Pwater = 25;//kPa
Ptotal = 101.3;//kPa
//Pwater / Ptotal = y / ( NN2 + x + y )
//we get, y = 0.32765 * x + 2.744            (1)
//Total balance Feed + G = W + (NN2 * 28 + x * 80 +
    y * 18.016)
//we get, W + 80*x + 18.016*y = 7727.32      (2)
//from 1 and 2, 84.9174*x + W = 7352.68      (3)
//SO3 balance, So3 eneterin with 50% H2SO4 + SO3 in
    feed gas = SO leaving with 75%H2SO4 + SO3 leaving
     in exit gas
//5000*0.5*80/98.016 + 34.09*80 = 80* x + 0.75*W *
    80/98.016    (4)
// from 3 and 4,
x = 9.74;
```

```
Nabsorbed = NSO3 - x;
Pabsorbed = Nabsorbed * 100 / NSO3;
disp("%",Pabsorbed,"Percentage of SO3 absorbed = ")
```

Scilab code Exa 9.17 Continuous distillation column

```
clc()
F = 200;//kmol/h
//F, D and W be the flow rates of the feed, the
   distillate and residue resp., xf , xd and xw be
   the mole fraction of ethanol in the fee,
   distillate and the residue resp.
xf = 0.10;
xd = 0.89;
xw = 0.003;
//total balance gives, F = D + W
//D + W = 200              (1)
//Alcohol balance gives, F*xf = D*xd + W*xw
//0.89*D+0.003*W = 20       (2)
//solving 1 and 2
D = 21.87;//kmol/h
W = 178.13;//kmol/h
Nawasted = W*xw;
mmakeup = Nawasted * 46*24;
disp("kg",mmakeup,"The make up alcohol required per
   day = ")
```

Scilab code Exa 9.18 Distillation operation for methanol solution

```
clc()
F = 100;//kg
//F, D and W be the flow rates of the feed, the
   distillate and bottom product resp., xf , xd and
```

```
xw be the mole fraction of methanol in the fee , distillate and the bottom product resp.
xf = 0.20;
xd = 0.97;
xw = 0.02;
//using , F = D + W and F*xf + D*xd + W*xw,we get
D = 18.95;//kg/h
W = 81.05;//kg/h
R = 3.5;
//R = L / D
//for distillate = 1kg
D1 = 1;//kg
L = R*D1;
//Taking balance around the condenser ,
G = L + D1;
mcondensed = G * D / F;
disp("kg",D,"(a)Amount of distillate = ")
disp("kg",W,"    Amount of Bottom Product = ")
disp("kg",G,"(b)Amount of vapour condensed per kg of distillate = ")
disp("kg",mcondensed,"(c)Amount of vapour condensed per kg of feed = ")
```

Scilab code Exa 9.19 Bypass operation

```
clc()
mdryair = 1;//kg
Pwater1 = 1.4;//kPa ( Partial pressure at 285K )
Pwater2 = 10.6;//kPa ( Partial pressure at 320K )
P = 101.3;// ( Total )
Ys1 = Pwater2 * 18 / ((P - Pwater2)*29);//( saturation humidity at 320K )
Ys2 = Pwater1 * 18 / ((P - Pwater1)*29);//( saturation humidity at 285K )
Ys = 0.03;//kg water / kg dry air. (final humidity)
```

```
// humidity of air leaving dehumidifier is Ys2 and
   humidity of bypassed air is Ys1. these 2 streams
   combine to give humidity of 0.03kg water / kg dry
    air.
//therefore, taking balance we get, 1*Ys2 + x * Ys1
   = (1 + x)*Ys
x = (1*Ys2 - 1*Ys)/(Ys - Ys1);
disp("kg dry air",x,"(a)Mass of dry air bypassed per
    kg of dry air sent through the dehumidifier = ")
mcondensed = Ys1 - Ys2;
mwetair = mdryair + Ys1;
Nwetair = mdryair/29 + Ys1/18.016;
Vstp = 22.4143;//m^3/kmol
Vstp1 = Nwetair * Vstp;
T = 320;//K
P = 101.3;//kPa
Tstp = 273.15;//K
Pstp = 101.325;//kPa
V = Vstp1 * Pstp * T / (P * Tstp);
Vgiven = 100;//m^3
mcondensed1 = mcondensed * Vgiven / V;
disp("kg",mcondensed1,"(b)mass of water vapour
   condensed in the dehumidifier per 100m^3 of air
   sent through it = ")
mfinal = mdryair + x;
mfinalair = mfinal * Vgiven / V;
N = mfinalair / 29;
Ysn = Ys * 29/18;//kmol water / kmol dry air
Ntotal = N * (Ysn + 1);
Vfinal = Ntotal * Vstp * Pstp * T / ( Tstp * P );
disp("m^3",Vfinal,"(c)Volume of final air obtained
   per 100 cubic metres f air passed through
   dehumidifier = ")
```

Scilab code Exa 9.20 Recycle operation centrifuge plus filter

```
clc()
F = 100;//kg/h
xf = 0.2;
xp = 0.93;
xr = 0.5/1.5;
xx = 0.65;
//R - recycle stream, P - Product stream , W - water separeted and removed
//component A balance, F * xf = P * xp, that is,
P = F * xf / xp;
//Total balance, F = P + W,therefore
W = F - P;
//x be the flow rate of strea entering the filter
//total balance, x = P + R                    (1)
//component A balance , 0.65 * x = 0.5*R/1.5 + 0.93P    (2)
//Solving 1 and 2, we get,
R = (xx * P - xp * P)/(xr - xx);
disp("kg/h",R,"Flow rate of the recycle stream = ")
```

Scilab code Exa 9.21 Recycle operation granulator and drier

```
clc()
F = 1000;//kg/h
xfwater = 0.7;
xpwater = 0.2;
xrwater = 0.20;
xswater = 0.5;
y1 = 0.0025;
y2 = 0.05;
//R - recycle, S - stream entering granulator, P - Product, G1 - air entering the drier, G2 - air leaving the drier,
//takin overall, moisture free balance, F * xf = P *
```

```
xp
P = F * ( 1 - xfwater )/(1 - xpwater );
// taking material balance at point where recycle strea joins the feed,
// F = R + S
//water balance, F*xfwater = R*xrwater + S*xswater, solving this we get,
R = (-F*xfwater +F*xswater)/(xrwater - xswater);
S = F + R;
mleaving = P + R;//solid leaving the drier
//dry air entering will there be in air leaving, therefore
//G1 * ( 1 - y1 ) = G2 * ( 1 - y2 )
// water balance over the drier gives, S*xswater+G1*y1=G2*y2+(P+R)*xpwater
//from above 2 equations , we get
G1 = ((mleaving*xpwater - S*xswater)/(y1 - y2*(1-y1)/(1-y2)));
disp("kg/h",R,"(a)Amount of solid recycled = ")
mdryair = G1 * (1 - y1);
disp("kg/h",mdryair,"(b)circulation rate of air in the drier on dry basis = ")
```

Scilab code Exa 9.22 Blowdown operation

```
clc()
xf = 500 * 10^-6;
xp = 50 * 10^-6;
xb = 1600 * 10^-6;
//F - Feed water rate, B - blow down rate, S - high pressure steam, P - process stream rate
// total balance, F = P + B
// Solid balance, F * xf + P * xp = B * xb
//eliminating P, we get, F * xf + (F - B)*xp = B * xb
```

```
//let F/B be X
X = (xb + xp)/(xf + xp);
disp(X,"the ratio of feed water to the blowdown
    water = ")
```

Chapter 10

Material Balance with Chemical Reaction

Scilab code Exa 10.1 Combustion of propane

```
clc()
mair = 500;//kg
mCO2 = 55;//kg
mCO = 15;//kg
//C3H8 + 5O2 = 3CO2 + 4H20
MCO2 = 44;
MCO = 28;
NCO2 = mCO2 / MCO2;
NCO = mCO / MCO;
Mair = 29;
Nair = mair / Mair;
//carbon balance gives ,
F = (NCO2 + NCO)/3;
MC3H8 = 44.064;
mC3H8 = MC3H8 * F ;
disp("kg",mC3H8,"(a)mass of propane burnt = ")
//one mole of propane requres 5 moles of oxygen for
   combustion
NO2 = F * 5;
```

```
Nairt = NO2 * 100 /21;//theoretical air required
Pexcess = (Nair - Nairt) * 100 / Nairt;
disp("%",Pexcess,"(b)The percent excess air = ")
//C3H8 + 7/2 * O2 = 3CO + 4H2O
NH2O = F * 4;
//Taking oxygen balance, unburned oxygen is
    calculated,
//O2 supplied = O2 present in form of CO2, CO and
    H2O + unburned O2
Nunburnt = Nair * 21 / 100 - NCO2 - NCO/2 - NH2O/2;
NN2 = Nair * 79 / 100;
Ntotal = NCO2 + NCO + NH2O + NN2 + Nunburnt;
PCO2 = NCO2 * 100 / Ntotal;
PCO = NCO *100/ Ntotal;
PH2O = NH2O *100/ Ntotal;
PN2 = NN2 *100/ Ntotal;
PO2 = Nunburnt *100 / Ntotal;
disp("%",PCO2,"(c)Percent composition of CO2 = ")
disp("%",PCO,"Percent composition of CO = ")
disp("%",PH2O,"Percent composition of H2O = ")
disp("%",PN2,"Percent composition of N2 = ")
disp("%",PO2,"Percent composition of O2 = ")
```

Scilab code Exa 10.2 Combustion of hydrogen free coke

```
clc()
Nflue = 100;//kmol
NCO2 = 14.84;
NCO = 1.65;
NO2 = 5.16;
NN2 = 78.35;
PCF = 85;//PERCENT CARBON IN FEED
PIF = 15;//PERCENT INERT IN FEED
//F - amount of coke charged, W - mass of coke left,
    W = 0.05F
```

```
NCflue = NCO2 + NCO ;
MC = 12;
mC = MC * NCflue ;
//carbon balance gives, F * PCF / 100 = W * PCF + mC
F = mC / ( PCF / 100 - 0.05*PCF / 100);
//let A kmol air supplied, taking N2 balance,
Nair = NN2 * 100/79;
NO2supplied = Nair - NN2;
Ntheoretical = F * PCF / (100 * MC);
Pexcess = ( NO2supplied - Ntheoretical ) * 100 / (
    Ntheoretical );
disp("%",Pexcess,"(a)Percentage excess air = ")
mair = Nair * 29;
m = mair / F ;//air supplied per kg of coke charged
disp("kg",m,"(b)air supplied per kg of coke charged
    = ")
P = 100;//kPa
T = 500;//K
V = Nflue *22.4143*101.325 * T / (F * P * 273.15);
disp("m^3",V,"(c)volume of flue gas per kg of coke =
    ")
W = 0.05*F;
mCr = W * PCF/100;//carbon in refuse
mir = F * (1-PCF/100);//inert in refuse
mr = mCr + mir;
C = mCr * 100 / mr;
I = mir *100/ mr;
disp("%",C,"(d)Carbon = ")
disp("%",I,"Inert = ")
```

Scilab code Exa 10.3 Combustion of fuel oil

```
clc()
Nflue = 100;//kmol
NCO2 = 9;
```

```
NCO = 2;
NO2 = 3;
NN2 = 86;
NCflue = NCO2 + NCO ;
MC = 12;
mC = MC * NCflue ;
//let A kmol air supplied , taking N2 balance ,
Nair = NN2 * 100/79;
NO2supplied = Nair - NN2;
// if CO in the flue gas was to be completely converted to CO2, then , the moles of oxygen present in the flue gas would be 3−1 =2kmol
Noexcess = NO2 - NCO/2;
Pexcess =  Noexcess * 100 / ( NO2supplied - Noexcess );
disp("%",Pexcess,"(a)Percentage excess air = ")
NwaterO = NO2supplied - NCO2 - NCO/2 - NO2;
NH2 = NwaterO*2;
mH2 = NH2 * 2;
xCF = 0.7
R = mC / mH2;
disp(R,"(b)Ratio of carbon to hydrogen in the fuel = ")
//let x be the amount of moisture in the feed , n it is given that 70% is carbon ,therefore ,
//0.7 = 3.32 / ( 1 + 3.32 + x )
x = R / xCF - 1 - R;
mH = x * 2.016 / 18.016;
mHtotal = mH + mH2;
Rtotal = mC / mHtotal;
disp(Rtotal,"(c)Ratio of carbon to total hydrogen in the fuel = ")
ntotal = R + 1  +x;
PH2 = 1*100/ntotal;
PH2O = x * 100 / ntotal;
disp("%",PH2,"(d)percentage of combustible hydrogen in the fuel = ")
disp("%",PH2O,"percentage of moisture in the fuel =
```

```
")
nH2Ototal = (PH2O + PH2 * 18.016 / 2.016)/100;
disp("kg",nH2Ototal,"(e)The mass of moisture in the
    flue gas per kg of fuel burned = ")
```

Scilab code Exa 10.4 Combustion of producer gas

```
clc()
Nflue = 100;//kmoles
NCO2 = 9.05;
NCO = 1.34;
NO2 = 9.98;
NN2 = 79.63;
PCO2F = 9.2;//% ( Feed )
PCOF = 21.3;//%
PH2F = 18;//%
PCH4F = 2.5;//%
PN2F = 49;//%
//Taking carbon balance,
F = (NCO2 + NCO )/ ( (PCO2F + PCOF + PCH4F)/100);
//Nitrogen balance gives,
Nair = (NN2 - F*PN2F/(100) )* 100 / 79;
R = Nair/F;
disp(R,"(a)molar Ratio of air to fuel = ")
Oexcess = NO2 - NCO / 2;
Pexcess = Oexcess *100/ (Nair*21/100 - Oexcess);
disp("%",Pexcess,"(b)Percent excess of air = ")
NN2F = F * PN2F / 100;
PN2F = NN2F *100/ NN2;
disp("%",PN2F,"(c)Percent of nitrogen in the flue
    gas that came from fuel = ")
```

Scilab code Exa 10.5 Combustion of coal

```
clc()
Nflue = 100;//kmole
NCO2 = 16.4;
NCO = 0.4;
NO2 = 2.3;
NN2 = 80.9;
PCF = 80.5;//% ( Feed )
PO = 5.0;//%
PHF = 4.6;//%
PN = 1.1;//%
Pash = 8.8;//%
//Taking Carbon balance,
W = (NCO2 + NCO)*12 / (PCF / 100);
mCO2 = NCO2 * 44;
mCO = NCO * 32;
mO2 = NO2 * 28;
mN2 = NN2 * 28.014;
mtotal = mCO2 + mCO + mO2 + mN2;
Mdryflue = mtotal * 100/ W;
disp("kg",Mdryflue,"(a)The weight of dry gaseous
   products formed per 100 kg of coal fired = ")
//taking nitrogen balance,
x = (mN2 - W*PN/100)/28.014;
Noxygen = x * 21 / 79;
Nrequired = W * (PCF /12 + PHF/(2*2.016) - PO/32)
   /100;
Pexcess = (Noxygen - Nrequired)*100/Nrequired ;
disp("%",Pexcess,"(b)Percent excess air supplied for
    combustion = ")
```

Scilab code Exa 10.6 Stoichiometric analysis of combustion of coal

```
clc()
mcoal = 100;//kg
mC = 63;//kg
```

```
mH = 12;//kg
mO = 16;//kg
mash  =9;//kg
mfixC = 39;//kg
mH2O = 10;//kg
mCvolatile = mC - mfixC;
mHH2O = mH2O *2.016/18.016;//(mass of hydrogen in moisture)
mHvolatile = mH - mHH2O;
mOH2O = mH2O - mHH2O;
mOvolatile = mO - mOH2O;
mtvolatile = mCvolatile + mHvolatile + mOvolatile;
PC = mCvolatile * 100 / mtvolatile;
PH = mHvolatile * 100 / mtvolatile;
PO = mOvolatile * 100 / mtvolatile;
disp("%",PC,"(a)percent carbon in volatile matter = ")
disp("%",PH,"   percent hydrogen in volatile matter = ")
disp("%",PO,"   percent oxygen in volatile matter = ")
PCflue = 10.8;//%
Pvflue = 9.0;//%
Pashflue = 80.2;//%
//taking ash balance, Wis the weight of the refuse,
W = mash *100 / Pashflue;
mvflue = Pvflue * W /100;
mCflue = W * PCflue / 100;
Ctflue = mCflue + mvflue * PC / 100;//total carbon in flue
Htflue = mvflue * PH / 100;
Otflue = mvflue * PO / 100;
PCflue = Ctflue *100/W;
PHflue = Htflue *100/W;
POflue = Otflue *100/W;
disp("%",PCflue,"(b)percent Carbon in refuse = ")
disp("%",PHflue,"   percent Hydrogen in refuse = ")
disp("%",POflue,"   percent Oxygen in refuse = ")
```

```
disp("%",Pashflue,"    percent Ash in refuse = ")
Coalburnt = mcoal - W;
NCburnt = (mC - Ctflue)/12;
NHburnt = (mH - Htflue)/2.016;
NOburnt = (mO - Otflue)/32;
PCO2 = 80;//Percentage of carbon burnt
NCO2 = PCO2 * NCburnt / 100;
NCO = ( 1 - PCO2/100 )*NCburnt;
Vair = 1000;//m^3
Nair = Vair / 22.4143;
NN2 = Nair * 79 / 100;
NO2 = Nair * 21 / 100;
Ocompounds = NCO2 + NCO/2 + NHburnt/2;//Oxygen
   present in CO2,CO and H2O
//Oxygen balance gives free oxygen as,
Ofree = NO2 + mO/32 - Otflue/32 - Ocompounds;
Ntotal = NN2 + Ofree + NCO2 + NCO;//dry basis
PCO21 = NCO2 *100/Ntotal;
PCO1 = NCO * 100/Ntotal;
PO21 = Ofree * 100/Ntotal;
PN21 = NN2 * 100/Ntotal;
disp("%",PCO21,"(c)percent CO2 in flue = ")
disp("%",PCO1,"    percent CO in flue = ")
disp("%",PO21,"    percent O2 in flue = ")
disp("%",PN21,"    percent N2 in flue = ")
NOrequired = mC/12 + mH/(2.016*2) - mO/32;
Oexcess = NO2 - NOrequired;
Pexcess = Oexcess * 100 / NOrequired;
disp("%",Pexcess,"(d)Percent excess air supplied = "
   )
NH2Oflue = NHburnt;
mH2O = NH2Oflue * 18.016;
m = mH2O * 100/Ntotal;
disp("g water vapour / 100kmol dry flue gas",m,"(e)
   mass of water vapour per 100 moles of dry flue
   gas = ")
```

Scilab code Exa 10.7 Orsat analysis

```
clc()
Pexcess = 20;//%
PSO3 = 5;//% ( Percent of sulphur burnt to SO3 )
//S + O2 = SO2
N = 1;//kmol sulphur
Orequired = N;//kmol
Osupplied = Orequired * ( 1 + Pexcess/100);
Nsupplied = Osupplied * 79/21;
NSO2 = (1-PSO3/100)*N;
NSO3 = PSO3 * N /100;
Oconsumed = NSO2 + 3/2 * PSO3/100;
Oremaining = Osupplied - Oconsumed;
Ntotal = NSO2 + NSO3 + Oremaining + Nsupplied;
PSO2 = NSO2 * 100 / Ntotal;
PSO3 = NSO3 * 100 / Ntotal;
PO2 = Oremaining * 100 / Ntotal;
PN2 = Nsupplied * 100 / Ntotal;
disp("%",PSO2,"Percent SO2 in burner gas = ")
disp("%",PSO3,"Percent SO3 in burner gas = ")
disp("%",PO2,"Percent O2 in burner gas = ")
disp("%",PN2,"Percent N2 in burner gas = ")
```

Scilab code Exa 10.8 Burning of pyrites

```
clc()
Nburner = 100;//kmol
NSO2b = 9.5;//kmol
NO2b = 7;//kmol
NN2 = Nburner - NSO2b - NO2b;
NOsupplied = NN2 * 21 / 79;//Oxygen supplied
```

```
//4FeS2 + 11O2 = 2Fe2O3 + 8SO2
//4FeS2 + 15O2 = 2Fe2O3 + 8SO3
NOtotal = NO2b + NSO2b + NSO2b * 3 / 8;
NOunaccounted = NOsupplied - NOtotal;
NSO31 = NOunaccounted * 8 /15;
NStotal = NSO2b + NSO31;
mS = NStotal * 32.064;
Pburnt = 50;//% ( percentage of pyrites burnt )
mFeS2 = mS * 100/ Pburnt;
disp("kg",mFeS2,"(a)Total pyrites burnt = ")
NFeS2 = NStotal / 2;
MFeS2 = 119.975;
mFeS21 = MFeS2 * NFeS2;
mgangue = mFeS2 - mFeS21;
NFe2O3 = NFeS2 * Pburnt / 100;
MFe2O3 = 159.694;
mFe2O3 = MFe2O3 * NFe2O3;
PSO3c = 2.5;//% ( percentage sulphur as SO3 in cinder )
mc = 100;//kg ( basis )
NSO3 = PSO3c / 32.064;
mSO3 = NSO3 * 80.064;
mremaining = mc - mSO3;// ( Fe2O3 + gangue )
//x be the weight of the cinder
x = (mFe2O3 + mgangue)*100/mremaining ;
disp("kg",x,"(b)weight of cinder produced = ")
Slost = x * NSO3 / 100;
PSlost = Slost *100/ NStotal;
disp("%",PSlost,"(c)Percent of total S lost in the cinder = ")
mSO3c = mSO3 * x / 100;
NSO3b = NSO31 - Slost;
P = NSO3b * 100 / NStotal;
disp("%",P,"(d)Percentage of S charged that is present as SO3 in the burner gas = ")
```

Scilab code Exa 10.9 Production of sulphuric acid

```
clc()
Ncgas = 100;//kmol ( basis - SO3 free converter gas
   )
NSO2 = 4.5;//kmol
NO2 = 7.5;//kmol
NN2 = 88.0;//kmol
NOsupplied = NN2 * 21/ 79;
NOconverter = NO2 + NSO2;
NOconsumed = NOsupplied - NOconverter;//(Oxygen
   consumed for SO3)
NSO3c = NOconsumed / 1.5;
NStotal = NSO3c + NSO2;
Nbgas = 100;//kmol ( basis - SO3 free burner gas )
NSO21 = 15;//%
NO21 = 5;//%
NN21 = 80;//%
NOburner = NO21 + NSO21;
NOsupplied1 = NN21 * 21 / 79;
NOconsumed1 = NOsupplied1 - NOburner;//(Oxygen
   consumed for SO3)
NSO3b = NOconsumed1 / 1.5;
NStotal1 = NSO3b + NSO21;
mS = 100;//kg ( basis - sulphur charged )
Pburned = 95;//%
mburned = mS * Pburned / 100;
Nburned = mburned / 32.064;
//let x be the SO3 free burner gas produced, then
   sulphur balance gives,
x = Nburned * Nbgas / NStotal1;
NSO2b = NSO21 * x / 100;
NO2b = NO21 * x / 100;
NN2b = NN21 * x / 100;
```

```
Ntotalb = NSO2b + NO2b + NN2b;
NSO3b1 = NSO3b * x / 100;
//let y be the no. of converter gas produced
y = Nburned * Ncgas / NStotal;
NSO2c = NSO2 * y / 100;
NO2c = NO2 * y / 100;
NN2c = NN2 * y / 100;
Ntotalc = NSO2c + NO2c + NN2c;
NSO3c1 = NSO3c * y / 100;
Nairsec = (NN2c - NN2b ) * 100 / 79;
P = 100;//kPa
T = 300;//K
V = Nairsec * 22.414 * 101.3 * T / (P * 273.15);
disp("m^3/h",V,"(a)The volume of secondary air at
    100kPa and 300K = ")
NSabsorbed = 95;//%
mSO3abs = NSabsorbed * NSO3c1 * 80.064 / 100;
//let z be the amount of 98% H2SO4, therefore , 100%
    H2SO4 produced = z + mSO3abs
// taking SO3 balance
z = (mSO3abs - mSO3abs * 80.064 / 98.08) / ( 80.064
    / 98.08 - 0.98 * 80.064/98.08);
disp("kg",z,"(b)98% H2SO4 required per hour = ")
w = z + mSO3abs;
disp("kg",w,"(c)100% H2SO4 produced per hour = ")
```

Scilab code Exa 10.10 Burning of limestone mixed with coke

```
clc()
mlime = 5;//kg
mcoke = 1;//kg
PCaCO3l = 84.5;//%
PMgCO3l = 11.5;//%
NCaCO3l = PCaCO3l * mlime / (100.09*100);
NMgCO3l = PMgCO3l * mlime / (84.312*100);
```

```
mInertsl = mlime * ( 100 - PCaCO3l - PMgCO3l ) /
    100;
PCc = 76;//%
Pashc = 21;//%
Pwaterc = 3;//%
NCc = mcoke *  PCc /(100*12);
Nwaterc = mcoke * Pwaterc / ( 100 * 18.016 );
mash = Pashc * mcoke / 100;
//CaCO3 + C + O2 = CaO + 2CO2
//MgCO3 + C + O2 = MgO + 2CO2
PCaCO3conv = 95;//(Percent calcination of CaCO3)
PMgCO3conv = 90;//(Percent calcination of MgCO3)
NCaO = PCaCO3conv * NCaCO3l / 100;
mCaO = NCaO * 56.08;
NMgO = PMgCO3conv * NMgCO3l / 100;
mMgO = NMgO * 40.312;
mCaCO3 = (NCaCO3l * (1-PCaCO3conv/100)*100.09);
mMgCO3 = (NMgCO3l * (1-PMgCO3conv/100)*84.312);
mtotal = mCaO + mMgO + mCaCO3 + mMgCO3 + mInertsl +
    mash;
PCaO = mCaO * 100 / mtotal;
disp("%",PCaO,"The weight percent of CaO in the
    product leaving the kiln = ")
```

Scilab code Exa 10.11 treating limestone with aqueous H2SO4

```
clc()
R = 100;//kg ( basis - residue )
MCaSO4 = 136.144;
MMgSO4 = 120.376;
mCaSO4r = 9;//kg
mMgSO4r = 5;//kg
mH2SO4r = 1.2;//kg
minertr = 0.5;//kg
mCO2r = 0.2;//kg
```

```
mH2O = 84.10;//kg
NCaSO4 = mCaSO4r / MCaSO4;
NMgSO4 = mMgSO4r / MMgSO4;
//CaCO3 + H2SO4 = CaSO4 + H2O + CO2
//MgSO4 + H2SO4 = MgSO4 + H2O + CO2
mCaCO3 = NCaSO4 * 100.08;
mMgCO3 = NMgSO4 * 84.312;
mtotallime = minertr + mCaCO3 + mMgCO3;
PCaCO3 = mCaCO3 * 100/ mtotallime;
PMgCO3 = mMgCO3 *100/ mtotallime;
Pinerts = minertr *100/ mtotallime;
disp("%",PCaCO3,"(a)Percentage of CaCO3 in limestone = ")
disp("%",PMgCO3,"   Percentage of MgCO3 in limestone = ")
disp("%",Pinerts,"   Percentage of inerts in limestone = ")
NH2SO4 = NCaSO4 + NMgSO4;
mH2SO4 = NH2SO4 * 98.08;
Pexcess = mH2SO4r * 100 / ( mH2SO4);
disp("%",Pexcess,"(b)The percentage excess of acid used = ")
macidt = mH2SO4 + mH2SO4r;
Pacidic = 12;//%
mwaterin = macidt * (100 - Pacidic)/ Pacidic;
mwaterr = (NCaSO4 + NMgSO4)*18.016;
mwatert = mwaterin + mwaterr;
mvaporized = mwatert - mH2O;
m = mvaporized * 100/mtotallime;//water vaporized per 100kg of limestone
disp("kg",m,"(c)the mass of water vaporized per 100 kg of limestone = ")
mCO2pr = (NCaSO4 + NMgSO4)*44;
mCO2rel = mCO2pr - mCO2r;
m1 = mCO2rel * 100 / mtotallime;//CO2 per 100kg of limestone
disp("kg",m1,"(d)the mass of CO2 per 100kg of limestone = ")
```

Scilab code Exa 10.12 Production of TSP

```
clc()
macid = 1000;//kg ( basis - dilute phosphoric acid )
Mphacid = 97.998;
P = 1.25;//% ( dilute % )
mphacid = macid * P /100;
Nphacid = mphacid / Mphacid;
//1mole of phosphoric acid - 1mole of trisodium phosphate
NTSP = Nphacid;
MTSP = 380.166;
mTSP = NTSP * MTSP;
disp("kg",mTSP,"(a)Maximum weight of TSP obtained = ")
NCO2 = NTSP;
Pwater = 6.27//kPa
//since gas is saturated with water vapour, vapour pressure = partial pressure
Nwater = NCO2 * Pwater / ( 100 - Pwater );
Ntotal = Nwater + NCO2;
P = 100;//kPa
T = 310;//K
V = Ntotal * 101.3 * T *22.4143 / ( P * 273.15 );
disp("m^3",V,"(b)Volume of CO2 = ")
```

Scilab code Exa 10.13 Production of sodium phosphate

```
clc()
mTSPd = 1000;//kg ( basis - 20% dilute TSP )
P = 20;//%
```

```
mTSP = mTSPd * P / 100;
NTSP = mTSP / 163.974;
msodaashd = NTSP * 106;
mphacidd = NTSP * 97.998;
mNaOHd = NTSP * 40.008;
Pphacid = 85;//% (85% solution phosphoric acid)
PNaOH = 50;//% (50% solution NaOH)
//let x be the water in soda ash,
//taking water balance,
x = (mTSPd - mTSP) - mNaOHd * PNaOH /(100 - PNaOH) -
    mphacidd * (100 - Pphacid) / Pphacid;
msodaash = msodaashd + x;
C = msodaashd *100 / msodaash;
disp("%",C,"(a)Concentration of soda ash solution =
  ")
mphacid = mphacidd * 100 / Pphacid;
R = msodaash / mphacid;
disp(R,"(b)Weight ratio in which soda ash and
  commercial phosphoric acid are mixed = ")
```

Scilab code Exa 10.14 Production of pig iron

```
clc()
m = 1000;//kg ( basis - pig iron produced )
//let x be the iron ore charged and y be the amount
  of flux added and z be the weight of slag
  produced
PFepg = 95;//% ( Fe% in product )
PCpg = 4;//%
PSipg = 1;//%
PFech = 85;//% (Fe% in feed )
mcoke = 1000;//kg
PCcoke = 90;//%
PSicoke = 10;//%
PSislag = 60;//%
```

```
PSiflux = 5;//%
PCaCO3fx = 90;//%
PMgCO3fx = 5;//%
PCMslag = 40;//%
//iron balance gives ,
x = PFepg * m *159.694 / ( PFech * 111.694);
//silicon balance gives ,
//x*(100 - PFech)*28.086/(100*60.086)+mcoke*Psicoke
   *28.086/(100*60.086)+y*PSiflux
   *28.086/(100*60.086) = 10 + z*Psislag*28.086 / (
   100*60.086 )
//taking (CaO + MgO) balance
//y * ((PCaCO3fx)*56.88/(100*100.88)+(PMgCO3fx
   *40.312/(100*84.312))=z*PCMslag/100
//solving above 2 equations , we get
y = 403.31;
disp("kg",y,"the amount of flux required to produce
   1000kg of pig iron = ")
```

Scilab code Exa 10.15 Production of nitric acid

```
clc()
N = 100;//mol(basis - scrubber)
NNOs = 2.4;//mol
NN2s = 92;//mol
NO2s = 5.6;//mol
PNOs = 20;//% ( Percentage NO leaving scrubber)
NNOreac = NNOs * 100 / PNOs;
//let x mol of nitroge be produced in the reaction ,
   then the amount of N2 present in the air = NN2s -
    x mol - (1)
//4NH3 + 5O2 = 4NO + 6H2O
//4NH3 + 3O2 = 2N2 + 6H2O
//4moles of NO - 5 moles of O2, 2moles of N2 - 3
   moles of O2
```

```
//Total oxygen used up, O  =  NNOreac * 5/4 + x*3/2
//total oxygen supplied , NOtotal= (O) + NO2s
//Nitrogen associated with O2 supplied NN2 = NOtotal *79/21 - (2)
//comparing 1 and 2,
x = 2.1835;
//12moles NO requires 12moles ammonia, 1 mole N2 requires 2 mole ammonia
Nammonia = x*2 + NNOreac;
Oreq = Nammonia * 5 / 4;
Osupp = NNOreac * 5/4 + x*3/2 + NO2s;
Pexcess = (Osupp - Oreq)*100/Oreq ;
disp("%",Pexcess,"(a)Percentage excess oxygen = ")
fr = x * 2 / Nammonia;
disp(fr,"Fraction of ammonia taking part in side reaction = ")
```

Scilab code Exa 10.16 Material balance in nitric acid production

```
clc()
m = 100;//kg (basis sodium nitrate reacted)
NNaNO3 = m/85;
//2NaNO3 + H2SO4 = 2HNO3 + Na2SO4
mh2so4 = NNaNO3 * 98.08/2;
mhno3 = NNaNO3*63.008;
mna2so4 = NNaNO3 * 142.064 /2;
Phno3 = 2;//%(percent nitric acid remaining in the cake)
mhno3cake = mhno3 * Phno3 / 100;
Ph2so4 = 35;//%
Pwater = 1.5;//%
mtotal = (mna2so4 + mhno3cake)*100/(100 - Ph2so4 - Pwater);
mwater = Pwater * mtotal / 100;
mh2so4c = Ph2so4 * mtotal / 100;
```

```
Pna2so4 = mna2so4 *100/mtotal;
Phno3c = mhno3cake * 100 / mtotal;
disp("kg",mna2so4,"(a)Mass of Na2SO4 in the cake = ")
disp("kg",mhno3,"Mass of HNO3 in the cake = ")
disp("kg",mwater,"Mass of water in the cake = ")
disp("kg",mh2so4c,"Mass of H2SO4 in the cake = ")
disp("%",Pna2so4,"Percentage of Na2SO4 in the cake = ")
disp("%",Phno3c,"Percentage of HNO3 in the cake = ")
disp("%",Pwater,"Percentage of water in the cake = ")
disp("%",Ph2so4,"Percentage of H2SO4 in the cake = ")
mh2so4req = mh2so4 + mh2so4c;
P = 95;//% (95% dilute sulphuric acid)
w = mh2so4req * 100 / P;
disp(mh2so4)
disp("kg",w,"(b)Weight of 95% sulphuric acid required = ")
mnitric = mhno3 - mhno3cake;
disp("kg",mnitric,"(c)weight of nitric acid product obtained = ")
mwaterd = w*(1-P/100)-mwater;
disp("kg",mwaterd,"(d)the water vapour tha tis distilled from the nitre cake = ")
```

Scilab code Exa 10.17 Electrolysis of brine

```
clc()
m = 50;//kg ( basis - mass of brine charged )
//let x be the amount of NaCl in the brine
Pelect = 50;//% ( electrolyzed )
//2NaCl + 2H2O = 2NaOH + Cl2 + H2
//amount of NaCl reacted =x*Pelect/(100*58.45)kmol=x
```

```
*Pelect/100kg    ( 1 )
//amount of water reacted = x * Pelect * 18.016 / ( 100 * 58.45 )kg ( 2 )
//Gases produced, Cl2 = x * Pelect / (100 * 58.45 * 2 )kmol = x * Pelect *71/ (100 * 58.45 * 2 )kg                                        ( 3 )
//H2 = x * Pelect / (100 * 58.45 * 2 )kmol = x * Pelect *2.016/ (100 * 58.45 * 2 )kg

( 4 )
Nwater = 0.03;//mol water vapour/mol of gas
//water vapour present = Nwater * 2*(Cl2 + H2)kmol = Nwater * 2*(Cl2 + H2)*18.016 kg

( 5 )
//NaoH = x * Pelect * 40.008/ (100 * 58.45 )kg                        ( 6 )
//water = water in brine - water reacted - water present in gas      ( 7 )
//= (m - Pelect/100) - water reacted ( 2 ) - water present in the gas( 5 )
//Total weight of solution = NaCl ( 1 ) + NaOH ( 6 ) + Water ( 7 )
//since NaOH is 10 percent of the total weight, we have NaOH = 0.1 * total weight, from these we get ,
x = 0.1 * 50 / (0.1* 0.3165 + 0.3422 );
NaOH = x * Pelect * 40.008/ (100 * 58.45 );
NaCl = x * Pelect / 100;
water = 34.5032;//kg
Pevap = 50;//NaOh percentage in solution leaving evaporator
//taking NaOH balance
mevap = NaOH * 100 / Pevap;
disp("kg",mevap,"(a)amount of 50% NaOH solution produced = ")
Cl2 = x * Pelect *71/ (100 * 58.45 * 2 );//kg
H2 = x * Pelect *2.016/ (100 * 58.45 * 2 );//kg
```

```
disp("kg",Cl2,"(b)Chlorine produced = ")
disp("kg",H2,"   Hydrogen produced = ")
Pleav = 1.5;//% NaCl leaving the evaporator
NaClleav = mevap * Pleav / 100;
mcrystal = NaCl - NaClleav;
disp("kg/h",mcrystal,"(c)Amount of NaCl crystallized = ")
mwaterleav = mevap - NaOH - NaClleav;
Mwaterevap = water - mwaterleav;
disp("kg",Mwaterevap,"(d)Weight of water evaporated = ")
```

Scilab code Exa 10.18 Preparation of Formaldehyde

```
clc()
m = 100;//mol ( basis reactore exit gas )
//CH3OH + O2 = HCOOH + H2O
//CH3OH + O2 / 2 = HCHO + H2O
Nn2 = 64.49;//mol
No2 = 13.88;//mol
Nh2o = 5.31;//mol
Nch3oh = 11.02;//mol
Nhcho = 4.08;//mol
Nhcooh = 1.22;//mol
//x be the moles of methanol reacted , taking C balance , we get ,
x = Nch3oh + Nhcho + Nhcooh;
Pconv = Nhcho * 100 / x ;
disp("%",Pconv,"(a)Percent conversion of formaldehyde = ")
Nair = Nn2 * 100 / 79;
R = Nair / x;
disp(R,"(b)Ratio of air to methanol in the feed = ")
```

Scilab code Exa 10.19 Recycle operation reactor and separator

```
clc()
NA = 100;//mol ( basi - 100 mol A in the fresh feed
    )
Pconv = 95;//%
NApro = NA * (100 - Pconv)/100;
//A = 2B + C
NB = NA * Pconv * 2 / 100;
NC = NA * Pconv/100;
PAent = 0.5;//%
NAent = NApro * 100 / PAent;
PBrec = 1;//%
NBent = NB * 100 / (100 - PBrec);
m = (NAent - NApro + NA);
conv = ((NAent - NApro + NA) - NAent)*100/(NAent -
    NApro + NA);
disp("%",conv,"(a)single pass converion = ")
Nrecycled = (NAent - NApro) + (NBent - NB);
R = Nrecycled/NA;
disp(R,"(b)recycle ratio = ")
```

Scilab code Exa 10.20 Conversion of sugar to glucose and fructose

```
clc()
m = 100;//kg ( basis - sucrose solution as fresh
    feed )
//R - recycle reactor exit , let x be the weight
    fraction of sucrose and y be the weight fracton
    of inversion sugar in the recycle stream , for
    combined stream  fraction of Glucose + fructose =
     0.04
```

```
//z be the weight fraction of sucrose in the combined stream entering the reactor
Psfeed = 25;//% percent sucrose in fresh feed
//sucrose balance gives, 25 + R*x = (100+R)* z (A)
//Glucose + fructose balance, R * y = (100 + R )*0.04 (B)
Sucrosecon = 71.7;//% sucrose consumed
//sucrose balance around the reactor,(100+R)z=0.717*(100+R)z+(100+R)x (C)
//From (C) , x = 0.283*z (D)
//Amount converted to Glucose + fructose = 0.717 ( 100 + R )* z
// = 0.717 ( 100 + R )* z * 360.192 / 342.176 kg
//Glucose and fructose balance around the reactor,
//(100+R)*0.04 + 0.717(100+R)*z*360.192/342.176 = (100+R)*y (E)
//Solving (E), y = 0.04 + 0.7548*z (F)
//Solving, (A), (B), (C) and (F)
x = 0.06;
y = 0.2;
z = 0.212;
R = 25;
disp("kg",R,"(a)Recycle flow = ")
disp("%",y*100,"(b)Combined concentration of Glucose and Fructose in the recycle stream = ")
```

Scilab code Exa 10.21 Purging operation

```
clc()
N = 1;//mol ( basis - combined feed )
//F - moles of fresh feed
Pinert = 0.5;//%
```

```
Pconv = 60;//%
P1inert = 2;//%
NA1 = N * ( 1- P1inert/100 );
NA2 = NA1 * ( 1 - Pconv / 100 );
NB2 = NA1 - NA2;
N1inert = N * P1inert / 100;
N2inert = N1inert;
//Let R be the moles recycled and P be the moles purged
//W = R + P
W = NA2 + N2inert;//                    (A)
PWinert = N2inert * 100/ ( NA2 + N2inert);
//component A balance , A fresh feed = A purge stream + A recycle stream
//F * 0.9 = P * 0.9515 + 0.588           (B)
//inert balance at the point where fresh feed is mixed with the recycle ,
//F*0.005 + R*0.0485 = 1* 0.02           (C)
//Solving (A) ,(B) and (C)
F = 0.6552;//mol
P = 0.0671;//mol
R = 0.3448;//mol
disp("mol",R,"(a)moles of recycle stream = ")
disp("mol",P,"(b)moles of purge stream = ")
NAconv = NA1 - NA2;
NAf = F * (1 - Pinert / 100);
Conv = NAconv *100/ NAf;
disp("%",Conv,"(c)Overall conversion = ")
```

Scilab code Exa 10.22 Purging operation for production of methanol

```
clc()
```

```
N = 100;//moles ( Basis - Fresh feed )
Pconv = 20;//%
xco = 0.33;
xh2 = 0.665;
xch4 = 0.005;
//R - recycle stream, P - purge stream
//x - mole fraction of CO in recycle stream ,
xch4r = 0.03;
//CO = x, H2 = 1 - xch4r - CO = 0.97- x;
//methane balance over the entire system,
P = xch4 * N / xch4r;
//taking caron balance, 33.5 = M + P ( 0.03 + x )
//Hydrogen balance, 66.5 + 2*0.5 = 2M + P(2*0.03 + 0.97 - x)
//substituting P, M + 16.67x = 33.0 and 2M - 16.67x = 50.33
M = (33.0 + 50.33)/3;
x = ((xco + xch4)*N - M ) / P - xch4r;
//methanol balance,(xco*N+Rx) * Poncv/100 = M
R = (M*100 / Pconv - (xco*N))/x;
disp("mol",R,"(a)moles of recycle stream = ")
disp("mol",P,"(b)moles of purge stream = ")
H2 = 1 - xch4r - x;
disp("%",xch4r*100,"(c)CH4 in purge stream = ")
disp("%",x*100,"CO in purge stream = ")
disp("%",H2*100,"hydrogen in purge stream = ")
disp("mol",M,"(d)Methanol produced = ")
```

Chapter 11

Energy Balance Thermophysics

Scilab code Exa 11.1 Power calculation

```
clc()
m = 75;//kg
g = 9.81//m^2/s
d = 10;//m
t = 2.5*60;//s
f = m*g;
w = f * d;
P = w / t;
disp("Nm",w,"The work done = ")
disp("W",P,"Power required = ")
```

Scilab code Exa 11.2 Kinetic energy calculation

```
clc()
PE = 1.5*10^3;//J
m = 10;//kg
g = 9.81;//m/s^2
v = 50;//m/s
```

```
//PE = mgz
z = PE / (m*g);
KE = m* (v^2) / 2;
disp("m",z,"Height of the body from the ground = ")
disp("kJ",KE/1000,"Kinetic energy of the body = ")
```

Scilab code Exa 11.3 Work done calculation for a gas confined in a cylinder

```
clc()
d = 100 /1000;//m
m = 50;//kg
P = 1.01325*10^5;//Pa
A = %pi * (d^2)/4;
Fatm = P * A;
Fwt = m * g;
Ftotal = Fatm + Fwt;
P = Ftotal / A;
disp("bar",P/10^5,"(a)Pressure of the gas = ")
z = 500/1000;//m
w = Ftotal * z;
disp("J",w,"(b)Work done by the gas = ")
```

Scilab code Exa 11.4 Power requirement of the pump

```
clc()
Sgr = 0.879;
F = 5;//m^3/h
D = Sgr * 1000;
m = F * D/3600;//kg/s
P = 3500;//kPa
W = P * m * 1000/ D;
disp("W",W,"Power requirement for the pump = ")
```

Scilab code Exa 11.5 Specific enthalpy of the fluid in the tank

```
clc()
d = 3;//m
m = 12500;//kg
P = 7000;//kPa
U = 5.3*10^6;//kJ
Vtank = 4*%pi*((d/2)^3) / 3;
Vliq = Vtank / 2;
H = U + P * Vliq;
disp("kJ/kg",H/m,"Specific enthalpy of the fluid in
    the tank = ")
```

Scilab code Exa 11.6 internal energy and enthalpy change calculation

```
clc()
P = 101.3;//kPa
SVl = 1.04 * 10^-3;//m^3/kmol
SVg = 1.675;//m^3/kmol
Q = 1030;//kJ
W = P * 10^3 * (SVg - SVl)/1000;
U = Q - W;
H = U +  P * 10^3 * (SVg - SVl)/1000;
disp("kJ/kmol",U,"Change in internal energy = ")
disp("kJ/kmol",H,"Change in enthalpy = ")
```

Scilab code Exa 11.7 change in internal energy

```
clc()
```

```
//work is done on the system, hence, W is negative
W = - 2 * 745.7;//J/s
//heat is transferres to the surrounding, hence,
    heat transferred is negative,
Q = -3000;//kJ/h
U = Q*1000/3600 - W;
disp("J/s",U,"Change in internal energy = ")
```

Scilab code Exa 11.8 reaction of iron with HCl

```
clc()
//Fe(s) + 2HCl(aq) = FeCl2(aq) + H2(g)
MFe = 55.847;
m = 1;//kg
Nfe = m * 10^3/MFe;
Nh2 = Nfe;//(since 1 mole of Fe produces 1 mole of
    H2)
T = 300;//K
R = 8.314;
//the change in volume is equal to the volume
    occupied by hydrogen produced
PV = Nh2 * R * T;
W = PV;
disp("kJ",W,"Work done = ")
```

Scilab code Exa 11.9 Thermic fluid

```
clc()
//Cp =1.436 + 2.18*10^-3*T;
m = 1000/3600;//kg/s
T1 = 380;//K
T2 = 550;//K
x = integrate('1.436 + 2.18*10^-3*T','T',T1,T2);
```

```
Q = m*x;
disp("kW",Q,"Heat load on the heater = ")
```

Scilab code Exa 11.10 Heat capacity

```
clc()
//Cp = 26.54 + 42.454*10^-3 * T - 14.298 * 10^-6 * T
    ^2;
T1 = 300;//K
T2 = 1000;//K
m = 1;//kg
N = m/44;//kmol
x = integrate('26.54 + 42.454*10^-3 * T - 14.298 *
    10^-6 * T^2','T',T1,T2);
Q = N*x;
disp("kJ",Q,"(a)Heat required = ")
//for temperature in t degree celsius
//Cp = 26.54 + 42.454*10^-3 * (t + 273.15) - 14.298
    * 10^-6 * (t + 273.15)^2
//Cp = 37.068 + 34.643 * 10^-3*t - 14.298* 10^-6 * t
    ^2 (kJ/kmolC)
//Cp = 8.854 + 8.274*10^-3*t -3.415*10^-6*t^2 ( Kcal
    /kmolC)
//For degree Fehreneit scale,replacet by ( t1 - 32)
    /18, we get
//Cp = 8.7058 + 4.6642 * 10^-3 *t1 - 1.0540 * 10^-6
    * t1^2 ( Btu/lbmolF)
```

Scilab code Exa 11.11 Enthalpy change when chlorine gas is heated

```
clc()
```

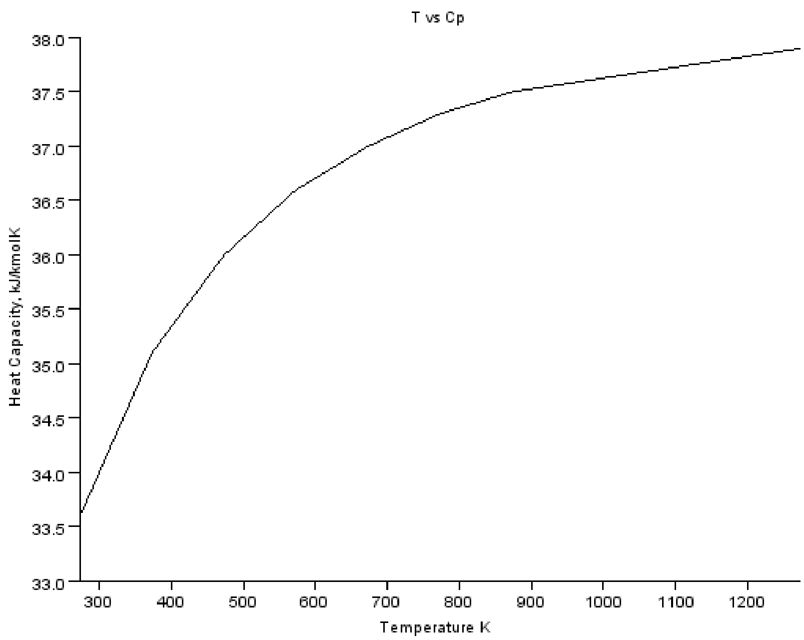

Figure 11.1: Enthalpy change when chlorine gas is heated

```
T = [273 373 473 573 673 773 873 973 1073 1173
   1273];
Cp = [33.6 35.1 36 36.6 37 37.3 37.5 37.6 37.7 37.8
   37.9];
plot2d(T,Cp,rect=[273,33,1273,38])
xtitle(" T vs Cp","Temperature K","Heat Capacity, kJ
   /kmolK")
// at constant Pressure, H = integration(Cp,T,T1,T2)
//Area under the curve form the graph ,is obtained
   as Area = 36828
H = 36828;//kJ/kmol
disp("kJ/kmol",H,"Enthalpy change = ")
```

Scilab code Exa 11.12 Molal heat capacity

```
clc()
//Cp = 26.586 + 7.582 * 10 ^-3 * T - 1.12 * 10^-6 *
   T^2
T1 = 500;//K
T2 = 1000;//K
x = integrate('26.586 + 7.582 * 10^-3 * T - 1.12 *
   10^-6 * T^2','T',T1,T2);
Cpm = 1 *x / ( T2 - T1 ) ;
disp("kJ/kmolK",Cpm,"(a)Mean molal heat capacity = "
   )
V = 500;//m^3;
N = V / 22.4143;
Q = N * Cpm * ( T2 - T1 );
disp("kJ/h",Q,"(b)Heat to be supplied = ")
T3 = 1500;//K
Q1 = Cpm * (T3 - T1);
y = integrate('26.586 + 7.582 * 10 ^-3 * T - 1.12 *
   10^-6 * T^2','T',T1,T3);
Q2 = y ;
disp(Q2)
```

```
Perror = (Q2 - Q1) * 100 / Q2;
disp("%",Perror,"(c)Percent error = ")
```

Scilab code Exa 11.13 Enthalpy change of a gas

```
clc()
T1 = 1500;//K
Tr = 273;//K
T2 = 400;//K
Cpm1 = 50;//kJ/kmol
Cpm2 = 35;//kJ/mol
H = Cpm1 * ( T1 - Tr ) - Cpm2 * ( T2 - Tr );
disp("kJ/kmol",H,"Enthalpy change = ")
```

Scilab code Exa 11.14 Combustion of solid waste

```
clc()
//CO,  26.586 + 7.582*10^-3*T - 1.12*10^-6*T^2
//CO2, 26.540 + 42.454*10^-3*T - 14.298*10^-6*T^2
//O2, 25.74 + 12.987*10^-3*T - 3.864*10^-6*T^2
//N2, 27.03 + 5.815*10^-3*T - 0.289*10^-6*T^2
//Cpmix = summation ( yi*Cpi ) = summation(yi*ai +
    yi*bi*T + yi*ci*T^2)
xco2 = 0.09;
xco = 0.02;
xo2 = 0.07;
xn2 = 0.82;
T1 = 600;//K
T2 = 375;//K
sumai = xco * 26.586 +xco2 * 26.540 + xo2 * 25.74 +
    xn2*27.03;
sumbi = xco * 7.582*10^-3 + xco2*2.454*10^-3+xo2
    *12.987*10^-3 + xn2*5.815*10^-3;
```

```
sumci = -(xco * 1.12*10^-6 + xco2*14.298*10^-6+xo2
    *3.864*10^-6+xn2*0.289*10^-6);
H = integrate('sumai+sumbi*T+sumci*T^2','T',T1,T2);
disp("kJ/kmol",H,"Enthalpy change = ")
```

Scilab code Exa 11.15 Heat capacity calculation for Na2SO4 10H2O

```
clc()
Hna = 26.04;//J/g-atomK
Hs = 22.6;//J/g-atomK
Ho = 16.8;//J/g-atomK
Hh = 9.6;//J/g-atomK
Hna2so410h2o = 2*Hna + Hs + 14*Ho  + 20*Hh;
Hexp = 592.2;//J/molK
Deviation = (Hexp - Hna2so410h2o)*100/Hexp;
disp("%",Deviation,"Deviation in heat capacity = ")
```

Scilab code Exa 11.16 Heat of vaporization calculation

```
clc()
P1 = 75;//kPa
T1 = 573;//K
Tvap = 365;//K
Tbasis = 273;//K
//Since, the boiling point of water at 75kPa is 375K
    , the vapour at 573K is superheated;
H1 = 3075;//kJ/kg
Cliq = 4.2;//kJ/kgK
Cvap = 1.97;//kJ/kg/K
m = 1;//kg
//let assume converting liq. water into superheated
    stream occurs in 3 steps,
```

```
//step1 - water is heated from 273K to 365 K at
    constant pressure,enthalpy change is the heat
    required to change the temperature,
Hc1 = m*Cliq * ( Tvap - Tbasis );
//step2 - the liq is vapurized at constant pressure
    and constant temperature, enthalpy change is
    equal to the heat of vapourisation, say Hc2
//step3 - the saturated vapour at 365K is heated to
    573K at constant pressure, the enthalpy change is
     the heat required to raise the temperature
Hc3 = m*Cvap*(T1 - Tvap);
//total enthalpy = 3075 = Hc1 + Hc2 + Hc3, therefore
Hc2 = H1 - Hc1 - Hc3;
disp("kJ/kg",Hc2,"Heat of vapourisation = ")
```

Scilab code Exa 11.17 Heat requirement

```
clc()
T1 = 250;//K
T = 273.15;//K
T2 = 400;//K
Cice = 2.037;//kJ/kgK
T3 = 373.15;//K
Cliq = 75.726;//kJ/kmolK
//Cp = 30.475 + 9.652*10^-3*T + 1.189*10^-6*T^2
Hfusion = 6012;//kJ/kmol
Hvap = 40608;//kJ/kmol
//1 - Heat for raising the temperature of ice, H1
H1 = Cice * (T - T1);
//2 - Latent heat of fusion of ice,  Hf
Hf = Hfusion / 18.016;//kJ
//3 - Sensible heat of raising the temperature of
    water, H2
H2 = Cliq * ( T3 - T)/18.016;
//4 - Latent heat of vaporization of water, Hv
```

```
Hv = Hvap / 18.016;
//5 - Sensible heat of raising the temperature of water vapou, H3
H3 = (integrate('30.475 + 9.652*10^-3*T + 1.189*10^-6*T^2','T',T3,T2))/18.016;
Q = H1 + H2 + H3 + Hf + Hv;
disp("kJ",Q,"Heat required = ")
```

Scilab code Exa 11.18 Equilibrium temperature of mixture

```
clc()
//Cp = 0.16 + 4.78 * (10^-3) * T ( organic liquid )
//Cp = 0.7935 + 1.298 * (10^-4) * T ( CCL4 )
Tb = 349.9;//K
Hv = 195;//kJ/kg
Cp = 0.4693;//kJ/kgK
//Let T be the final temperature
//integration(T - 650)(0.16 + 4.78 * (10^-3) * T)dt = integration(295 - T)(0.7935 + 1.298 * (10^-4) * T)dt
// the above equation yields, 2.4549*(10^-3)*T^2 + 0.9535*T - 1353.51 = 0, from this we get
T = 573.3;//K
//since this temperature is above boiling point of CCl4,
//heat balance is, integration(T - 650)(0.16 + 4.78 * (10^-3) * T)dt = integration(295 - 349.9)(0.7935 + 1.298 * (10^-4) * T)dt + Hv + integration(349.9 - T)*0.4693*dT
//solving above equation, we get,
T1 = 540.1;//K
disp("K",T1,"equilibrium temperature of the mixture = ")
```

Scilab code Exa 11.19 Estimation of mean heat of vaporisation

```
clc()
T1 = 363;//K
T2 = 373;//K
P1s = 70.11;//kPa
P2s = 101.3;//kPa
R = 8.314;//kJ/kmolK
// ln(P2s / P1s) = Hv / R * (1/T1 - 1/T2);
Hv = (log(P2s/P1s)*R)/(1/T1 - 1/T2);
Hv1 = Hv / (18);
disp("kJ/kg",Hv1,"Mean heat of vaporization = ")
```

Scilab code Exa 11.20 Heat of vaporization of methyl chloride

```
clc()
T = 273.15 - 30;//K
//lnPs = 14.2410 - 2137.72 / (T-26.72)
//dlnPs/dT = Hv / RT2
Hv = 2137.72 * R * T^2 / ( T - 26.72 )^2;
disp("kJ/kmol",Hv,"Heat of vaporization = ")
```

Scilab code Exa 11.21 Watson equation

```
clc()
Hv1 = 2256;//kJ/kg
T1 = 373;//K
T2 = 473;//K
Tc = 647;//K
```

```
Tr1 = T1 / Tc;
Tr2 = T2 / Tc;
//Hv2 / Hv1 = ((1-Tr2)/(1-Tr1))^0.38
Hv2 = Hv1*(((1-Tr2)/(1-Tr1))^0.38);
disp("kJ/kg",Hv2,"Latent heat of vaporization of
    water at 473K = ")
```

Scilab code Exa 11.22 Kistyakowsky equation

```
clc()
//Cp = a + b*T
T1 = 293.15;//K
Cp1 = 131.05;//J/molK
T2 = 323;//K
Cp2 = 138.04;//J/molK
//a + 293*b = 131.05
//a + 323*b = 138.04
b = (Cp1 - Cp2)/(T1 - T2);
a = Cp1 - b * T1;
//Cp = 62.781 + 0.233*T
// Hvb / Tb = 36.63 + 8.31lnTb
Tb = 273.15 + 80.1;//K
Hvb = (36.63 + 8.31*log(Tb)) * Tb;
m = 100;//kg
H = m*(10^3) * (integrate('62.781 + 0.233*T','T',T1,
    Tb))/78.048 + m*(10^3)*Hvb/78.048;
disp("J",H,"Heat required = ")
```

Scilab code Exa 11.23 Quality of steam

```
clc()
P = 10;//kPa
T1 = 323.15;//K
```

```
T2 = 373.15;//K
T = 358.15;//K
H1 = 2592.6;//kJ/kg
H2 = 2687.5;//kJ/kg
//H by interpolation ,
H = H1 + ((H2 - H1)/(T2 - T1))*(T - T1);
Hl = 697.061;//kJ/kg
Hg = 2762;//kJ/kg
//H = x*Hl + ( 1 - x )* Hg
x = (H - Hg)/(Hl - Hg) ;
Pmois = x*100;
Psteam = ( 1 - x )*100;
disp("%",Pmois,"Percentage of moisture = ")
disp("%",Psteam,"Percentage of dry saturated steam = ")
```

Scilab code Exa 11.24 Heat calculation

```
clc()
P = 3500;//kPa
T = 673.15;//K
SV = 0.08453;//m^3/kg
Vcondensed = 1/2;
m = 100;//kg
V = m * SV / (m/2);
//m*(Vl+Vg)*Vcondensed = m * SV
//But Vl is negligible ,
Vg = m * SV / (m * Vcondensed);
//using steam table
T1 = 459.5;//K
P1 = 1158;//kPa
//internal energy of superheated steam from steam table
I = 2928.4;//kJ/kg
U1 = m * I;
```

```
U1 = 790;//kJ/kg
Ug = 2585.9;//kJ/kg
U2 = m*Vcondensed*Ul + m*(1-Vcondensed)*Ug;
Q = U2 - U1;
disp("kJ",Q,"The amount of heat removed fromt he
    system = ")
```

Scilab code Exa 11.25 Enthalpy balance for evaporation process

```
clc()
m = 1000;//kg/h ( basis  mass of 10% NaOH solution )
Pfeed = 10;//%
Ppro = 50;//(Percentage NaOH in product)
//Taking NaOH balance,P being the weight of the
    product
P = Pfeed * m / Ppro;
//W be the weight of water evaporized
W = m - P;
//step1 - cooling 1000kg/h of 10% solution from 305K
     to 298K
T1 = 305;//K
T2 = 298;//K
Cliq = 3.67;//kJ/kgK
H1 = m*Cliq * (T2 - T1);
//step2 - separation into pure components
Hsolution = -42.85;//kJ/mol
H2 = -Pfeed * m *1000 *Hsolution/ (40*100);
//step3 - W kg water is converted to water vapour
Hvap = 2442.5;//kJ/kg
H3 = W * Hvap;
//step4 - water vapour at 298K is heated to 373.15K
Cvap = 1.884;//kJ/kgK
T3 = 373.15;//K
H4 = W * Cvap * ( T3 - T2 );
//step5 - formation of 200kg of 50% NaOH solution at
```

```
   298K
Hsolu = -25.89;//kJ/mol
H5 = Pfeed * m *1000 *Hsolu/ (40*100);
//step6 - Heating the solution from 298K to 380K
Csolu = 3.34;//kJ/kg
T4 = 380;//K
H6 = P * Csolu * (T4 - T2);
Htotal = H1 + H2 + H3 + H4 + H5 + H6;
disp("kJ",Htotal,"The enthalpy change accompanying
   the complete process = ")
```

Scilab code Exa 11.26 Mean heat capacity of ethanol water solution

```
clc()
Nwater = 0.8;//moles
Nethanol = 0.2;//moles
T = 323;//K
Cwater = 4.18*10^3;//J/kgK
Cethanol = 2.58*10^3;//J/kgK
Hmixing1 = -758;//J/mol ( at 298K )
Hmixing2 = -415;//J/mol ( at 323K )
T1 = 298;//K
T2 = 523;//K
//step1 - 0.8 mol of water is cooled from 323 K to
   298K
H1 = Nwater * 18 * Cwater * ( T1 - T )/ 1000;
//step2 - 0.2 mol ethanol cooled from 323K to 298K
H2 = Nethanol * 46 * Cethanol * ( T1 - T )/1000;
//step3 - 0.8 mol water and 0.2 mol ethanol are
   mixed together,
H3 = Hmixing1;
//step4 solution is heated to 323K, H4 = Cpm * (T -
   T1)
//Hmixing2 = H1 + H2 + H3 + H4
H4 = Hmixing2 - H1 - H2 - H3;
```

```
Cpm = H4 / ( T - T1 );
disp("J/molK",Cpm,"The mean heat capacity of a 20
   percent solution = ")
```

Scilab code Exa 11.27 Evaporation of NaOH solution

```
clc()
F = 1000;//kg/h
H1 = 116.3;//kJ/kg ( enthalpy of feed solution − 10%
    NaOH, 305 K )
H2 = 560.57;//kJ/kg ( enthalpy of thick liquor − 50%
    NaOH, 380 K )
Hsteam = 2676;//kJ/kg ( 1atm , 373.15K )
//by doing material balances,
P = 200;//kg/h
mvap = 800;//kg/h
//Enthalpy balance gives, F*H1 + Q = mvap*Hsteam + P
   *H2
Q = (mvap*Hsteam + P*H2)-F*H1;
disp("kJ/h",Q,"Heat to be supplied = ")
```

Scilab code Exa 11.28 Heat transfer to air

```
clc()
U2 = 0.35*10^3;//kJ
U1 = 0.25*10^3;//kJ
//since the tank is rigid the volume does not change
    during heating, Under constant volume, the
   change in the internal energy is equal to the
   heat supplied
Q = U2 - U1;
disp("kJ",Q,"Heat transferred to the air = ")
```

Scilab code Exa 11.29 change in internal energy

```
clc()
W = -2.25*745.7;//W ( work done on the system and 1
    hp = 745.7W)
Q = -3400;//kJ/h ( Heat transferred to the
    surrounding )
U = Q*1000/3600 - W;
disp("J/s",U,"Rise in the Internal energy of the
    system = ")
```

Scilab code Exa 11.30 Heat liberation in oxidation of iron fillings

```
clc()
//2Fe + 3/2O2 = Fe2O3
Hliberated = 831.08;//kJ
Q = -Hliberated*1000;
disp("J",Q,"Q = ")
//P(V) = (n)RT
//W = P(V) = (n)RT
n = -1.5;
R = 8.314;
T = 298;//K
W = (n) * R * T;
disp("J",W,"W = ")
U = Q - W;
disp("J",U,"U = ")
```

Scilab code Exa 11.31 Saturated steam and saturated water

```
clc()
Vgas = 0.09;//m^3
Vliq = 0.01;//m^3
SVliq = 1.061*10^-3;//m^3/kg
SVvap = 0.8857;//m^3/kg
mvap = Vgas / SVvap;
mliq = Vliq / SVliq;
Ul = 504.5;//kJ/kg
Ug = 2529.5;//kJ/kg
U1 = Ul * mliq + Ug * mvap;
SVtotal = (Vgas + Vliq)/(mvap + mliq);
//using steam table , these value of specific volume
    corresponds to pressure of 148.6bar and internal
    energy of 2464.6kJ/kg
U = 2464;//kJ/kg
Utotal = U * (mvap + mliq);
//Utotal - U1 = Q - W, but W = o, hence,
Q = Utotal - U1;
disp("kJ",Q,"Heat to be added = ")
```

Scilab code Exa 11.32 constant volume and constant pressure process

```
clc()
m = 10;//kg(air)
N = m / 29;//kmol
P1 = 100;//kPa
T1 = 300;//K
R = 8.314;
V1 = N * R * T1 / P1;
V2 = V1;
T2 = 600;//K
Cv = 20.785;//kJ/kmolK
Cp = 29.099;//kJ/kmolK
U = N * Cv * (T2 - T1);
Q = U;
```

```
W = Q - U;
H = U + N * R * ( T2 - T1 );
disp("kJ",U,"(a)Change in internal energy at constant volume = ")
disp("kJ",Q,"heat supplied at constant volume = ")
disp("kJ",W,"Work done at constant volume = ")
disp("kJ",H,"Change in Enthalpy at constant volume = ")
P2 = P1;
H2 = N * Cp * ( T2 - T1 );
Q2 = H2;
U2 = H2 - N * R * (T2 - T1);
W2 = Q2 - U2;
disp("kJ",U2,"(b)Change in internal energy at constant Pressure = ")
disp("kJ",Q2,"heat supplied at constant Pressure = ")
disp("kJ",W2,"Work done at constant Pressure = ")
disp("kJ",H2,"Change in Enthalpy at constant Pressure = ")
```

Scilab code Exa 11.33 series of operations

```
clc()
Cp = 29.3;//kJ/kmol
R = 8.314;
Cv = Cp - R;
T1 = 300;//K
P1 = 1;//bar
P2 = 2;//bar
//step1 - Volume remains constant, therefore the work done is zero and heat supplied is Cv, Also T2/T1 = P2/P1
T2 = P2 * T1 / P1;
Q1 = Cv * ( T2 - T1 );
```

```
W1 = 0;
disp("kJ",W1,"Work done at constant volume = ")
disp("kJ",Q1,"Heat supplied at constant volume = ")
//step2 - Process is abdiabatic
Q2 = 0;
r = 1.4;
T3 = T2 * (( P1 / P2 )^((r - 1)/r));
W2 = Cv * ( T2 - T3 );
disp(T3)
disp("kJ",W2,"Work done in adiabatic process = ")
disp("kJ",Q2,"Heat supplied in adiabatic process = ")
//step3 - process is isobaric
Q3 = Cp * (T1 - T3);
U3 = Cv * (T1 - T3);
W3 = Q3 - U3;
disp("kJ",W3,"Work done at constant pressure = ")
disp("kJ",Q3,"Heat supplied at constant pressure = ")
```

Scilab code Exa 11.34 change in internal energy and enthalpy and heat supplied and work done

```
clc()
P1 = 5;//bar
P2 = 4;//bar
T1 = 600;//K
V = 0.1;//m^3
T2 = 400;//K
T = 298;//K
Cp = 30;//J/molK
//step1 - isothermal condition
U1 = 0;
H1 = 0;
P = 1;//bar
```

```
R = 8.314;
W1 = R*T1*log(P1/P2);
Q1 = W1;
disp("kJ/kmol",U1,"(a)Change in the internal energy in isothermal condition = ")
disp("kJ/kmol",H1,"Change in the enthalpy energy in isothermal condition = ")
disp("kJ/kmol",W1,"Work done in isothermal condition = ")
disp("kJ/kmol",Q1,"Heat supplied in isothermal condition = ")
N = P * (1.01325 * 10^5) * V / ( R * T );
Cv = Cp - R;
U2 = Cv * (T2 - T)*N;
H2 = Cp * (T2 - T)*N;
W2 = 0;
Q2 = U2 + W2;
disp("kJ/kmol",U2,"(b)Change in the internal energy at constant volume condition = ")
disp("kJ/kmol",H2,"Change in the enthalpy energy at constant volume condition = ")
disp("kJ/kmol",W2,"Work done at constant volume condition = ")
disp("kJ/kmol",Q2,"Heat supplied at constant volume condition = ")
```

Scilab code Exa 11.35 Heat removed in condenser

```
clc()
m = 1;//kg
u2 = 0.5;//m/s
u1 = 60;//m/s
H = -3000;//kJ/kg
//KE = (u^2)/2
KE = ((u2 ^ 2) - (u1^2))/2000;
```

```
g = 9.81; //m/s^2
Z1 = 7.5; //m
Z2 = 2; //m
//PE = g * (Z)
PE = g * (Z2 - Z1)/1000;
W = 800; //kJ/kg
Q = H + PE + KE + W;
disp("kJ/kg",Q,"Heat removed from the fluid = ")
```

Scilab code Exa 11.36 Throttling process

```
clc()
PE = 0;
W = 0;
Q = 0;
//(H) + (u^2)/2 = 0
//according to the realtion u1 * v1 = u2 * v2
//(u^2)/2 is negligible, change in enthalpy is 0
T1 = 623; //K
P1 = 6000; //kPa
H1 = 3045.8; //kJ/kg ( Enthalpy of the steam using
    steam table )
P2 = 1000; //kPa
T2 = 570; //K ( value of temperature corresponding to
    the enthalpy and pressure using the steam table
    )
disp("K",T2,"Temperature of superheated steam = ")
```

Scilab code Exa 11.37 water pumping and energy balances

```
clc()
g = 9.81; //m/s^2
z = 55;
```

```
PE = g * z;
KE = 0;
T2 = 288;//K
f = 1.5*10^-2;//m^3/min
D = 1000;//kg/m^3
m = f * D;
Qsupp = 500;//kJ/min
Qlost = 400;//kJ/min
Qnet = (Qsupp - Qlost) * D / m ;
W = 2*745.7;//W
Ws = -W * 0.6 / (m/60);
H = Qnet - Ws - PE - KE;
Cp = 4200;
T1 = H / Cp;
T = T1 + T2;
disp("K",T,"The temperature of exit water = ")
```

Scilab code Exa 11.38 Energy balance on rotary drier

```
clc()
m = 1000;//kg/h (dried product)
// S be the amount of dry solid in the product
   stream
Pmoisture1 = 4;//%
Pmoisture2 = 0.2;//%
S = m *(1 - P/1000);
X1 = Pmoisture1/(100 - Pmoisture1);
X2 = Pmoisture2/(100 - Pmoisture2);
//let G be the weight of dry air in the air stream
Y1 = 0.01;//kg water/kg dry solid
Cp = 1.507;
Cw = 4.2;
T1 = 298;//K
T = 273;//K
T2 = 333;//K
```

```
Tg1 = 363; //K
Tg2 = 305; //K
Hs1 = (Cp + X1 * Cw) * (T1 - T);
Hs2 = (Cp + X2 * Cw) * (T2 - T);
//Hg = Cs(Tg - To) + Y*L
//Cs = 1.005 + 1.884*Y
L = 2502.3; //kJ/kg dry air
Hg1 = (1.005 + 1.884 * Y1)*(Tg1 - T) + Y1 * L;
Q = -40000; //kJ/h
//Calculating for T2, Hg2 = 32.16 + 2562.59*Y
//change in enthalpy = Q
//H1 = S * Hs1 + G * HG1 = 37814.22 + 117.17G
//H2 = 100728.14 + G* (32.16 + 2561.59*Y)
//change in enthalpy = Q
//62913.92 + G *(-85.01 + 2561.59*Y) + 40000 = 0
//102913.92 + G *(-85.01 + 2561.59*Y) = 0
                (1)
//moisture balance, S*X1 + G*Y1 = S*X2 + G*Y2
//G*(Y-0.01) = 39.62
                                         (2)
//solving simultaneously ( 1 ) and ( 2 ),
Gdry = 3443; //kg/h
G = Gdry*(1 + Y1);
disp("kg/h",G,"Air requirement = ")
```

Scilab code Exa 11.39 Energy balance on the fractionator

```
clc()
m = 1000; //kg/h ( feed solution )
//F - mass of feed distilled , W - mass of the bottom
    product , D - mass of the distillate , xf , xd and
    xw - weight fraction of actone in feed ,
    distillate and residue resp.
//total balance , F = D + W
//Acetone balance , F*xf = D*xd + w*xw
```

```
F = 1000;
xf = 0.10;
xd = 0.9;
xw = 0.01;
//substituting in above equations,
D = F * (xf - xw) / (xd - xw);
W = F - D;
R = 8;
L = R * D;
//material balance around the condenser,G vapour reaching the condenser
G = L + D;
Td = 332;//K
T2 = 300;//K
Tw = 370;//K
Tf = 340;//K
Lacetone1 = 620;//kJ/kg
Lwater1 = 2500;//kJ/kg
Ld = xd * Lacetone1 + (1 - xd) * Lwater1;
Cpacetone = 2.2;//kJ/kgK
Cpwater = 4.2;//kJ/kgK
Cp = xd * Cpacetone + (1-xd)*Cpwater;
H = Ld + Cp * ( Td - T2 );
Cpc = 4.2;//kJ/kg
Tc = 30;//K ( change in temperature allowable for cooling water )
m = G * H / ( Cpc * Tc );
disp("kg/h",m,"(a)The circulation rate of cooling water = ")
Qc = G * H;
Hd = 0;
Hw = (xw * Cpacetone + (1-xw)*Cpwater)*(Tw - T2);
Hf = (xf * Cpacetone + (1-xf)*Cpwater)*(Tf - T2);
Qb = D * Hd + W * Hw + Qc - F * Hf;
Hcondensation = 2730;//kJ/kg
msteam = Qb/Hcondensation;
disp("kg/h",msteam,"(b)Amount of steam supplied = ")
```

Chapter 12

Energy Balance Thermochemistry

Scilab code Exa 12.1 Heat liberated calculation

```
clc()
N = 100;//mol gas mixture burned
//CO(g) + 1/2 O2(g) = CO2 -                    Hr1 = - 282.91kJ/mol
//H2(g) + 1/2 O2(g) = H2O -                    Hr2 = - 241.83kJ/mol
Hr1 = - 282.91;//kJ/mol
Hr2 = - 241.83;//kJ/mol
Nco1 = 20;
Nh21 = 30;
Nn21 = 50;
Htotal = Nco1*Hr1 + Nh21*Hr2;
disp("kJ",-Htotal,"the amount of heat liberated on the complete combustion of 100mol of the gas mixture = ")
Ncoreac = Nco1 * 0.9;
Nh2reac = Nh21 * 0.8;
Htotal1 = Ncoreac*Hr1 + Nh2reac*Hr2;
disp("kJ",-Htotal1,"the amount of heat liberated if
```

```
    only 90% of CO and 80% of H2 react of 100mol of
    the gas mixture = ")
```

Scilab code Exa 12.2 Heat of formation of methane

```
clc()
//C(s) + 2H2(g) = CH4(g)            Hf = ?
Hc = -393.51;//kJ/mol
Hh2 = -285.84;//kJ/mol
Hch4 = - 890.4;//kJ/mol
//heat of reaction can be calculated from the heat
    of combustion data using following equation, the
    heat of reaction is the sum of the heat of
    combustion of all the reactants in the desired
    reaction minus the sum of the heat of combustion
    of all the products of the desired reaction. Here
     the reactants are one mole of Carbon and two
    moles hydrogen, and the product is one mole of
    methane,there heat of reaction is
Hf = 1 * Hc + 2 * Hh2 - 1 * Hch4;
disp("kJ",Hf,"Heat of formation of methane = ")
```

Scilab code Exa 12.3 Net heating value of coal

```
clc()
m = 1;//kg of coal burned
xc = 0.7;
xh2 = 0.055;
xn2 = 0.015;
xs = 0.03;
xo = 0.13;
xash = 0.07;
Hvap = 2370;//kJ/kg
```

```
C = 29000;//kJ/kg
Nh2 = xh2 * m / 2.016;
Nwater = Nh2;// ( amount of water formed )
mwater = Nwater * 18.016;
Hreq = mwater * Hvap;
Hnet = C - Hreq;
disp("kJ/kg",Hnet,"Net heating value of coal = ")
```

Scilab code Exa 12.4 Heat of reaction for esterification of ethyl alcohol

```
clc()
//C2H5OH(l) + CH3COOH(l) = C2H5COOCH3(l) + H2O(l) H = ?
Hc2h5oh = -1366.91;//kJ/mol
Hch3cooh = -871.69;//kJ/mol
Hc2h5cooch3 = -2274.48;//kJ/mol
//to calculate heat of reaction from the heat of combustion data ,
//Hreac = Hreac - Hprod
Hreac = Hc2h5oh + Hch3cooh - Hc2h5cooch3;
disp("kJ",Hreac,"Heat of reaction for the esterification of ethyl alcohol with acetic acid = ")
```

Scilab code Exa 12.5 Vapour phase hydration of ethylene to ethanol

```
clc()
//C2H4(g) + H2O(g) = C2H5OH(g)
//2CO2(g) + 3H2O(l) = C2H5OH(l) + 3O2(g)      H = 1366.91kJ   (A)
Hc2h4 = -1410.99;//kJ/mol
Hvap = 44.04;//kJ/mol
Hc2h5oh = 42.37;//kJ/mol
```

```
//C2H4(g) + 3H2O(l) = C2H5OH(l) + 3O2(g)        H = −1410.99kJ (B)
//H2O(l) = H2O(g)                               H = 44.04kJ     (C)
//C2H5OH(l) = C2H5OH(g)                         H = 42.37kJ     (D)
//A + B + D − C gives the required reaction
Ha = 1366.91;//kJ
Hb = -1410.99;//kJ
Hc = 44.04;//kJ
Hd = 42.37;//kJ
Hreac = Ha + Hb + Hd - Hc;
disp("kJ",Hreac,"The standard heat of reaction = ")
```

Scilab code Exa 12.6 Standard heat of formation of acetylene

```
clc()
//C2H5(g) + 5/2O2(g) = 2CO2(g) + H2O(l)
    H1 = −1299.6kJ     (A)
//C(s) + O2(g) = CO2(g)
    H2 = −393.51kJ     (B)
//H2(g) + 1/2O2(g) = H2O(l)
    H3 = −285.84kJ     (C)
//2C(s) + H2(g) = C2H2(g)
    H = ?
H1 = -1299.6;//kJ
H2 = -393.51;//kJ
H3 = -285.84;//kJ
Hreac = 2 * H2 + H3 - H1;
disp("kJ",Hreac,"Heat of formation of acetylene = ")
```

Scilab code Exa 12.7 Standard heat of roasting of iron pyrites

```
clc()
m = 100;//kg of pyrites charged
xfes2in = 0.8;
xgangueìn = 0.2;
xfes2out = 0.05;
//let x be the FeS2 in the feed, then, Fe2O3 = (80 - x)*159.69 / (119.98*2) and gangue = 20, total = 73.24 + 0.3345, be FeS2 is only 5 % in the product, hence
x = 0.05 * 73.24 / (1 - 0.05*0.3345);
mfes2reacted = m*xfes2in - x;
//4FeS2 + 11O2 = 2Fe2O3 + 8SO2
Hfes2 = -178.02;//kJ/mol
Hfe2o3 = -822.71;//kJ/mol
Hso2 = -296.9;//kJ/mol
Hreac = 2 * Hfe2o3 + 8 * Hso2 - 4 * Hfes2;
N = mfes2reacted *1000/ 119.98;
H = Hreac * N / 4;
H1 = H/m;//(heat of reaction per kg of coal burnt)
disp("kJ",H1,"Heat of reaction per 1 kg of coal burned = ")
```

Scilab code Exa 12.8 Standard heat of formation of liquid methanol

```
clc()
//CH3OH(l) + 3/2O2(g) = CO2(g) + 2H2O(l)          H = -726.55kJ
H1 = -726.55;//kJ
Hco2 = -393.51;//kJ/mol
Hh2o = -285.84;//kJ/mol
Hch3oh = Hco2 + 2 * Hh2o - H1;
disp("kJ",Hch3oh,"Heat of formation of liquid methanol = ")
```

Scilab code Exa 12.9 Gross heating value and Net heating value calculation

```
clc()
N = 100;//mol fuel gas
Nco = 21;
Nh2 = 15.6;
Nco2 = 9.0;
Nch4 = 2;
Nc2h4 = 0.4;
Nn2 = 52;
Hco = 282.99;//kJ/mol ( heat of combustion )
Hh2 = 285.84;//kJ/mol ( heat of combustion )
Hch4 = 890.4;//kJ/mol ( heat of combustion )
Hc2h4 = 1410.99;//kJ/mol ( heat of combustion )
Hvap = 44.04;//kJ/mol
H = Nco * Hco + Nh2 * Hh2 + Nch4*Hch4 + Nc2h4*Hc2h4;
   //kJ
V = N * 22.4143/1000;
H1 = H / V;//kJ/m^3
//on combustion, 1 mol hydrogen gives 1 mol of water
   , 1 mol of methane gives 2 mol of water and 1 mol
    of ethylene gives 2 moles of water
Nwater = Nh2 + 2 * Nch4 + 2 * Nc2h4;
Hvap1 = Hvap * Nwater;
Hnet = H1 - Hvap1;
disp("kJ",Hnet,"Net heating value of the fuel = ")
```

Scilab code Exa 12.10 Standard heat of reaction calculation

```
clc()
// C5H12(g) + 8O2(g) = 5CO2(g) + 6H20(l)
```

```
Hfco2 = -393.51;//kJ
Hfh2o = - 241.826;//kJ
Hfc5h12 = -146.4;//kJ
Hvap = 43.967;//kJ/mol
H1 = 6*Hfh2o +5*Hfco2 - Hfc5h12;
H2 = 6 * (-Hvap);
Hreac = H1 + H2;
disp("kJ",Hreac,"Standard heat of reaction = ")
```

Scilab code Exa 12.11 Constant pressure heat of combustion

```
clc()
m = 1;//kg of oil burned
mc = 0.9;//kg
mh2 = 0.1;//kg
Mc = mc / 12;//kmol
//C(s) + O2(g) = CO2(g)
Nh2 = mh2 / 2.016;//kmol
//change in the no. of gaseous components
   accompanying the combustion of 1 mole of hydrogen
    in liquid state is -1/2 mol, therefore for Nh2
   mol
R = 8.314;
T = 298;//K
x = Nh2 * R * T / (-2);
Qv = -43000;//kJ/kg
Qp = Qv + x;
disp("kJ/kg",Qp,"the constant pressure heat of
   combustion = ")
```

Scilab code Exa 12.12 Heat of reaction for ammonia synthesis

```
clc()
```

```
//1 - N2, 2 - H2, 3 - NH3
a1 = 27.31;
a2 = 29.09;
a3 = 25.48;
b1 = 5.2335*10^-3;
b2 = -8.374*10^-4;
b3 = 36.89 * 10^-3;
c1 = -4.1868 * 10^-9;
c2 = 2.0139*10^-6;
c3 = -6.305*10^-6;
H1 = -46191;//J
T1 = 298;//K
//1/2 N2 + 3/2 H2 = NH3                    H = -46.191kJ
//Ht = H + a*T + b*T^2 / 2+ c*T^3 / 3
//at 298,
a = a3 - a1 / 2 - 3 * a2 / 2;
b = b3 - b1 / 2 - 3 * b2 / 2;
c = c3 - c1 / 2 - 3 * c2 / 2;
H = H1 -a * T1 - b * (T1^2) / 2 - c * (T1^3) / 3;
T2 = 700;//K
H2 = H + a * T2 + b * (T2^2) / 2 + c * (T2^3) / 3;
disp(H);
disp("kJ",H2,"Heat of reaction at 700K = ")
```

Scilab code Exa 12.13 Standard heat of reaction of methanol synthesis

```
clc()
//CO(g) + 2H2(g) = CH3OH(g)
T1 = 298;//K
T2 = 1073;//K
//Cp(CH3OH) = 18.382 + 101.564 * 10^-3 * T - 28.683
    * 10^-6 * T^2
//Cp(CO) = 28.068 + 4.631 * 10^-3 * T - 2.5773 *
    10^4 * T^-2
//Cp(H2)  = 27.012 + 3.509 * 10^-3 * T + 6.9006 *
```

```
   10^4 * T^-2
//for reactants,
H1 = integrate('28.068 + 4.631 * 10^-3 * T - 2.5773
   * 10^4 * T^-2','T',T2,T1) + 2 * integrate('27.012
    + 3.509 * 10^-3 * T + 6.9006 * 10^4 * T^-2','T',
   T2,T1);
//for product,
H2 = integrate('18.382 + 101.564 * 10^-3 * T -
   28.683 * 10^-6 * T^2','T',T1,T2);
//H298 = Hproducts - Hreactants;
//CO + 2H2 = CH3OH                 Ha1 = -238.64kJ
Ha1 = -238.64;//kJ
//CH3OH(l) = CH3OH(g)              Hvap = 37.98kJ
Hvap = 37.98;//kJ
//CO(g) + 2H2(g) = CH3OH(g)        Ha2 = -200.66kJ
Ha2 = Ha1 + Hvap;//kJ
Hco = -110.6;//kJ/mol
H298 = Ha2 - (Hco);
Htotal = H1/1000 + H298 + H2/1000;
disp("kJ/mol",Htotal,"The heat of reaction at 773K =
    ")
```

Scilab code Exa 12.14 Combustion of CO

```
clc()
Nco = 1;//mol CO reacted
//CO + 1/2 O2 = CO2
No2 = Nco / 2;
Pexcess = 100;
Nosupp = No2 * ( 1 + Pexcess / 100 );//oxygen
   supplied
Nn2 = Nosupp * 79 / 21;
Nco2 = Nco;
Noremain = Nosupp - No2;
T1 = 298;//K
```

```
T2 = 400;//K
Hr1 = -282.99;//kJ
T3 = 600;//K
SHco = 29.1;//J/molK
SHo2 = 29.7;//J/molK
SHn2 = 29.10;//J/molK
SHco2 = 41.45;//J/molK
H1 = (Nosupp * SHo2 + Nn2 * SHn2 + Nco * SHco) * (T1 - T2);//enthalpy of cooling of reactants from 298 to 400 K
H2 = (Nco2 * SHco2 + Nn2 * SHn2 + Noremain * SHo2) * (T3 - T1);//enthalpy of heating the products from 298K to 600K
H = H1/1000 + Hr1 + H2/1000;
disp("kJ",H,"Heat change at 600K = ")
```

Scilab code Exa 12.15 Heat added or removed calculation

```
clc()
//CO(g) + H2O(g) = CO2(g) + H2(g)                H298 = -41.190
T1 = 298;//K
Pconv = 75;//%
T2 = 800;//K
H298 = -41.190;//kJ
Hco = 30.35;//J/molK
Hco2 = 45.64;//J/molK
Hwater = 36;//J/molK
Hh2 = 29.3;//J/molK
Nco = 1;//mol
Nh2o = 1;//mol
Ncofinal = Nco * (1 - Pconv/100);
Nwaterf = Ncofinal;
Nco2final = Nco - Ncofinal;
Nh2final = Nco2final;
```

```
H2 = (Nco2final * Hco2 + Nh2final * Hh2 + Ncofinal * Hco + Nwaterf * Hwater) * (T2 - T1);
Hr1 = H298 * (Nco - Ncofinal);
Hr2 = Hr1 * 1000 + H2;
mh2 = Nh2final * 2.016 * 10^-3;//kg
//therfore for 1000k H2,
Hr = Hr2 * 1000 / (mh2 * 1000);//kJ
disp("kJ",Hr,"Amount of heat change for 1000kg of hydrogen produced = ")
```

Scilab code Exa 12.16 CO2 O2 and N2 passed through a bed of C

```
clc()
//CO2(g) + C(s) = 2CO(g)                    H1298 = 170 kJ/mol
//O2(g) + 2C(s) = 2CO(g)                    H2298 = -221.2kJ/mol
T2 = 1298;//K
T1 = 298;//K
Hc = 0.02;//kJ/molK
Ho = 0.03;//kJ/molK
Hco = 0.03;//kJ/molK
Hco2 = 0.05;//kJ/molK
//let the flue gas contain x mol CO2 per mole of oxygen, product contains 2(1+x)mol CO. Nitrogen in reactant and product remain the same
//enthalpy of cooling xmol CO2, 1 mol O2 and 2 + xmol carbon from 1298 to 298K is given as, H1 = (Hco2 * x + Ho * 1 + Hc * (2 + x)) * (298 - 1298)
//H1 = (-70x - 70)kJ
//enthalpy of heating the product, H2 = 2 * ( 1 + x )* Hco * (1298 - 298)
//H2 = 60 + 60x kJ
//Hr = 170x - 221.2
//Htotal = 0 = H1 + H2 + Hr
```

```
x = (221.2 + 70 - 60)/(170 + 60 - 70);
disp("mol",x,"moles of CO2 present per mol of oxygen in feed stream = ")
```

Scilab code Exa 12.17 Partial oxidation of natural gas

```
clc()
N = 100;//mol flue gas
//Carbon balance,
//x is the feed of methane, w is water in flue ga, y is the oxygen supplied
xco2 = 0.019;
xch2o = 0.117;
xo2 = 0.038;
xch4 = 0.826;
xc = xco2 + xch2o + xch4;
Nc = xc * N;
Nch4i = Nc;
//Hydrogen balance,
xh2 = xch2o + xch4*2;
w = 2 * (Nch4i) - xh2*N;
//oxygen balance
No2s = (xco2 + xch2o/2 + xo2)*N + w/2;
y = No2s;
T1 = 298;//K
T2 = 573;//K
T3 = 673;//K
//oxygen cooled from 573K and methane from 673 to 298K
Ho573 = 30.5;//J/molK
Hch4673 = 45.9;//J/molK
H1 = y * Ho573 * (T1 - T2) + Nch4i * Hch4673 * (T1 - T3);
//CH4 + O2 = CH2O + H2O          Hr1 = -282.926kJ
//CH4 + 2O2 = CO2 + 2H2O         Hr2 = -802.372kJ
```

```
Hr1 = -282.926;//kJ
Hr2 = -802.372;//kJ
H2 = xch2o*N*Hr1 + xco2*N*Hr2;
T4 = 873;//K
Ho = 31.9
Hch4 = 51.4;
Hco2 = 46.3;
Hch2o = 47.1;
Hh2o = 36.3;
H3 = ((xco2 * Hco2 + xo2 * Ho + xch4 * Hch4 + Hch2o*xch2o)*N + w * Hh2o)*(T4 - T1);
Htotal = H1/1000 + H2 + H3/1000;
Nch2o = xch2o * N;
mch2o = Nch2o * 30.016/1000;//kg
//for 1000 kg of formaldehyde produced,
H = Htotal * 1000 / mch2o;
disp("kJ",H,"The amount of heat to be removed per 1000kg of formaldehyde produced = ")
```

Scilab code Exa 12.18 Maximum allowable conversion calculation

```
clc()
Nn2 = 1;//kmol/s ( basis - feed conisting of 1 kmol of N2 and 3 kmol of H2 )
Nh2 = 3;//kmol/s
//let x be the fraction converted
T1 = 700;//K
Hr1 = -94.2;//kJ/mol
//heat liberated = Hr1 * x
//Product consists of 2x kmol NH3, (1-x)kmol N2, and 3(1-x)kmol Hydrogen
T2 = 800;//K
Hn2 = 0.03;//kJ/molK
Hh2 = 0.0289;//kJ/molK
Hnh3 = 0.0492;//kJ/molK
```

```
//H2 = (1-x)*0.03*10^3 * 100 + 3*(1-x)
    *0.0289*1000*100 + 2*x*0.0492*1000*100
//H2 = 11.67*1000 - 1.83*10^3*x kJ
//reaction is adiabatic, hence, H1 = H2
//solving this we get,
x = 0.1215;
Convmax = x * 100;
disp("%",Convmax,"The maximum conversion for
    nitrogen should be ")
```

Scilab code Exa 12.19 Theoretical flame temperature calculation

```
clc()
Nco = 1;//mol CO
// CO + 1/2 O2 = CO2
O2r = 1;//mol
N2r = 3.76;//mol
COr = 1;//mol
O2p = 0.5;//mol
N2p = 3.76;//mol
CO2p = 1;//mol
Hco = 29.23;//J/molK
Ho2 = 34.83;//J/molK
Hn2 = 33.03;//J/molK
Hco2 = 53.59;//J/molK
Hcomb1 = -282.99;//kJ/mol
T1 = 298;//K
T2 = 373;//K
H1 = (O2r * Ho2 + N2r * Hn2 + COr * Hco) * (T1 - T2)
    ;
//For product at temp T, H2 = (O2p * Ho2 + N2p * Hn2
     + CO2p * Hco2) * (T - T1)
//For adiabatic condition, -(H1 + Hcomb1) = H2
T = -(H1 + Hcomb1 * 1000) / (O2p * Ho2 + N2p * Hn2 +
     CO2p * Hco2) + T1;
```

```
disp("K",T,"Theoretical flame temperature = ")
```

Scilab code Exa 12.20 Temperature of products on burning of hydrogen gas

```
clc()
N = 1;//kmol hydrogen burned
No = N/2;
Nosupplied = 2 * No;
Nair = Nosupplied * 100 / 21;
Nn2 = Nair - Nosupplied;
//Reactants, H2 = 1kmol, Air = 4.762 kmol
//Product, Water vapour = 1kmol, Oxygen = 0.5kmol, N2 = 3.762kmol
//Cp(water) = 30.475 + (9.652*10^-3)*T + 1.189 * 10^-6 * T^2
//Cp(nitrogen) = 27.034 + 5.815 * 10^-3 *T - 0.2889 * 10^-6 * T^2
//Cp(oxygen) = 25.611 + 13.260 * 10^-3 * T - 4.2077 * 10^-6 * T^2
//H2 = integration(298 to T of (1 * Cp(water) + 0.5 * Cp(oxygen) + 3.762 * Cp(nitrogen)))
//therefore, H2 = 140.34 * T + 31.222 * 10^-3 * T^2 - 4.928 * 10^-6 * T^2 - 44463.54 kJ
H298 = -241.826 * 10^3;//kJ
//H2 = -H1 - H298
//H1 = 0
//therefore using equation H2, the value of T is obtained to be
T = 1609.8;//K
disp("K",T,"Temperature of the reaction products = ")
```