

Scilab Textbook Companion for
Stoichiometry And Process Calculations
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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

```
1 //clc()
2 funcprot(0)
3 V1 = 15; //ft^3/min
4 ft = 0.3048; //m
5 min = 60; //secs
6 V = V1*ft^3/min;
7 disp("m^3/s",V,"Volumetric flowrate = ")
8 D = 1000; //kg/m^3
9 M = V * D;
10 disp("kg/s",M,"mass flowrate = ")
```

Scilab code Exa 2.2 Poundal to Newton

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

Scilab code Exa 2.3 Conversion of N per m2

```
1 //clc ()
2 funcprot (0)
3 kgf = 9.80665; //N
4 cm = 10^-2; //m
5 P = kgf/cm^2;
6 disp("N/m^2",P,"1 kgf/cm^2 = ")
7 lbf = 32.174; //lb*ft //s^2
8 lb = 0.4535924; //kg
9 ft = 0.3048; //m
10 in = 0.0254; //m
11 P1 = lbf*lb*ft/in^2;
12 disp("N/m^2",P1,"1 lbf/in^2 = ")
```

Scilab code Exa 2.4 Thermal conductivity

```
1 //clc ()
2 Q1 = 10000; //kJ/hr
3 kJ = 1000; //J
4 hr = 3600; //s
5 Q = Q1*kJ/hr; //J/s
6 disp("J/s",Q,"Q = ")
7 x = 0.1; //m
8 A = 1//m^2
9 T = 800; //K
10 k = x*Q/(A*T);
11 disp("W/(m*K)",k,"thermal conductivity = ")
12 J = 1/4.1868; //cal
13 k1 = k*J*hr/1000;
14 disp("kcal/(h*m*C)",k1,"thermal conductivity = ")
```

Scilab code Exa 2.5 Mass and FPS system

```
1 // clc ()
2 F = 300; //N
3 a = 9.81; //m/s^2
4 m = F/a; //kg
5 disp("kg",m,"mass in kg = ")
6 lb = 4.535924/10; //kg
7 m1 = m/lb;
8 disp("lb",m1,"mass in pounds = ")
```

Scilab code Exa 2.6 Kinetic energy calculation

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

Scilab code Exa 2.7 Force and pressure for piston cylinder

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

```

5 D1 = 4; //inch
6 D = D1 * 2.54 * 10^-2; //m
7 A = 3.1415 * (D^2)/4; //m^2
8 F1 = P * A; //N
9 F2 = m * g; //N
10 F = F1 + F2;
11 disp("N",F,"Total force acting on the gas = ")
12 P1 = F / A; //N/m^2
13 P2 = P1/100000; //bar
14 P3 = P1/(6.894757 * 10^3); //psi
15 disp("N/m^2",P1,"Pressure in N/m^2 = ")
16 disp("bar",P2,"Pressure in bar = ")
17 disp("psi",P3,"Pressure in psi = ")
18 d = 0.4; //m
19 W = F * d;
20 disp("J",W,"Work done = ")
21 PE = m * g * d;
22 disp("J",PE,"Change in potential energy = ")

```

Scilab code Exa 2.8 units conversion

```

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

```

```

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

```

Scilab code Exa 2.9 units conversion

```

1 //clc ()
2 //Cp = 7.13 + 0.577 * (10^-3) * t + 0.0248 * (10^-6)
    * t^2
3 //Cp - Btu/lb-mol F, t - F
4 //Cp1 - kJ/kmol K , t1 - K
5 a = 7.13;
6 b = 0.577 * 10^-3;
7 c = 0.0248 * 10^-6;
8 //t = 1.8 * t1 - 459.67
9 Cp = 4.1868; //Cp1 (Btu/lb-mol F = 4.1868 * (kJ/kmol
    K) )
10 //substituting the above, we get ,
11 //Cp1 = 28.763 + 4.763 * (10^-3) * t1 + 0.3366 *
    (10^-6) * t1^2
12 a1 = 28.763;
13 b1 = 4.763 * (10^-3);
14 c1 = 0.3366 * (10^-6);
15 disp(a1,"a1 = ")
16 disp(b1,"b1 = ")
17 disp(c1,"c1 = ")
18 // this are the co efficients for the following
    equation;
19 // 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

```
1 //clc ()
2 m = 1000 * 0.4536; //kg/min
3 M = 30.24; //gm/mol
4 m1 = m * 60 / M;
5 disp("kmol/hr",m1,"molar flow rate = ")
```

Scilab code Exa 3.2 Number of molecules

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

```

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

```

Scilab code Exa 3.3 Moles of sodium sulphate

```

1 //clc()
2 Na = 23; //gm/mol
3 MNa = 100; //kg
4 N = MNa * 1000 / Na ; //g-atoms
5 NNa2S04 = N / 2;
6 disp(" kmol",NNa2S04," (a) moles of sodium sulphate =
    ")
7 MNa2S04 = 142.06;
8 m = NNa2S04 * MNa2S04/1000;
9 disp(" kg",m," (b) kilograms of sodium sulphate = ")

```

Scilab code Exa 3.4 Pyrites and oxygen moles

```

1 //clc()
2 MFe = 55.85;
3 MO = 16;
4 MS = 32;
5 MFeS2 = MFe + MS * 2;
6 MFe2O3 = MFe * 2 + MO * 3;
7 MSO3 = MS + MO * 3;
8 m1SO3 = 100; //kg
9 N1 = m1SO3 / (MSO3); //kmol
10 NFeS2 = N1 / 2;
11 mFeS2 = NFeS2 * MFeS2;
12 disp(" kg",mFeS2," mass of pyrites to obtain 100kg of
    SO3 =")
13 m2SO3 = 50; //kg

```

```

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

```

Scilab code Exa 3.5 Volume of oxygen

```

1 //clc()
2 MKC103 = 122.55
3 mKC103 = 100; //kg
4 NKC103 = mKC103 / MKC103;
5 NO2 = 3 * NKC103 / 2;
6 V1 = 22.4143; //m^3/kmol;
7 V = V1 * NO2;
8 disp("m^3",V,"volume of oxygen produced = ")

```

Scilab code Exa 3.6 Reaction of iron and steel

```

1 //clc()
2 mH2 = 100; //kg
3 NH2 = mH2/2.016;
4 NFe = 3 * NH2 / 4;
5 mFe = NFe * 55.85;
6 disp("kg",mFe,"(a)mass of iron required = ")
7 NH2O = NH2 ;
8 mH2O = NH2O * 18;
9 disp("kg",mH2O,"mass of steam required =")
10 V1 = 22.4143; //m^3/kmol;
11 V = V1 * NH2;
12 disp("m^3",V,"Volume of hydrogen = ")

```

Scilab code Exa 3.7 Equivalent weight

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

Scilab code Exa 3.8 Specific gravity calculation

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

Scilab code Exa 3.9 Specific gravity of mixture

```
1 //clc ()
2 m1 = 10; //kg
3 m2 = 5; //kg
4 sp.g1 = 1.17;
5 sp.g2 = 0.83;
6 Dwater = 1000; //kg/m3
7 DA = Dwater * sp.g1;
8 DB = Dwater * sp.g2;
9 V1 = m1 / DA;
```

```

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

```

Scilab code Exa 3.10 Baume scale

```

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

```

Scilab code Exa 3.11 Density using API scale

```

1 //clc ()
2 API1 = 30; //API
3 sp.g1 = 141.5/(131.5 + API1); // (since , API = 141.5/
    sp.g -131.5)
4 Dwater = 999; //kg/m^3;
5 Doil1 = sp.g1 * Dwater;
6 V1 = 250; //m^3
7 m1 = V1 * Doil1;
8 API2 = 15; //API
9 sp.g2 = 141.5/(131.5 + API2); // (since , API = 141.5/
    sp.g -131.5)
10 Dwater = 999; //kg/m^3;
11 Doil2 = sp.g2 * Dwater;
12 V2 = 1000; //m^3
13 m2 = V2 * Doil2;
14 Dmix = (m1 + m2)/(V1 + V2);
15 disp("kg/m^3",Dmix,"density of the mixture =")

```

Scilab code Exa 3.12 Drying Ammonium sulphate

```
1 //clc()
2 m1 = 250; //kg
3 mwater1 = 50; //kg
4 mdrysolid1 = m1 - mwater1;
5 wfe1 = mwater1 / m1;
6 wr1 = mwater1 / mdrysolid1;
7 wtpercentw1 = mwater1 * 100 / m1;
8 wtpercentd1 = mwater1 * 100 / mdrysolid1;
9 a = 90; //%
10 mwater2 = mwater1 * (1 - a/100);
11 m2 = mdrysolid1 + mwater2;
12 wfe2 = mwater2 / m2;
13 wr2 = mwater2 / mdrysolid1;
14 wtpercentw2 = mwater2 * 100 / m2;
15 wtpercentd2 = mwater2 * 100 / mdrysolid1;
16 disp(wfe1,"(a) weight fraction of water at entrance =
    ")
17 disp(wfe2,"weight fraction of water at exit = ")
18 disp(wr1,"(b) weight ratio of water at entrance = ")
19 disp(wr2,"weight ratio of water at exit = ")
20 disp(wtpercentw1,"(c) weight percent of moisture on
    wet basis at entrance = ")
21 disp(wtpercentw2,"weight percent of moisture on wet
    basis at exit = ")
22 disp(wtpercentd1,"(d) weight percent of moisture on
    dry basis at entrance = ")
23 disp(wtpercentd2,"weight percent of moisture on dry
    basis at exit = ")
```

Scilab code Exa 3.13 Percentage of water removed

```

1 //clc ()
2 mdrysolid = 100; //kg
3 percentin = 25;
4 mwaterin = mdrysolid * percentin / 100;
5 percentout = 2.5;
6 mwaterout = mdrysolid * percentout / 100;
7 mremoved = mwaterin - mwaterout;
8 percentremoved = mremoved *100 / mwaterin ;
9 disp(percentremoved,"percentage of water removed = "
    )

```

Scilab code Exa 3.14 Amount and percentage water removed

```

1 //clc ()
2 m = 1; //kg
3 percent1 = 20; // %
4 mwaterin = m * percent1 / 100;
5 mdrysolid = m - mwaterin;
6 percent2 = 2.44; // %
7 mout = mdrysolid / (1 - percent2/100);
8 mwaterout = mout - mdrysolid;
9 mremoved = mwaterin - mwaterout;
10 percentremoved = mremoved * 100 / mwaterin ;
11 disp("kg",mremoved,"weight of water removed = ")
12 disp("%",percentremoved,"percentage of water removed
    = ")

```

Scilab code Exa 3.15 NaCl solution

```

1 //clc ()
2 mwater = 100; //kg
3 mNaCl = 35.8; //kg
4 msolu = mwater + mNaCl;

```

```

5 mfr = mNaCl / msolu;
6 mpr = mfr * 100;
7 MNaCl = 58.45; //kg/kmol
8 NNaCl = mNaCl / MNaCl;
9 MH2O = 18; //kg/kmol
10 NH2O = mwater / MH2O;
11 Mfr = NNaCl / (NNaCl + NH2O);
12 Mpr = Mfr * 100;
13 N = NNaCl *1000 / mwater;
14 disp(mfr,"(a)mass fraction of NaCl =")
15 disp(mpr,"mass percent of NaCl= ")
16 disp(Mfr,"(b)mole fraction of NaCl =")
17 disp(Mpr,"mole percent of NaCl = ")
18 disp(N,"kmol NaCl per 1000 kg of water =")

```

Scilab code Exa 3.16 Molal absolute humidity

```

1 //clc ()
2 Y = 0.015; //kg water vapour/kg dry air
3 Mair = 29; //kg/kmol
4 Mwater = 18.016; //kg/kmol
5 Nwater = Y / Mwater; //kmol
6 Nair = 1 / Mair; //kmol
7 Mpr = Nwater *100 / (Nwater + Nair);
8 Mr = Nwater / Nair;
9 disp(Mpr,"(a)mole percent of water vapour = ")
10 disp("kmol water/kmol dry air",Mr,"(b) molal
    absolute humidity =")

```

Scilab code Exa 3.17 K₂CO₃ solution

```

1 //clc ()
2 msolu = 100; //g

```



```

3 MK2C03 = 138.20; //g/mol
4 percent1 = 50; //%
5 mK2C03 = percent1 *msolu / 100;
6 NK2C03 = mK2C03 / MK2C03;
7 mwater = msolu - mK2C03;
8 Nwater = mwater / 18.06;
9 Mpr = NK2C03 * 100 / (NK2C03 + Nwater);
10 sp.gr =1.53;
11 Vsolu = msolu/sp.gr; //mL
12 Vwater = mwater / 1; //mL
13 Vpr = Vwater * 100/ Vsolu;
14 Molality = NK2C03 / (mwater * 10^-3);
15 Molarity = NK2C03 / (Vsolu * 10^-3);
16 Eq.wt = MK2C03 / 2;
17 No = mK2C03/Eq.wt;
18 N = No / (Vsolu * 10^-3);
19 disp("%",Mpr,"(a)Mole prcent of salt = ")
20 disp("%",Vpr,"(b)Volume percent of water = ")
21 disp("mol/kg",Molality,"(c)Molality = ")
22 disp("mol/L",Molarity,"(d)Molarity = ")
23 disp("N",N,"(e)Normality")

```

Scilab code Exa 3.18 Molarity and Molality of Alcohol solution

```

1 //clc()
2 msolu = 100; //kg
3 percent1 = 60; //%
4 Dwater = 998; //kg/m^3
5 Dalco = 798; //kg/m^3
6 Dsolu = 895; //kg/m^3
7 Vsolu = msolu/Dsolu;
8 malco = msolu * percent1 / 100;
9 Valco = malco / Dalco;
10 Vpr = Valco * 100 / Vsolu;
11 Malco = 46.048; //kg/kmol

```

```

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

```

Scilab code Exa 3.19 CO to phosgene

```

1 //clc ()
2 //CO + CL2 = COCl2
3 Np = 12; //moles
4 NCl2 = 3; //moles
5 NCO = 8; //moles
6 N1Cl2 = NCl2 + Np;
7 N1CO = NCO + Np;
8 pr.ex = (N1CO - N1Cl2)* 100/N1Cl2;
9 pr.co = (N1Cl2-NCl2) * 100/ N1Cl2;
10 T = Np + NCl2 + NCO;
11 T1 = N1Cl2 + N1CO;
12 N = T / T1;
13 disp("%",pr.ex,"(a)percent excess of CO = ")
14 disp("%",pr.co,"(b)percent conversion = ")
15 disp(N,"(c)Moles of total products per mole of total
    reactants = ")

```

Scilab code Exa 3.20 Extent of reaction

```

1 //clc ()
2 Nn2 = 2; //moles
3 Nh2 = 7; //moles

```

```

4 Nnh3 = 1; //mole
5 n0 = Nn2 + Nh2 + Nnh3;
6 v = 2 - 1- 3;
7 //YN2 = (2 - E)/(10 - 2*E)
8 //Yh2 = (7-3*E)/(10 - 2*E)
9 //Ynh3 = (1 + 2*E)/(10 - 2*E)
10 disp("mole fraction of N2 = (2 - E)/(10 - 2*E)")
11 disp("mole fraction of H2 = (7-3*E)/(10 - 2*E)")
12 disp("mole fraction of NH3 = (1 + 2*E)/(10 - 2*E)")

```

Scilab code Exa 3.21 ethylene to ethanol

```

1 //clc()
2 msolu = 100; //g
3 MK2C03 = 138.20; //g/mol
4 percent1 = 50; //%
5 mK2C03 = percent1 *msolu / 100;
6 NK2C03 = mK2C03 / MK2C03;
7 mwater = msolu - mK2C03;
8 Nwater = mwater / 18.06;
9 Mpr = NK2C03 * 100 / (NK2C03 + Nwater);
10 sp.gr =1.53;
11 Vsolu = msolu/sp.gr; //mL
12 Vwater = mwater / 1; //mL
13 Vpr = Vwater * 100/ Vsolu;
14 Molality = NK2C03 / (mwater * 10^-3);
15 Molarity = NK2C03 / (Vsolu * 10^-3);
16 Eq.wt = MK2C03 / 2;
17 No = mK2C03/Eq.wt;
18 N = No / (Vsolu * 10^-3);
19 disp("%",Mpr,"(a)Mole prcent of salt = ")
20 disp("%",Vpr,"(b)Volume percent of water = ")
21 disp("mol/kg",Molality,"(c)Molality = ")
22 disp("mol/L",Molarity,"(d)Molarity = ")
23 disp("N",N,"(e)Normality")

```


Chapter 4

Ideal Gases and Gas Mixtures

Scilab code Exa 4.1 gas constant R

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

Scilab code Exa 4.2 Molar volume of air

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

```

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

```

Scilab code Exa 4.3 Ideal gas equation

```

1 //clc()
2 P = 10; //bar
3 T = 300; //K
4 V = 150; //L
5 P1 = 1.01325; //bar ( \suffix 1 represents at STD)
6 T1 = 273.15; //K
7 V2 = T1 * P * V / (T * P1); //m^3
8 V1 = 22.4143; //m^3/mol
9 N = V2 / V1; //mol
10 M02 = 32;
11 m = N * M02 / 1000;
12 disp("kg", m, "Mass of oxygen in the cylinder = ")

```

Scilab code Exa 4.4 Maximum allowable temperature of tyre

```

1 //clc()
2 P = 195; //kPa
3 T = 273; //K
4 P1 = 250; //kPa
5 T1 = P1 * T / P;
6 disp("K", T1, "Maximum temperature to which tyre may
  be heated = ")

```

Scilab code Exa 4.5 Pressure calculation

```
1 // clc ()
2 V = 250; //L
3 T = 300; //K
4 V1 = 1000; //L
5 P1 = 100; //kPa
6 T1 = 310; //K
7 P = T * P1 * V1 / (T1 * V);
8 disp("kPa", P, "Original pressure in the cylinder = ")
```

Scilab code Exa 4.6 weight composition and density calculation

```
1 // clc ()
2 Vper1 = 70; //% ( 1 = HCl)
3 Vper2 = 20; //% ( 2 = Cl2)
4 Vper3 = 10; //% ( 3 = CCl4)
5 M1 = 36.45;
6 M2 = 70.90;
7 M3 = 153.8;
8 m1 = Vper1 * M1;
9 m2 = Vper2 * M2;
10 m3 = Vper3 * M3;
11 mper1 = m1 * 100 / (m1 + m2 + m3);
12 mper2 = m2 * 100 / (m1 + m2 + m3);
13 mper3 = m3 * 100 / (m1 + m2 + m3);
14 disp(mper1, " (a) weight percent of HCl= ")
15 disp(mper2, "weight percent of Cl2= ")
16 disp(mper3, "weight percent of CCl4= ")
17 m = (m1 + m2 + m3) / (Vper1 + Vper2 + Vper3);
18 disp("kg", m, "(b) average molecular weight = ")
19 v = 22.4143; //m^3/kmol
```

```

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

```

Scilab code Exa 4.7 calculations for natural gas

```

1 //clc()
2 per1 = 93; //% ( 1 = methane)
3 per2 = 4.5; //% ( 2 = ethane)
4 per3 = 100 - (per1 + per2); //% ( 3 = N2);
5 T = 300; //K
6 p = 400; //kPa
7 P3 = p * per3 / 100;
8 v = 10; //m^3
9 V2 = per2 * v / 100;
10 M1 = 16.032;
11 M2 = 30.048;
12 M3 = 28;
13 N1 = per1;
14 N2 = per2;
15 N3 = per3;
16 m1 = M1 * N1;
17 m2 = M2 * N2;
18 m3 = M3 * N3;
19 m = m1 + m2 + m3;
20 Vstp = 100 * 22.4143 * 10^-3; //m3 at STP
21 D = m / (1000 * Vstp);
22 Pstp = 101.325; //kPa
23 T1 = 273.15; //K
24 V = T * Pstp * Vstp / ( T1 * p);
25 D1 = m / (1000 * V);
26 Mavg = m / 100;
27 mper1 = m1 * 100 / (m1 + m2 + m3);
28 mper2 = m2 * 100 / (m1 + m2 + m3);

```



```

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

```

Scilab code Exa 4.8 Volume of gas from absorption columnn

```

1 //clc()
2 per1 = 20; //% ( 1 = ammonia)
3 Vstp = 22.4143; //m^3/kmol
4 Pstp = 101.325; //kPa
5 Tstp = 273.15; //K
6 V1 = 100; //m^3
7 P1 = 120; //kPa
8 T1 = 300; //K
9 P2 = 100; //kPa
10 T2 = 280; //K
11 per2 = 90; //% (absorbed)
12 N = V1 * P1 * Tstp / (Vstp * Pstp * T1); //kmol
13 Nair = (1 - per1 / 100) * N;
14 N1 = per1 * N/100;
15 Nabs = per2 * N1 / 100;
16 N2 = N1 - Nabs; //leaving
17 Ntotal = Nair + N2;
18 Vstp1 = Ntotal * Vstp; //m^3
19 V2 = Vstp1 * Pstp * T2 / (Tstp * P2);
20 disp("m^3",V2,"Volume of gas leaving = ")

```

Scilab code Exa 4.9 dehumidification

```
1 //clc()
2 V = 100; //m^3
3 Ptotal = 100; //kPa
4 Pwater = 4; //kPa
5 Pair = Ptotal - Pwater;
6 T = 300; //K
7 T1 = 275; //K
8 Vstp = 22.4143; //m^3/kmol
9 Tstp = 273.15; //K
10 Pstp = 101.325; //kPa
11 Pwater1 = 1.8; //kPa
12 Pair1 = Ptotal - Pwater1;
13 V1 = V * Pair * T1 / ( T * Pair1);
14 Nwater = V * Pwater * Tstp / (Vstp * Pstp * T);
15 Nwater1 = V1 * Pwater1 * Tstp / (Vstp * Pstp * T1);
16 m = (Nwater - Nwater1) * 18.02;
17 disp("m^3",V1,"(a) volume of air after
      dehumidification = ")
18 disp("kg",m,"(b) Mass of water vapour removed = ")
```

Scilab code Exa 4.10 Absorption column for H2S

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

```

8 Tstp = 273.15; //K
9 Vstp = 22.414; //m^3/kmol
10 Vstp1 = V * P * Tstp / ( T * Pstp)
11 N = Vstp1 / Vstp;
12 N1 = N * per1 / 100;
13 N2 = N - N1; // ( 2 = inerts )
14 Nleaving = N2 / ( 1 - per2 / 100);
15 N1leaving = per2 * Nleaving / 100;
16 mabsorbed = (N1 - N1leaving) * 34.08; //( molecular
    wt. = 34.08)
17 mgiven = 100; //kg/h
18 Vactual = mgiven * V / mabsorbed;
19 Nactual = Nleaving * Vactual / V; // actual moles
    leaving
20 Vstp1 = Nactual * Vstp; // volume leaving at STP
21 P2 = 500; //kPa
22 T2 = 290; //K
23 V2 = Vstp1 * Pstp * T2 / ( P2 * Tstp);
24 Precovery = (N1 - N1leaving)*100 / N1;
25 disp("m^3/h",Vactual,"(a)Volume of gas entering per
    hour")
26 disp("m^3/h",V2,"(b)Volume of gas leaving per hour")
27 disp("%",Precovery,"(c)Percentage recovery of H2S")

```

Scilab code Exa 4.11 Reaction stoichiometry for preparation of ammonia

```

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

```

```

7 T1 = 350; //K
8 P2 = 5; //bar
9 T2 = 290; //K
10 V3 = 3 * V1 * P1 * T2 / ( P2 * T1);
11 disp("m^3",V3,"(b)Volume required at 50 bar and 290K
      = ")
12 m = 1000; //kg ( ammonia )
13 N = m / 17.03; //kmol
14 N1 = N/2; // ( nitrogen )
15 N2 = N * 3 / 2; //(hydrogen)
16 P3 = 50; //bar
17 T3 = 600; //K
18 Pstp = 1.01325; //bar
19 Tstp = 273.15; //K
20 Vstp = 22.414; //m^3/kmol
21 V1stp = N1 * Vstp;
22 V4 = V1stp * Pstp * T3 / (P3 * Tstp); // ( nitrogen
      at 50 bar and 600K)
23 V5 = V4 * 2 ; // ( ammonia at 50 bar and 600K)
24 V6 = V4 * 3 ; // ( hydrogen at 50 bar and 600K)
25 disp("m^3",V4,"(c)Volume of nitrogen at 50 bar and
      600K")
26 disp("m^3",V6," Volume of hydrogen at 50 bar and
      600K")
27 disp("m^3",V5," Volume of ammonia at 50 bar and
      600K")

```

Scilab code Exa 4.12 Reaction stoichiometry for preparation of producer gas

```

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

```

```

6 P4 = 68; // % ( Nitrogen )
7 N1 = N * P1/100;
8 N2 = N * P2/100;
9 N3 = N * P3/100;
10 N4 = N * P4/100;
11 NC = N1 + N2;
12 m = NC * 12;
13 Ngas = N / m; // moles of gas for 1 kg of Carbon
14 Vstp = 22.4143; // m^3/kmol
15 Vstp1 = Vstp * Ngas;
16 P = 1; // bar
17 T = 290; // K
18 Pstp = 1.01325; // bar
19 Tstp = 273.15; // K
20 V = T * Vstp1 * Pstp / (Tstp * P );
21 disp("m^3",V,"(a) Volume of gas at 1 bar and 290 K
      per kg Carbon = ")
22 // CO + 1/2 * O2 = CO2
23 Nrequired = N1/2 - N3; // (oxygen required)
24 Nsupplied = Nrequired * 1.2;
25 P01 = 21; // % ( Oxygen percent in air )
26 Nair = Nsupplied * 100/P01;
27 V1 = 100; // m^3;
28 Vair = V1 * Nair / N;
29 disp("m^3",Vair,"(b) Volume of air required = ")
30 NC02 = N2 + N1;
31 N02 = Nsupplied - Nrequired;
32 NN2 = N4 + (Vair * (1 - P01/ 100));
33 Ntotal = NC02 + N02 + NN2;
34 PC02 = NC02 * 100 / Ntotal;
35 P02 = N02 * 100 / Ntotal;
36 PN2 = NN2 * 100 / Ntotal;
37 disp("%",PC02,"Percent composition of Carbon Dioxide
      = ")
38 disp("%",P02,"Percent composition of Oxygen = ")
39 disp("%",PN2,"Percent composition of Nitrogen = ")

```

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

```
1 //clc()
2 //4HCl + O2 = 2Cl2 + 2H2O
3 n = 1; //mol ( Basis 1 mol of HCl )
4 NO2 = n / 4;
5 NO2supp = 1.5 * NO2;
6 Nair = NO2supp * 100 / 21;
7 V = 100; //m^3
8 Vair = V * Nair / n;
9 disp("m^3",Vair,"(a)Volume of air admitted = ")
10 P1 = 80; //% ( HCl converted)
11 Ncon = n * P1 / 100;
12 N2 = Ncon/4; // oxygen required
13 NH2O = Ncon / 2;
14 NCl2 = Ncon / 2;
15 nHCl = n - Ncon;
16 nO2 = NO2supp - N2;
17 Nnitro = Nair - NO2supp;
18 Ntotal = nHCl + nO2 + NH2O + NCl2 + Nnitro;
19 V1 = V * Ntotal;
20 P1 = 1; //bar
21 T1 = 290; //K
22 P2 = 1.2; //bar
23 T2 = 400; //K
24 V2 = V1 * P1 * T2 / ( P2 * T1);
25 disp("m^3",V2,"(b)Volume of gas leaving = ")
26 VCl2 = NCl2 * V;
27 Pstp = 1.01325; //bar
28 Tstp = 273; //K
29 Vstp = 22.4143; //m^3/kmol
30 Vstp1 = Tstp * P1 * VCl2 / (T1 * Pstp);
31 Nstp = Vstp1/Vstp;
```

```

32 m = Nstp * 70.90;
33 disp("kg",m,"(c) Kilograms of Chlorine produced = ")
34 Ntotaldry = nHCl + nO2 + NCl2 + Nnitro;//dry basis
35 p1 = nHCl*100/Ntotaldry;
36 p2 = nO2*100/Ntotaldry;
37 p3 = NCl2*100/Ntotaldry;
38 p4 = Nnitro*100/Ntotaldry;
39 disp("%",p1,"(d) Percent composition of HCl in exit
    stream = ")
40 disp("%",p2,"    Percent composition of Oxygen in
    exit stream = ")
41 disp("%",p3,"    Percent composition of Chlorine in
    exit stream = ")
42 disp("%",p4,"    Percent composition of nitrogen in
    exit stream = ")

```

Scilab code Exa 4.14 Reaction stoichiometry for dissociation of Carbon Dioxide

```

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

```

```
15 // CO2 = (1 - x)mol, CO = xmol, O2 = (0.5*x)mol
16 //total moles = 1 - x + x + 0.5 * x = 1 + 0.5 * x
17 V = 350; //L
18 N1 = V * P1 * Tstp / (Vstp * Pstp * T1);
19 // 1 + 0.5 * x = N1, therefore
20 x = (N1 - 1) / 0.5 ;
21 p = x*100;
22 disp("%",p,"(b)CO2 converted = ")
```

Chapter 5

Properties of Real Gases

Scilab code Exa 5.1 Van der waals equation

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

Scilab code Exa 5.2 Van der waals equation for CO2 gas

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

```

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

```

Scilab code Exa 5.3 Redlich Kwong equation for gaseous ammonia

```

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

```

Scilab code Exa 5.4 Molar Volume calculation for gaseous ammonia

```

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

```

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

Scilab code Exa 5.5 virial equation of state

```
1 //clc ()
2 B = -2.19 * 10^-4; //m^3/mol
3 C = -1.73 * 10^-8; //m^6/mol^2
4 P = 10; //bar
5 T = 500; //K
6 //virial equation is given as,  $Z = PV/RT = 1 + B/V + C/V^2$ 
7 //  $V = (RT/P) * (1 + B/V + C/V^2)$ 
8 // 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
9 //by trial and error we get ,
10 V = 3.92 * 10^-3; //m^3
11 disp("m^3",V,"Molar volume of methanol = ")
```

Scilab code Exa 5.6 Lyderson method for n butane

```
1 //clc ()
2 T = 510; //K
3 P = 26.6; //bar
4 Tc = 425.2; //K
5 Pc = 38; //bar
6 Zc = 0.274;
7 R = 8.314;
8 Pr = P / Pc;
9 Tr = T / Tc;
10 disp(Pr,"Pr = ")
```

```

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

```

Scilab code Exa 5.7 Pitzer correlation for n butane

```

1 //clc()
2 T = 510; //K
3 P = 26.6; //bar
4 Tc = 425.2; //K
5 Pc = 38; //bar
6 w = 0.193;
7 R = 8.314;
8 Pr = P / Pc;
9 Tr = T / Tc;
10 disp(Pr,"Pr = ")
11 disp(Tr,"Tr = ")
12 //From fig. 5.6 and 5.7 from the text book
13 Z0 = 0.855;
14 Z1 = 0.042;
15 Z = Z0 + w*Z1;
16 disp(Z,"Z = ")
17 V = R * T * Z / (P * 10^5);
18 disp("m^3/mol",V,"Molar volume of n-butane = ")

```

Scilab code Exa 5.8 Molar volume by different methods

```

1 //clc()
2 P = 6000; //kPa

```

```

3 T = 325; //K
4 xn2 = 0.4;
5 xethane = 0.6;
6 an2 = 0.1365; //N m^4 / mol^2
7 bn2 = 3.86 * 10^-5; //m^3/mol
8 aethane = 0.557; //N m^4 / mol^2
9 bethane = 6.51 * 10^-5; //m^3/mol
10 Pcn2 = 3394; //kPa
11 Tcn2 = 126.2; //K
12 Pcethane = 4880; //kPa
13 Tcethane = 305.4; //K
14 R = 8.314;
15 V = R * T / (P*1000);
16 disp("m^3/mol",V,"(a)Molar volume by ideal gas
    equation =")
17 a = (xn2 * (an2^0.5) + xethane * (aethane^0.5))^2;
18 b = (xn2*bn2 + xethane*bethane);
19 //substituting the above values in van der waals
    equation , and solving , we get
20 V1 = 3.680 * 10^-4; //m^3/mol
21 disp("m^3/mol",V1,"(b)Molar volume by van der waals
    equation =")
22 Prin2 = P/Pcn2;
23 Trin2 = T/Tcn2;
24 Priethane = P/Pcethane;
25 Triethane = T/Tcethane;
26 // using compressibility chart ,
27 Zn2 = 1;
28 Zethane = 0.42;
29 Z = xn2 * Zn2 + xethane * Zethane;
30 V2 = Z * R * T / P;
31 disp("m^3/mol",V2,"(c)Molar volume based on
    compressibility factor =")
32 Pri1n2 = xn2*P/Pcn2;
33 Tri1n2 = T/Tcn2;
34 Pri1ethane = xethane*P/Pcethane;
35 Tri1ethane = T/Tcethane;
36 // using compressibility chart ,

```

```

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

```

Scilab code Exa 5.9 Van der waals equation and Kays method

```

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

```

```

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

```

Chapter 6

Vapour Pressure

Scilab code Exa 6.1 Quality of steam

```
1 //clc ()
2 P = 500; //kPa
3 SV = 0.2813; //m^3/kg
4 Vsaturatedl = 1.093 * 10^-3; //m^3/kg
5 Vsaturatedv = 0.3747; //m^3/kg
6 // let the fraction of vapour be y
7 //(1-y)*Vsaturatedl + y*Vsaturatedv = SV
8 //then we get , (1-y)*(1.093*10^-3) + y*(0.3747) =
   0.2813
9 y = (SV - Vsaturatedl)/(Vsaturatedv - Vsaturatedl);
10 P1 = y * 100;
11 P2 = 100 - P1;
12 disp("%",P1,"Percentage of Vapour = ")
13 disp("%",P2,"Percentage of Liquid = ")
```

Scilab code Exa 6.2 Calculation of vapour pressure

```
1 //clc ()
```



```

2 T1 = 363; //K
3 T2 = 373; //K
4 P2s = 101.3; //kPa
5 J = 2275 * 18; //kJ/kmol
6 R = 8.314; //kJ/kmolK
7 //ln (P2s/P1s) = J * (1/T1 - 1/T2) / R
8 P1s = P2s/exp(J * (1/T1 - 1/T2) / R);
9 disp("kPa",P1s,"Vapour pressure of water at 363 K =
    ")

```

Scilab code Exa 6.3 Clausius Clapeyron equation for acetone

```

1 //clc()
2 P1s = 194.9; //kPa
3 P2s = 8.52; //kPa
4 T1 = 353; //K
5 T2 = 273; //K
6 T3 = 300; //K
7 Pair = 101.3; //kPa
8 //log (P2s/P1s) = J * (1/T1 - 1/T2) / R
9 //let J / R = L
10 L = log (P2s/P1s)/(1/T1 - 1/T2);
11 P3s = P1s * exp(L * (1/T1 - 1/T3)) ;
12 Ptotal = P3s + Pair; //at saturation vapour pressure
    = partial pressure
13 disp("kPa",Ptotal,"(a)Final pressure of the mixture
    = ")
14 MP = P3s * 100 / Ptotal;
15 // mole percent = moles of acetone * 100 / total
    moles
16 // = Partial pressure of acetone * 100 / total
    Pressure
17 disp("%",MP,"(b)Mole percent of acetone in the final
    mixture = ")

```

Scilab code Exa 6.4 Antoine equation for n heptane

```
1 //clc ()
2 A = 13.8587;
3 B = 2911.32;
4 C = 56.56;
5 T1 = 325; //K
6 //Pressure at normal condition = 101.3kPa
7 P2 = 101.3; //kPa
8 //Antoine equation - lnP = A - B / (T - C)
9 lnP = A - (B / (T - C));
10 P1 = exp(lnP);
11 disp("kPa",P1,"(a)Vapour pressure of n-heptane at
      325K = ")
12 T2 = B/(A - log(P2)) + C;
13 disp("K",T2,"(b)Normal boiling point of n-heptane =
      ")
```

Scilab code Exa 6.5 Cox chart

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

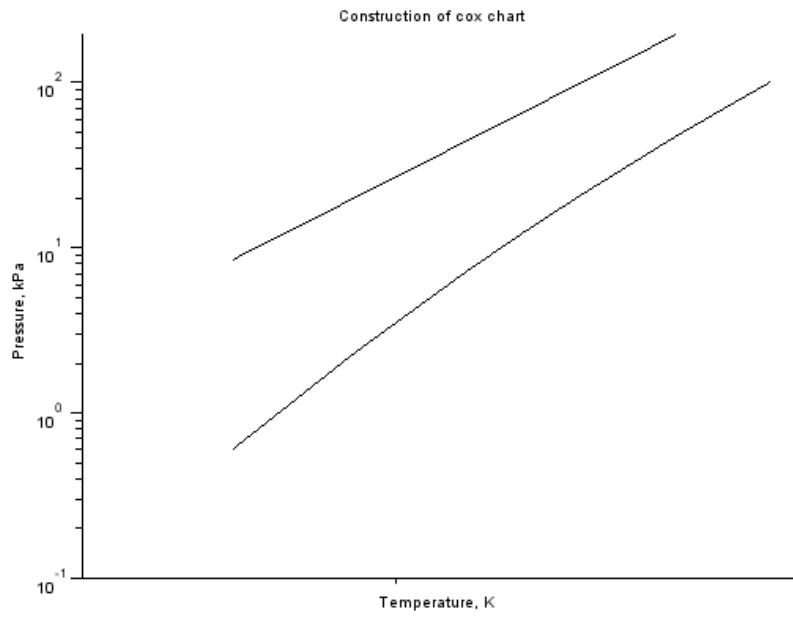


Figure 6.1: Cox chart

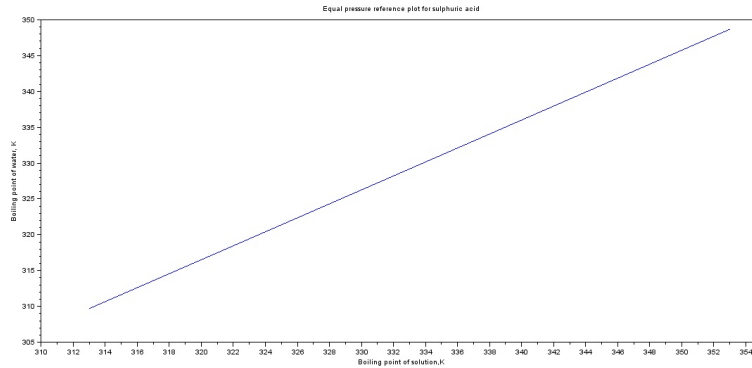


Figure 6.2: Duhring line

Scilab code Exa 6.6 Duhring line

```

1 //clc()
2 Pswater1 = 6.08; //kPa
3 T1 = 313; //K
4 //lnPs = 16.26205 - 3799.887/(T - 46.854)
5 Tb1 = 3799.887/(16.26205 - log(Pswater1)) + 46.854;
6 disp("K",Tb1,"boiling point of water at 6.08kPa
       vapour pressure = ")
7 Pswater2 = 39.33; //kPa
8 T2 = 353; //K
9 Tb2 = 3799.887/(16.26205 - log(Pswater2)) + 46.854;
10 disp("K",Tb2,"boiling point of water at 39.33 kPa
       vapour pressure = ")
11 Tb = [Tb1 Tb2];
12 T = [T1 T2];
13 plot(T,Tb);

```

```
14 xtitle('Equal pressure reference plot for sulphuric
    acid', 'Boiling point of solution ,K', 'Boiling
    point of water , K');
15 T3 = 333; //K
16 //corresponding to T3 on x axis , on y we get
17 Tb3 = 329; //K
18 Pswater3 = exp(16.26205 - 3799.887/(Tb3 - 46.854));
19 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

```
1 //clc ()
2 Pas = 71.2; //kPa
3 Pbs = 48.9; //kPa
4 P = 65; //kPa
5 //P=(Pas-Pbs)*xa+Pbs, xa=mole fraction of n-heptane ,
   liq . condition , therefore
6 xa = (P - Pbs)/(Pas - Pbs);
7 //ya = Pa / P , Vapour condition
8 ya = Pas * xa / P;
9 P1 = xa * 100;
10 P2 = ya * 100;
11 disp("%",P1,"Percentage of hepatne in liquid = ")
12 disp("%",P2,"Percentage of hepatne in vapour = ")
```

Scilab code Exa 7.2 Composition and total pressure calculation

```
1 //clc ()
```

```

2 P1 = 100; //kPa ( Vapour pressure of liq A )
3 P2 = 60; //kPa ( Vapour pressure of liq B )
4 T = 320; //K
5 //Pa = xa * P1 = 100 * xa
6 //Pa = xb * P2 = 60 * xb
7 //P = xa * P1 + ( 1 - xa ) * P2
8 // = 100xa + ( 1 - xa ) * 60
9 // = 60 + 40*xa
10 //ya = Pa / P
11 //0.5 = 100*xa / ( 60 + 40 * xa)
12 xa = 60 * 0.5 / (100 - 20);
13 Per1 = xa * 100;
14 disp("%",Per1,"(a) Percentage of A in liquid = ")
15 Ptotal = 60 + 40 * xa;
16 disp("kPa",Ptotal,"(b) Total pressure of the vapour =
    ")

```

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

```

1 //clc()
2 xa = 0.25;
3 xb = 0.30;
4 xc = 1 - xa - xb;
5 Ptotal = 200; //kPa
6 Pcs = 50; //kPa(Vapour pressure of c)
7 Pc = xc * Pcs; //(partial pressure of c)
8 yc = Pc / Ptotal;
9 yb = 0.5;
10 ya = 1 - yb - yc;
11 per1 = ya * 100;
12 disp("%",per1,"Percentage of A in vapour = ")

```

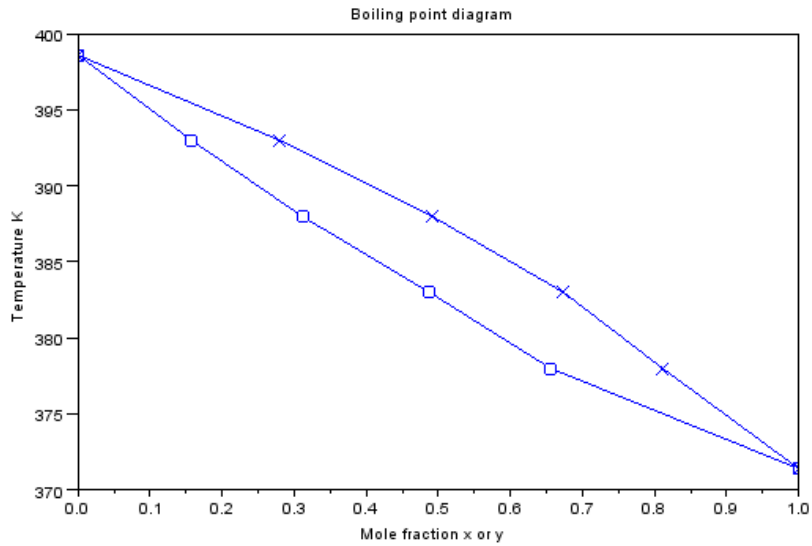


Figure 7.1: Boiling point diagram

Scilab code Exa 7.4 Flash vapourization of benzene toluene mixture

```

1 //clc()
2 P = 101.3; //kPa
3 Pbs = 54.21; //kPa
4 Pas = 136.09; //kPa
5 xf = 0.65;
6 xw = (P - Pbs)/(Pas - Pbs);
7 yd = xw * Pas / P ;
8 // f = ( xf - xw ) / ( yd - xw )
9 f = ( xf - xw ) / ( yd - xw );
10 per1 = f * 100;
11 disp("%",per1,"mole percent of the feed that is
    vapourised = ")

```

Scilab code Exa 7.5.a Boiling point diagram

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

Scilab code Exa 7.5.b Equilibrium Diagram

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

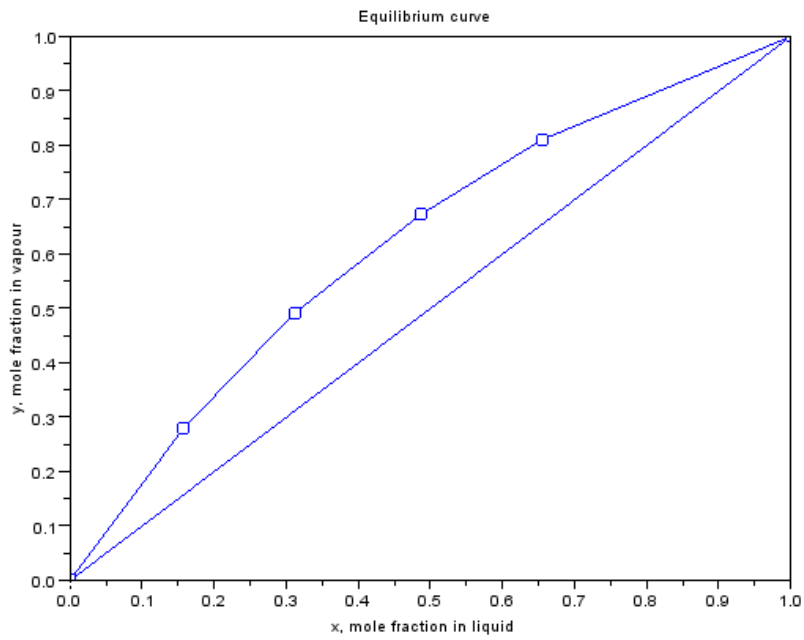


Figure 7.2: Equilibrium Diagram

```

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

```

Scilab code Exa 7.6 Bubble point temperature and vapour composition

```

1 //clc()
2 Ps = 100; //kPa
3 A1 = 13.8587; //(1 = n-heptane)
4 A2 = 13.8216; //(2 = n-hexane)
5 B1 = 2911.32;
6 B2 = 2697.55;
7 C1 = 56.51;
8 C2 = 48.78;
9 //lnPs = A - B / ( T - C)
10 T1 = B1 / (-log(Ps)+A1) + C1;
11 T2 = B2 / (-log(Ps)+A2) + C2;
12 x2 = 0.25;

```

Scilab code Exa 7.7 Dew point temperature pressure and concentration

```

1 //clc()
2 //lnPas = 14.5463 - 2940.46/(T - 35.93)
3 //lnPbs = 14.2724 - 2945.47 / (T - 49.15)
4 //xa = (P - Pbs)/(Pas - Pbs)
5 //Ya = Pas * (P - Pbs)/(P * (Pas - Pbs))
6 Ya = 0.4;
7 P = 65; //kPa
8 //various temperature value are assumed and tried
    till LHS = RHS, we get
9 T = 334.15; //K
10 Pas = exp(14.5463 - 2940.46/(T - 35.93));
11 Pbs = exp(14.2724 - 2945.47 / (T - 49.15));

```

```

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

```

Scilab code Exa 7.8 Partial pressure of acetaldehyde

```

1 //clc()
2 MW = 44.032;
3 Mwater = 18.016;
4 x = 2; //%
5 Pa = 41.4; //kPa
6 Mfr = (x/MW)/(x/MW + (100-x)/Mwater);
7 //henry's law gives Pa = Ha * xa
8 Ha = Pa / Mfr;
9 Molality = 0.1;
10 Mfr1 = Molality / (1000/Mwater + Molality);
11 Pa1 = Ha * Mfr1;
12 disp("kPa",Pa1,"Partial Pressure = ")

```

Scilab code Exa 7.9 Raoult's law application

```

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

```

```

3 x1 = 0.6;
4 x2 = 0.25;
5 x3 = 0.15;
6 A1 = 13.8183;
7 A2 = 13.8216;
8 A3 = 13.8587;
9 B1 = 2477.07;
10 B2 = 2697.55;
11 B3 = 2911.32;
12 C1 = 39.94;
13 C2 = 48.78;
14 C3 = 56.51;
15 //As raoults law is applicable ,  $K_i = y_i/x_i = P_i/P$ 
16 //  $y_i = x_i * P_i/P$ 
17 //  $\ln P = A - B/(T-C)$ 
18 //Assuming ,
19 P = 400; //kPa
20 T = 369.75; //K
21 Pas1 =exp(A1 - B1 / (T - C1));
22 Pas2 =exp(A2 - B2 / (T - C2));
23 Pas3 =exp(A3 - B3 / (T - C3));
24 Yi = (x1*Pas1 + x2*Pas2 + x3*Pas3)/P;
25 disp("K",T,"(a) bubble point temperature of the
      mixture = ")
26 y1 = x1*Pas1/P;
27 y2 = x2*Pas2/P;
28 y3 = x3*Pas3/P;
29 disp("%",y1*100,"(b) composition of n-pentane in
      vapour = ")
30 disp("%",y2*100,"composition of n-hexane in vapour =
      ")
31 disp("%",y3*100,"composition of n-heptane in vapour
      = ")
32 T1 = 300; //K
33 Ps1 =exp(A1 - B1 / (T1 - C1));
34 Ps2 =exp(A2 - B2 / (T1 - C2));
35 Ps3 =exp(A3 - B3 / (T1 - C3));
36 P1 = x1*Ps1 + x2*Ps2 + x3*Ps3;

```

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

Scilab code Exa 7.10 Dew point temperature and pressure

```
1 //clc()
2 //1 - pentane, 2 - hexane, 3 - heptane
3 y1 = 0.6;
4 y2 = 0.25;
5 y3 = 0.15;
6 A1 = 13.8183;
7 A2 = 13.8216;
8 A3 = 13.8587;
9 B1 = 2477.07;
10 B2 = 2697.55;
11 B3 = 2911.32;
12 C1 = 39.94;
13 C2 = 48.78;
14 C3 = 56.51;
15 P = 400; //kPa
16 T = 300; //K
17 //As raoults law is applicable,  $K_i = y_i/x_i = P_i^s/P$ 
18 //  $x_i = y_i*P/P_i^s$ 
19 //  $\ln P = A - B/(T-C)$ 
20 //Assuming,
21 T1 = 385.94; //K
22 Pas1 =exp(A1 - B1 / (T1 - C1));
23 Pas2 =exp(A2 - B2 / (T1 - C2));
24 Pas3 =exp(A3 - B3 / (T1 - C3));
25 disp("K",T,"(a)Dew point temperature of the mixture
    = ")
26 Ps1 =exp(A1 - B1 / (T - C1));
27 Ps2 =exp(A2 - B2 / (T - C2));
28 Ps3 =exp(A3 - B3 / (T - C3));
29 P1 = 1/(y1/Ps1 + y2/Ps2 + y3/Ps3);
30 disp("kPa",P1,"(b)Dew point pressure = ")
```

Scilab code Exa 7.11 bubble point and dew point

```
1 //clc()
2 //1 - methanol, 2 - ethanol, 3 - propanol
3 x1 = 0.45;
4 x2 = 0.3;
5 x3 = 1 - (x1 + x2);
6 P = 101.3; //kPa
7 // by drawing the temperature vs vapour pressure
  graph and interpolation, assuming,
8 T = 344.6; //K
9 Ps1 = 137.3;
10 Ps2 = 76.2;
11 Ps3 = 65.4;
12 y1 = x1 * Ps1 / P;
13 y2 = x2 * Ps2 / P;
14 y3 = x3 * Ps3 / P;
15 disp("K",T,"(a)Bubble point temperature = ")
16 disp("%",y1*100,"Composition of methanol in vapour =
  ")
17 disp("%",y2*100,"Composition of ethanol in vapour =
  ")
18 disp("%",y3*100,"Composition of propanol in vapour =
  ")
19 //again, for xi = 1
20 T1 = 347.5; //K
21 P1 = 153.28;
22 P2 = 85.25;
23 P3 = 73.31;
24 xa = x1 * P / P1;
25 xb = x2 * P / P2;
26 xc = x3 * P / P3;
27 disp("K",T1,"(b)Dew point temperature = ")
28 disp("%",xa*100,"Composition of methanol in liquid =
```

```

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

```

Scilab code Exa 7.12 component calculations

```

1 //clc()
2 xp = 0.25;
3 xnb = 0.4;
4 xnp = 0.35;
5 P = 1447.14; //kPa
6 //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,
7 Tb = 361; //K
8 disp("K",Tb,"(a) The bubble point temperature = ")
9 //At 361,
10 Kip = 2.12;
11 Kinb = 0.85;
12 Kinp = 0.37;
13 xp1 = Kip * xp;
14 xnb1 = Kinb * xnb;
15 xnp1 = Kinp * xnp;
16 disp(xp1," concentration of propane at bubble point =
    ")
17 disp(xnb1," concentration of n-butane at bubble point
    = ")
18 disp(xnp1," concentration of n-pentane at bubble
    point = ")
19 //At dew point  $Y_i/K_i = 1$ , at 377.6K this is 1.1598

```



```

    and at 388.8K it is 0.9677, by interpolation dew
    point is found to be
20 Td = 387;//K
21 Kip1 = 2.85;
22 Kinb1 = 1.25;
23 Kinp1 = 0.59;
24 yp1 = xp/Kip1;
25 ynb1 = xnb/Kinb1;
26 ynp1 = xnp/Kinp1;
27 disp("K",Td,"(b) The dew point temperature = ")
28 disp(yp1,"concentration of propane at dew point = ")
29 disp(ynb1,"concentration of n-butane at dew point =
    ")
30 disp(ynp1,"concentration of n-pentane at dew point =
    ")
31 //summation zi / (1 + L/VKi)= 0.45, using trial and
    error , we find
32 T = 374.6;//K
33 L = 0.55;
34 V = 0.45;
35 Kip2 = 2.5;
36 Kinb2 = 1.08;
37 Kinp2 = 0.48;
38 t = (xp/(1+L/(V*Kip2)))+(xnb/(1+L/(V*Kinb2))) + (xnp
    /(1+L/(V*Kinp2)));
39 yp2 = (xp/(1+L/(V*Kip2)))/t;
40 ynb2 = (xnb/(1+L/(V*Kinb2)))/t;
41 ynp2 = (xnp/(1+L/(V*Kinp2)))/t;
42 xp2 = (xp - V * yp2)/L;
43 xnb2 = (xnb - V * ynb2)/L;
44 xnp2 = (xnp - V * ynp2)/L;
45 disp("K",T,"(c) Temperature of the mixture = ")
46 disp(yp2,"vapour phase concentration of propane = ")
47 disp(ynb2,"vapour phase concentration of n-butane =
    ")
48 disp(ynp2,"vapour phase concentration of n-pentane =
    ")
49 disp(xp2,"liquid phase concentration of propane = ")

```

```

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

```

Scilab code Exa 7.13 equilibrium temperature and composition

```

1 //clc ()
2 P = 93.30; //kPa
3 T1 = 353; //K
4 T2 = 373; //K
5 Pwater1 = 47.98; //kPa
6 Pwater2 = 101.3; //kPa
7 Pliq1 = 2.67; //kPa
8 Pliq2 = 5.33; //kPa
9 T = T1 + (T2 - T1)*(P - (Pwater1 + Pliq1))/(Pwater2
    + Pliq2 - (Pwater1 + Pliq1));
10 disp("K",T,"(a)The equilibrium temperature = ")
11 Pwater = 88.50;
12 y = Pwater * 100 /P;
13 disp("%",y,"(b)Water vapour in vapour mixture = ")

```

Scilab code Exa 7.14 Temperature composition diagram

```

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

```

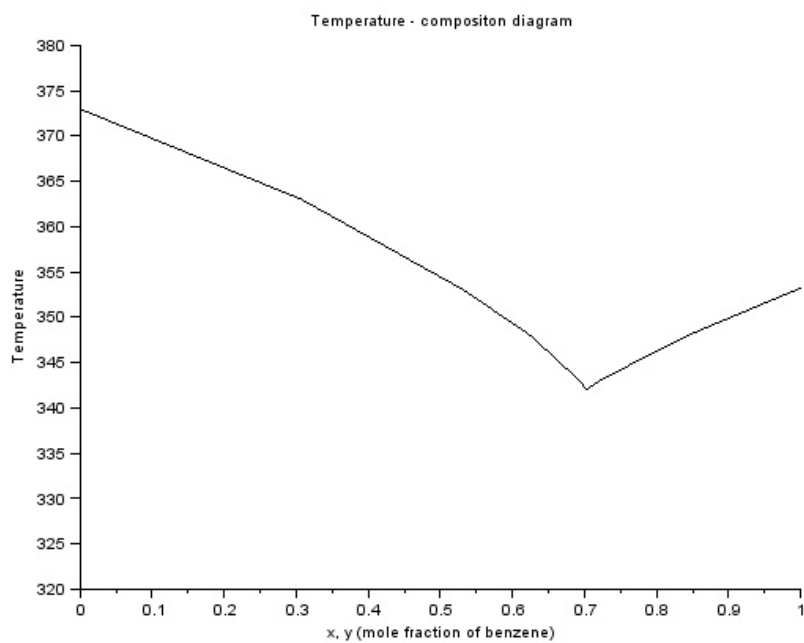


Figure 7.3: Temperature composition diagram

```

6 P = 101.3; //kPa
7 for i = 1:4
8     y1(i) = 1 - (Ps1(i))/P;
9 end
10 for i = 1:6
11     y2(i) = 1 - (Ps2(i))/P;
12 end
13 plot2d(y2,T);
14 plot2d(1-y1,T,rect = [0,320,1,380]);
15 xtitle('Temperature - compositon diagram', 'x', y (
    mole fraction of benzene)', 'Temperature')

```

Scilab code Exa 7.15 Boiling point calculation

```

1 //clc()
2 T = 379.2; //K
3 P = 101.3; //kPa
4 Ps = 70; //kPa
5 Molality = 5;
6 Pws = exp(16.26205 - 3799.887/(T - 46.854));
7 k = P / Pws;
8 Pws1 = Ps / k;
9 T1 = 3799.887 / (16.26205 - log( Pws1)) + 46.854;
10 disp("K",T1,"Boiling point of the solution = ")

```

Chapter 8

Humidity and Humidity chart

Scilab code Exa 8.1 Nitrogen and ammonia gas mixture

```
1 //clc()
2 T = 280; //K
3 P = 105; //kPa
4 Pas = 13.25; //kPa ( Vpaour pressure of acetone )
5 Pa = Pas; // ( As gas is saturated , partial pressure
    = vapour pressure )
6 Mfr = Pa / P; //(Mole fraction)
7 Mpr = Mfr * 100;
8 disp("%",Mpr,"(a)The mole percent of acetone in the
    mixture = ")
9 Ma = 58.048; //(molecular weight of acetone)
10 Mn = 28; //(molecular weight of nitrogen)
11 N = 1; //mole
12 Na = Mfr * N;
13 Nn = N - Na;
14 ma = Na * Ma ;
15 mn = Nn * Mn;
16 mtotal = ma + mn;
17 maper = ma *100 / mtotal;
18 mnper = mn *100/ mtotal;
19 disp("%",maper,"(b)Weight percent of acetone = ")
```

```

20 disp("%",mper," Weight percent of nitrogen = ")
21 Vstp = 22.4; //m^3/kmol
22 Pstp = 101.3; //kPa
23 Tstp = 273.15; //K
24 V = Vstp * Pstp * T / ( Tstp * P );
25 C = ma/V;
26 disp("kg/m^3",C," (c) Concentration of vapour = ")

```

Scilab code Exa 8.2 Benzene vapour air mixture

```

1 //clc()
2 P = 101.3; //kPa
3 Per1 = 10; //%
4 Pa = P * Per1 / 100; // ( a - benzene )
5 Ps = Pa; //( saturation )
6 //lnPs = 13.8858 - 2788.51/(T - 52.36)
7 T = 2788.51 / ( 13.8858 - log(Ps)) + 52.36;
8 disp("K",T," Temperature at which saturation occurs = ")

```

Scilab code Exa 8.3 Evaporation of acetone using dry air

```

1 //clc()
2 Pdryair = 101.3; //kPa
3 Pacetone = 16.82; //kPa
4 Nratio = Pacetone / (Pdryair - Pacetone);
5 mratio = Nratio * 58.048 / 29; // ( Macetone =
    58.048, Mair = 29 )
6 macetone = 5; //kg ( given )
7 mdryair = macetone / mratio;
8 disp("kg",mdryair," Minimum air required = ")

```

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

```
1 //clc()
2 Pa = 15;//kPa ( partial pressure of acetone)
3 Ptotal = 101.3;//kPa
4 Mfr = Pa / Ptotal;
5 disp(Mfr,"(a)Mole fraction of acetone = ")
6 Macetone = 58.048;
7 Mnitrogen = 28;
8 mafr = Mfr * Macetone / ( Mfr * Macetone + (1-Mfr)*
    Mnitrogen );
9 disp(mafr,"(b)Weight fraction of acetone = ")
10 Y = Mfr / ( 1 - Mfr );
11 disp("moles of acetone/moles of nitrogen",Y,"(c)
    Molal humidity = ")
12 Y1 = Y * Macetone / Mnitrogen ;
13 disp("kg acetone/kg nitrogen",Y1,"(d)Absolute
    humidity = ")
14 Pas = 26.36;//kPa ( vapour pressure)
15 Ys = Pas / ( Ptotal - Pas);//saturation humidity
16 disp("moles of acetone/moles of nitrogen",Ys,"(e)
    Saturation humidity = ")
17 Y1s = Ys * Macetone / Mnitrogen;
18 disp("kg acetone/kg nitrogen",Y1s,"(f)Absolute
    saturation humidity = ")
19 V = 100;//m^3
20 Vstp =22.4143;//m^3/kmol
21 Pstp = 101.3;//kPa
22 Tstp = 273.15;//K
23 T = 295;//K
24 N = V * Ptotal * Tstp / (Vstp * Pstp * T );
25 Nacetone = N * Mfr;
26 macetone = Nacetone * Macetone;
```

```
27 disp("kg",macetone,"(g)Mass of acetone in 100m3 of  
the total gas = ")
```

Scilab code Exa 8.5 Percent saturation and relative saturation

```
1 //clc();  
2 Pa = 15;//kPa ( Partial pressure )  
3 Pas = 26.36;//kPa ( Vapour pressure )  
4 RS = Pa * 100 / Pas ;  
5 Y = 0.1738;  
6 Ys = 0.3517;  
7 PS = Y * 100 / Ys;  
8 disp("%",RS,"Relative humidity = ")  
9 disp("%",PS,"Percent humidity = ")
```

Scilab code Exa 8.6 Analysis of Moist air

```
1 //clc()  
2 mwater = 0.0109;//kg  
3 V = 1;//m3  
4 T = 300;//K  
5 P = 101.3;//kPa  
6 Vstp =22.4143;//m3/kmol  
7 Pstp = 101.3;//kPa  
8 Tstp = 273.15;//K  
9 N = V * P * Tstp / (Vstp * Pstp * T );  
10 Nwater = mwater / 18.016;  
11 Nfr = Nwater / N;  
12 Pwater = Nfr * P;  
13 disp("kPa",Pwater,"(a)Partial pressure of water  
vapour = ")  
14 Ps = exp(16.26205 - 3799.887/(T - 46.854));  
15 RS = Pwater * 100 / Ps;
```



```

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

```

Scilab code Exa 8.7 Heating value calculation for a fuel gas

```

1 //clc ()
2 T = 300; //K
3 P = 100; //kPa
4 S = 25000 //kJ/m^3
5 T1= 295; //K
6 P1 = 105; //kPa
7 RS = 50; //%
8 Ps = 3.5; //kPa
9 Ps1 = 2.6; //kPa
10 Vstp = 22.4143; //m^3/kmol
11 Pstp = 101.3; //kPa
12 Tstp = 273.15; //K
13 V = 1; //m^3
14 N = V * P * Tstp/(Vstp * Pstp * T);
15 Nfuel = N * (P - Ps)/P;
16 Smol = S / Nfuel; //kJ/kmol
17 N1 = V * P1 * Tstp/(Vstp * Pstp * T1);
18 Pwater = Ps1 * RS /100;

```

```

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

```

Scilab code Exa 8.8 Analysis of nitrogen benzene mixture

```

1 //clc()
2 T = 300; //K
3 T1 = 335; //K
4 P = 150; //kPa
5 //lnPs = 13.8858 - 2788.51 / ( T - 52.36)
6 Ps = exp(13.8858 - 2788.51 / ( T - 52.36));
7 Ps1 = exp(13.8858 - 2788.51 / ( T1 - 52.36));
8 Pa = Ps; //(Vapour pressure at dew point is equal to
      the partial pressure of the vapour)
9 Y = Pa / ( P - Pa);
10 Ys = Ps1 / ( P - Ps1);
11 PS = Y * 100 / Ys;
12 disp("%",PS,"(a)Percent saturation = ")
13 Ma = 78.048;
14 Mb = 28;
15 Q = Y * Ma / Mb ;
16 disp("kg benzene/kg nitrogen",Q,"(b)Quantity of
      benzene per kilgram of nitrogen = ")
17 V = 1; //m^3 ( basis )
18 Vstp = 22.4143; //m^3/kmol
19 Pstp = 101.3; //kPa
20 Tstp = 273.15; //K
21 N = V * P * Tstp/(Vstp * Pstp * T1);
22 y = Y / ( 1 + Y );
23 Nbenzene = N * y;
24 C = Nbenzene * Ma;
25 disp("kg/m^3",C,"(c)Kilogram of benzene per m^3 of
      nitrogen = ")

```

```

26 P1 = 100; //kPa
27 Pbenzene = y * P1;
28 T1 = 2788.51 / ( 13.8858 - log (Pbenzene)) + 52.36;
29 disp("K",T1,"(d)Dew point = ")
30 Per1 = 60; //%
31 Y2 = Y * (1- Per1/100);
32 //Y2 = Pa / (P - Pa)
33 P = Pa / Y2 + Pa;
34 disp("kPa",P,"(e)Pressure required = ")

```

Scilab code Exa 8.9 Drying

```

1 //clc()
2 T = 300; //K
3 T1 = 285; //K
4 Pwater = 3.56; //kPa
5 Pwater1 = 1.4; //kPa
6 V = 1; //m^3 ( Basis )
7 Vstp = 22.4143; //m^3/kmol
8 N = V / Vstp;
9 Pstp = 101.3; //kPa
10 Y = Pwater / (Pstp - Pwater);
11 Y1 = Pwater1 / (Pstp - Pwater1);
12 Nremoved = Y - Y1;
13 Ndryair = N * 1 / (1 + Y);
14 mremoved = Ndryair * Nremoved * 18.016;
15 disp("kg",mremoved,"(a)amount of water removed = ")
16 Nremaining = Ndryair * Y1 ;
17 V1 = (Ndryair + Nremaining) * Vstp ;
18 disp("m^3",V1,"(b)Volume of gas at stp after drying
    = ")

```

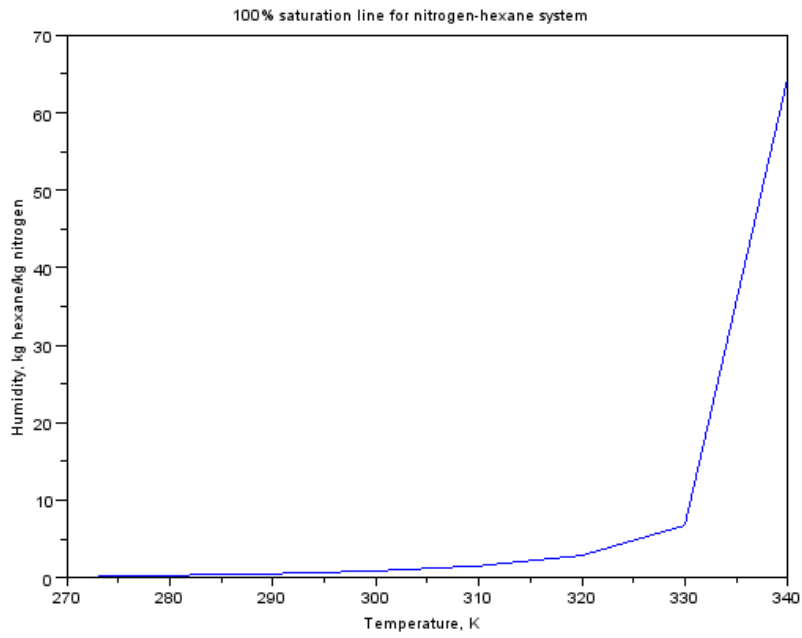


Figure 8.1: Saturation lines for hexane

Scilab code Exa 8.10 Saturation lines for hexane

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

Scilab code Exa 8.11 Psychometric chart application

```
1 //clc ()
2 Td = 328; //K ( dry bulb )
3 P = 101.3; //kPa
4 PS = 10; //%
5 //referring to the psychometric chart , corresponding
   to 328 K and 10% saturation
6 Y1 = 0.012; //kg water / kg dry air
7 disp("kg water / kg dry air",Y1,"(a) Absolute
   humidity = ")
8 //Y1 = Pa * 18 / ( P - Pa ) * 29
9 Pa = Y1 * P * 29 / ( 18 + Y1 * 29 );
```

```

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

```

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

```

1 //clc ()
2 Ca = 1.884; //kJ/kgK
3 Cb = 1.005; //kJ/kgK
4 Y1 = 0.012;
5 //Cs = Cb + Y1 * Ca
6 Cs = Cb + Y1 * Ca;
7 disp("kJ/kgK",Cs,"Humid heat of the sample = ")
8 P = 101.3; //kPa
9 V = 100; //m^3
10 R = 8.314;
11 T = 328; //K
12 T1 = 373; //K
13 N = P * V / ( R * T );
14 Pa = 1.921; //kPa

```

```

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

```

Scilab code Exa 8.14 wet bulb temperature and dry bulb temperature

```

1 //clc ()
2 P = 101.3; //kPa
3 MW = 58;
4 T1 = 280.8; //K
5 Ps = 5; //kPa
6 pr = 2; //kJ/kgK ( Psychometric ratio )
7 Hvap = 360; //kJ/kg
8 Tw = T1;
9 Yw1 = Ps * MW / (( P - Ps) * 29);
10 // Tw = Tg - Hvap * ( Yw1 - Y1) / (hG / kY), where
    hG/kY is the psychometric ratio pr
11 Y1 = 0;
12 Tg = Tw + Hvap * ( Yw1 - Y1) / pr;
13 disp("K",Tg,"The air temperature = ")

```

Scilab code Exa 8.15 Humidity calculation

```

1 //clc ()
2 Td = 353.2; //K
3 Tw = 308; //K
4 Hvap = 2418.5; //kJ/kg
5 pr = 0.950; //kJ/kg
6 Ps = 5.62; //kPa
7 P = 101.3; //kPa
8 Yw1 = (Ps * 18) / (( P - Ps) * 29);
9 Y1 = Yw1 - pr * ( Td - Tw ) / Hvap;

```

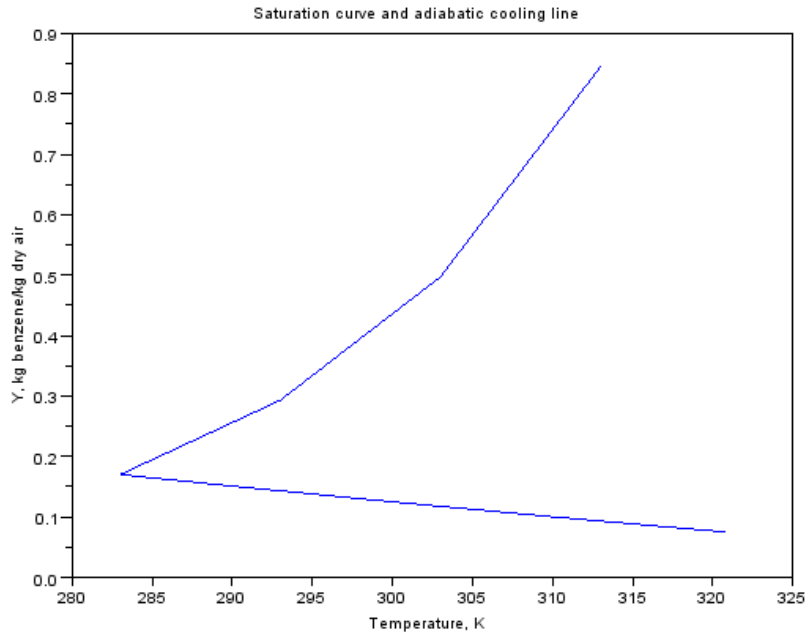


Figure 8.2: SATuration curve and adiabatic cooling line

```

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

```

Scilab code Exa 8.16 SATuration curve and adiabatic cooling line

```

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

```



```

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

```

Scilab code Exa 8.17 Adiabatic drier

```

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

```

```

13 MY = Y * 29 / 18; //molal humidity
14 Ndryair = N / ( 1 + MY );
15 mdryair = Ndryair * 29;
16 mwaterin = mdryair * Y;
17 mwaterout = mwaterin + mremoved;
18 Yout = mwaterout / mdryair;
19 // percent humidity is calculated using the chart,
    and is
20 PY = 55; //%
21 disp("kg water /kg dry air",Yout,"(b) exit air
    humidity = ")
22 disp("%",PY,"Percent humidity = ")
23 //from the humidity chart
24 Twet = 313.2; //K
25 Td = 322.2; //K
26 disp("K",Twet,"(c) exit air wet bulb temperature = ")
27 disp("K",Td,"(c) exit air dry bulb temperature = ")
28 MYout = Yout * 29 / 18;
29 Nout = Ndryair * ( 1 + MYout ) / 1;
30 V1 = Nout * Vstp * Td / Tstp;
31 disp("m^3",V1,"(d) Volume of exit air = ")

```

Scilab code Exa 8.18 Psychometric chart application

```

1 //clc()
2 P = 101.3; //kPa
3 Td = 303; //K
4 Tw = 288; //K
5 //using psychometric chart,
6 Y1 = 0.0045; //kg water/ kg dry air
7 PY = 18; //%
8 Theated = 356.7; //K
9 Cb = 1.005;
10 Ca = 1.884;
11 Cs = Cb + Y1 * Ca;

```

```

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

```

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

```

1 //clc ()
2 Tw = 313; //K
3 Td = 333; //K
4 //Using th psychometric chart ,
5 Y = 0.04; //kg water/ kg dry air
6 PS = 26.5; //%
7 VS = 1.18; //m^3/kg dry air ( volume of saturated air
    )
8 VD = 0.94; //m^3/kg dry air ( volume of dry air )
9 VH = VD + PS * (VS - VD )/100;
10 HS = 470; //J / kg dry air ( enthalpy of saturated
    air )
11 HD = 60; //J / kg dry air ( enthalpy of dry air )
12 H = HD + PS * ( HS - HD )/100;
13 disp("kg water/ kg dry air",Y,"(a)Absolute Humidity
    of the air = ")
14 disp("%",PS,"(b)Percent humidity = ")
15 disp("m^3/kg dry air",VH,"(c)Humid volume = ")
16 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

```
1 //clc ()
2 PC1 = 85; //% ( Percent carbon in coal )
3 PA1 = 15; //% ( Percent ash in coal )
4 PA2 = 80; //% ( Percent ash in cinder )
5 PC2 = 20; //% ( Percent carbon in cinder )
6 m = 100; //kg (weight of coal )
7 mash = PA1 * m / 100;
8 w = mash * 100 / PA2; // weight of cinder
9 mcarbon = w - mash;
10 Plost = mcarbon * 100 / ( m - mash );
11 disp("kg",w,"weight of cinder formed = ")
12 disp("%",Plost,"Percent fuel lost = ")
```

Scilab code Exa 9.2 Drying of wood

```
1 //clc ()
```

```

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

```

Scilab code Exa 9.3 Effluent discharge

```

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

```

Scilab code Exa 9.4 benzene requirement calculation

```

1 //clc()
2 D = 100; //kg of overhead product
3 xfa = 0.956;
4 xdw = 0.074;
5 xdb = 0.741;
6 xda = 0.185;
7 //water balance gives
8 F = D * xdw / (1 - xfa) ;
9 W = F * xfa - xda * D;

```

```

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

```

Scilab code Exa 9.5 Fortification of waste acid

```

1 //clc()
2 //let, W – waste acid, S – Sulfuric acid, N – nitric
   acid, M – mixed acid
3 xsh2so4 = 0.95;
4 xsh2o = 0.5;
5 xwh2so4 = 0.3;
6 xwhno3 = 0.36;
7 xwh2o = 0.34;
8 xmh2so4 = 0.4;
9 xmhno3 = 0.45;
10 xmh2o = 0.15;
11 xnhno3 = 0.8;
12 xnh2o = 0.2;
13 M = 1000; //kg
14 // total material balance, W + S + N = 1000;
15 //H2SO4 balance, xwh2so4 * W + xsh2so4 * S = xmh2so4
   *M
16 //HNO3 balance, xwhno3 * W + xnhno3 * N = xmhno3*M
17 //H2O balance, xwh2o*W+xnh2o*N + xsh2o*S = xmh2o*M
18 //solving the above equations simultaneously, we get
   ,
19 W = 70.22; //kg
20 S = 398.88; //kg
21 N = 530.9; //kg
22 disp("kg",W,"Waste acid = ")
23 disp("kg",S,"Concentrated H2SO4 = ")
24 disp("kg",N,"Concentrated HNO3 = ")

```

Scilab code Exa 9.6 Triple effect evaporator

```
1 //clc ()
2 F = 1000; //kg
3 Psolute1 = 20; //%
4 Psolute2 = 80; //%
5 //taking solute balance
6 L3 = F * Psolute1 / Psolute2;
7 //taking total material balance
8 V = (F -L3) / 3;
9 //for first effect , total balance gives ,
10 L1 = F - V;
11 //solute balance gives ,
12 Psolute3 = F * Psolute1 / L1;
13 //For second effect , total balance gives ,
14 L2 = L1 - V;
15 //solute balnce gives ,
16 Psolute4 = L1 * Psolute3 / L2;
17 disp("%",Psolute3,"solute entering second effect = ")
18 )
19 disp("kg",L1,"Weight entering second effect")
20 disp("%",Psolute4,"solute entering third effect = ")
21 disp("kg",L2,"Weight entering third effect")
```

Scilab code Exa 9.7 Crystallization operation

```
1 //clc ()
2 F = 100; //kg
3 xf = 0.25;
4 x2 = 7/107;
5 P1 = 10; //%
```

```

6 W3 = P1 * F * (1-xf)/100; //(W3 – weight of water
  evaporated)
7 // let W1 and W2 be weight of crystal and weight of
  mother liquor remaining after crystallization
  resp. ,
8 //F = W1 + W2 + W3
9 //100 = W1 + W2 + 7.5
10 //solute balance gives , F*xf = W1*x1 + W2*x2
11 //100*0.25 = W1*1+W2 * 0.0654
12 W2 = (F - W3 - F*xf)/(1-x2);
13 W1 = F - W3 - W2;
14 disp("kg",W1,,,"yeild of the crystals = ")

```

Scilab code Exa 9.8 Evaporation of Na₂CO₃

```

1 //clc ()
2 F = 100; //kg
3 xf = 0.15;
4 P1 = 80; //% ( Carbonate recovered )
5 M1 = 106; //(Molecular weight of Na2CO3)
6 M2 = 286; //(Molecular weight of Na2CO3.10H2O)
7 x1 = M1 / M2; //(Weight fraction of Na2CO3 in
  crystals)
8 Mrecovered = P1 * F * xf / 100;
9 Wcrystal = Mrecovered / x1;
10 disp("kg",Wcrystal, "(a)quantity of crystals formed =
  ")
11 //Na2CO3 balance gives , F*xf = Wcrystal*x1 + W2*x2
12 //W2 weight of mother liquor remaining after
  crystallization
13 //let M = W2 * x2, therefore
14 M = F * xf - Mrecovered;
15 x2 = 0.09;
16 W2 = M/x2;
17 W3 = F - Wcrystal - W2; //weight of water evaporated

```


18 `disp("kg",w3,"(b)Weight of water evaporated = ")`

Scilab code Exa 9.9 Crystallization

```
1 //clc ()
2 m = 100; //kg (of 60% solution)
3 //w - water added to the original solution
4 //w1 - wt. of Na2S2O3.5H2O crystallized
5 //w2 - wt. of mother liquor obtained
6 //w3 - solution carried away by the crystals
7 xf = 0.6;
8 Mna2s2o3 = 158;
9 Mna2s2o35h2o = 248;
10 mcrystals = m * xf * Mna2s2o35h2o / Mna2s2o3;
11 // free water available = m + w - 1 - mcrystals
12 //concentration of impurity = 1/(w+4.823)
13 //total balance, 100 - 1 + w = w1 + w2 + w3
14 //w1 + w2 + w3 - w = 99
15 //Na2S2O3 balance, 60 = (w1 + w2 * 1.5/2.5 + w3 *
    1.5/2.5)*158/248
16 //w1 + 0.6 * w2 + 0.6 * w3 = 94.177
17 //each gram crystals carry 0.05 kg solution,
18 //w3 = 0.05 * w1
19 //impurity % = 0.1
20 //impurity = w3 / (2.5 * (w+4.823))
21 //solving above equations, we get
22 w = 14.577; //kg
23 w1 = 65.08; //kg
24 w2 = 45.25; //kg
25 w3 = 0.05 * w1;
26 disp("kg",w,"(a)amount of water added = ")
27 disp("kg",w1,"(b)amount of Na2S2O3.5H2O crystals
    added = ")
28 m1 = w1 * Mna2s2o3 / Mna2s2o35h2o + w3 * 1.5 *
    Mna2s2o3 / (2.5 * Mna2s2o35h2o);
```

```

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

```

Scilab code Exa 9.10 Extraction

```

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

```

Scilab code Exa 9.11 Leaching operation

```

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

```

```

8 Pwater = 100 - Poil1 - Ppulp1 - Psalts1;
9 Phexane2 = 25; //%(2 - underflow)
10 Psalts2 = 2.5; //%
11 Poil2 = 15; //%
12 Pwater2 = 7.5; //%
13 Ppulp2 = 100 - Phexane2 - Poil2 - Pwater2 - Psalts2
    ;
14 Poil3 = 25; //% ( 3 - extract )
15 //taking pulp ( inert ) balance
16 U = Ppulp1 * F / Ppulp2;
17 //oil balance gives , F * Poil1 = U * Poil2 + R *
    Poil3 ,from these , we get
18 R = (F * Poil1 - U * Poil2)/Poil3;
19 S = U + R - F;
20 disp("kg",S,"(a)The amount of solvent used for
    extraction = ")
21 Precovered = 95; //%
22 mhexane2 = Phexane2 * U / 100;
23 mrecovered = mhexane2 * Precovered / 100;
24 P = mrecovered * 100 / S ;
25 disp("%",P,"(b)Percent of hexane used that is
    recovered from the underflow = ")
26 Poil = Poil3 * R * 100 / (F * Poil1 );
27 disp("%",Poil,"(c)Percent recovery of oil = ")

```

Scilab code Exa 9.12 Dryer and oven

```

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

```

```

7 //moisture free solid balance for drier ,  $F * ( 1 -$ 
       $xf) = S1 * ( 1 - x1 )$ 
8  $S1 = F * ( 1 - xf ) / (1 - x1);$ 
9 //total balance for drier ,  $F = S1 + V1$ 
10  $V1 = F - S1;$ 
11 //For oven ,  $S1 * ( 1 - x1 ) = S2 * ( 1 - x2 )$ 
12  $S2 = S1 * ( 1 - x1 ) / (1 - x2);$ 
13 //Also ,  $S1 = S2 + V2$ 
14  $V2 = S1 - S2;$ 
15 disp("kg",S1,"(a)Weight of product leaving the drier
      = ")
16 disp("kg",S2," Weight of product leaving the oven
      = ")
17  $P1 = V1 * 100 / (F * xf);$ 
18  $P2 = V2 * 100 / (F * xf);$ 
19 disp("%",P1,"(b)Percentage of original water removed
      in drier = ")
20 disp("%",P2," Percentage of original water removed
      in oven = ")

```

Scilab code Exa 9.13 Adiabatic drier

```

1 //clc()
2 //Ss = solid flow rate ,
3 Pwaterin = 25; //%
4 Pwaterout = 5; //%
5  $X1 = Pwaterin / (100 - Pwaterin);$  //kg water/kg dry air
6  $X2 = Pwaterout / (100 - Pwaterout);$  //kg water/kg dry
      air
7 //form humidity chart ,
8  $Y2 = 0.015;$  //kg water/kg dry air
9  $Y1 = 0.035;$  //kg water/kg dry air
10  $m = 1;$  //kg of dry air
11 //  $Ss * X1 + Y2 = Ss * X2 + Y1$ 
12  $Ss = (Y1 - Y2) / (X1 - X2);$ 

```

```

13 T = 87.5 + 273.15; //K
14 P = 101.3; //kPa
15 Tstp = 273.15; //K
16 Pstp = 101.3; //kPa
17 Vstp = 22.4143; //m^3/mol
18 V = 100; //m^3
19 N = V * P * Tstp / ( Vstp * Pstp * T);
20 Nr2 = Y2 * 29 / 18; //kmol of water / kmol of dry air
21 Ndryair = N * 1 / (1 + Nr2);
22 mdryair = Ndryair * 29;
23 mevaporated = mdryair * ( Y1 - Y2 );
24 disp("kg",mevaporated,"(a)total moisture evaporated
      per 100m^3 of air entering = ")
25 Ss1 = mdryair * Ss;
26 mproduct = Ss1 * ( 1 + X2 );
27 disp("kg",mproduct,"(b)mass of finished product per
      100m^3 of air entering = ")

```

Scilab code Exa 9.14 Extraction of isopropyl alcohol

```

1 //clc()
2 //F = feed , E = extract , S = solvent , R = Raffinate
3 xwaterF = 0.7; //Feed
4 xalcoholF = 0.3;
5 xwaterR = 0.71; //raffinate
6 xalcoholR = 0.281;
7 xethyR = 0.009;
8 xwaterE = 0.008; //Extract
9 xalcoholE = 0.052;
10 xethyE = 0.94;
11 //Total balance , R + E = F + S
12 F = 100; //kg
13 //R + E = 100 + S (1)
14 //Isopropyl balance , xalcoholR * R + xalcoholE * E =
      xalcoholF * F

```

```

15 //0.281*R + 0.052 * E = 30 (2)
16 //Ethylene tetra chloride balance , xethyR * R +
    xethyE * E = S
17 //0.009*R + 0.94*E = S (3)
18 //Solving equation 1, 2 and 3 simultaneously , we get
    ,
19 S = 45.1;
20 E = 47.04;
21 R = 98.06;
22 disp("kg",S,"(a)Amount of solvent used = ")
23 disp("kg",E,"(b)Amount of extract = ")
24 disp("kg",R," Amount of raffinate = ")
25 mextracted = E * xalcoholE;
26 P1 = mextracted * 100 / (F * xalcoholF);
27 disp("%",P1,"(c)Percent of isopropyl alcohol
    extracted = ")

```

Scilab code Exa 9.15 Absorption of acetone

```

1 //clc()
2 G1 = 100; //kmol
3 //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.,
4 y1 = 0.25; //%
5 y2 = 0.05; //%
6 //air balance gives , G1 * ( 1-y1 ) = G2 * ( 1-y2 )
7 G2 = G1 * ( 1-y1 ) / (1 - y2);
8 maleaving = G2 * y2;
9 maentering = G1 * y1;
10 Pabsorbed = (maentering - maleaving) * 100 / (
    maentering);
11 disp("%",Pabsorbed,"Percentage of acetone absorbed =
    ")

```

Scilab code Exa 9.16 Absorption of SO₃

```

1 //clc ()
2 F = 5000; //kg/h
3 P1 = 50; //% (H2O4 in)
4 MH2SO4 = 98.016;
5 P1gas = 65; //(nitrogen in gas entering)
6 P2gas = 35; // ( SO3)
7 MN2 = 28;
8 MSO3 = 80;
9 Mavg = ( MN2 * P1gas + MSO3 * P2gas)/100; //avg
    molecular wt. of entering gas
10 G = 4500; //kg/h
11 Ng = G / Mavg;
12 NN2 = Ng * P1gas / 100;
13 NSO3 = Ng - NN2;
14 P2 = 75; //% (H2O4 out)
15 //W be the mass of 75% H2SO4, x and y be the moles
    of SO3 and water vapour leaving resp.,
16 Pwater = 25; //kPa
17 Ptotal = 101.3; //kPa
18 //Pwater / Ptotal = y / ( NN2 + x + y )
19 //we get , y = 0.32765 * x + 2.744 (1)
20 //Total balance Feed + G = W + (NN2 * 28 + x * 80 +
    y * 18.016)
21 //we get , W + 80*x + 18.016*y = 7727.32 (2)
22 //from 1 and 2, 84.9174*x + W = 7352.68 (3)
23 //SO3 balance , So3 eneterin with 50% H2SO4 + SO3 in
    feed gas = SO leaving with 75%H2SO4 + SO3 leaving
    in exit gas
24 //5000*0.5*80/98.016 + 34.09*80 = 80* x + 0.75*W *
    80/98.016 (4)
25 // from 3 and 4,
26 x = 9.74;

```

```

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

```

Scilab code Exa 9.17 Continuous distillation column

```

1 //clc()
2 F = 200; //kmol/h
3 //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.
4 xf = 0.10;
5 xd = 0.89;
6 xw = 0.003;
7 //total balance gives, F = D + W
8 //D + W = 200 (1)
9 //Alcohol balance gives, F*xf = D*xd + W*xw
10 //0.89*D+0.003*W = 20 (2)
11 //solving 1 and 2
12 D = 21.87; //kmol/h
13 W = 178.13; //kmol/h
14 Nawasted = W*xw;
15 mmakeup = Nawasted * 46*24;
16 disp("kg",mmakeup,"The make up alcohol required per
   day = ")

```

Scilab code Exa 9.18 Distillation operation for methanol solution

```

1 //clc()
2 F = 100; //kg
3 //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.
4  xf = 0.20;
5  xd = 0.97;
6  xw = 0.02;
7  //using ,  $F = D + W$  and  $F*xf + D*xd + W*xw$ ,we get
8  D = 18.95; //kg/h
9  W = 81.05; //kg/h
10 R = 3.5;
11 //R = L / D
12 //for distillate = 1kg
13 D1 = 1; //kg
14 L = R*D1;
15 //Taking balance around the condenser ,
16 G = L + D1;
17 mcondensed = G * D / F;
18 disp("kg",D,"(a)Amount of distillate = ")
19 disp("kg",W," Amount of Bottom Product = ")
20 disp("kg",G,"(b)Amount of vapour condensed per kg of
    distillate = ")
21 disp("kg",mcondensed,"(c)Amount of vapour condensed
    per kg of feed = ")

```

Scilab code Exa 9.19 Bypass operation

```

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

```

```

9 // 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.
10 //therefore , taking balance we get ,  $1*Ys2 + x * Ys1$ 
    =  $(1 + x)*Ys$ 
11  $x = (1*Ys2 - 1*Ys)/(Ys - Ys1);$ 
12 disp("kg dry air",x,"(a)Mass of dry air bypassed per
  kg of dry air sent through the dehumidifier = ")
13 mcondensed = Ys1 - Ys2;
14 mwetair = mdryair + Ys1;
15 Nwetair = mdryair/29 + Ys1/18.016;
16 Vstp = 22.4143; //m^3/kmol
17 Vstp1 = Nwetair * Vstp;
18 T = 320; //K
19 P = 101.3; //kPa
20 Tstp = 273.15; //K
21 Pstp = 101.325; //kPa
22  $V = Vstp1 * Pstp * T / (P * Tstp);$ 
23 Vgiven = 100; //m^3
24 mcondensed1 = mcondensed * Vgiven / V;
25 disp("kg",mcondensed1,"(b)mass of water vapour
  condensed in the dehumidifier per 100m^3 of air
  sent through it = ")
26 mfinal = mdryair + x;
27 mfinalair = mfinal * Vgiven / V;
28 N = mfinalair / 29;
29 Ysn = Ys * 29/18; //kmol water / kmol dry air
30 Ntotal = N * (Ysn + 1);
31 Vfinal = Ntotal * Vstp * Pstp * T / ( Tstp * P );
32 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

```

1 //clc ()
2 F = 100; //kg/h
3 xf = 0.2;
4 xp = 0.93;
5 xr = 0.5/1.5;
6 xx = 0.65;
7 //R - recycle stream , P - Product stream , W - water
   separated and removed
8 //component A balance , F * xf = P * xp, that is ,
9 P = F * xf / xp;
10 //Total balance , F = P + W, therefore
11 W = F - P;
12 //x be the flow rate of strea entering the filter
13 //total balance , x = P + R
                                     (1)
14 //component A balance , 0.65 * x = 0.5*R/1.5 + 0.93P
                                     (2)
15 //Solving 1 and 2, we get ,
16 R = (xx * P - xp * P)/(xr - xx);
17 disp("kg/h",R,"Flow rate of the recycle stream = ")

```

Scilab code Exa 9.21 Recycle operation granulator and drier

```

1 //clc ()
2 F = 1000; //kg/h
3 xfwater = 0.7;
4 xpwater = 0.2;
5 xrwater = 0.20;
6 xswater = 0.5;
7 y1 = 0.0025;
8 y2 = 0.05;
9 //R - recycle , S - stream entering granulator , P -
   Product, G1 - air entering the drier , G2 - air
   leaving the drier ,
10 //taken overall , moisture free balance , F * xf = P *

```

```

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

```

Scilab code Exa 9.22 Blowdown operation

```

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

```

```
9 //let F/B be X
10 X = (xb + xp)/(xf + xp);
11 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

```
1 //clc ()
2 mair = 500; //kg
3 mCO2 = 55; //kg
4 mCO = 15; //kg
5 //C3H8 + 5O2 = 3CO2 + 4H2O
6 MCO2 = 44;
7 MCO = 28;
8 NCO2 = mCO2 / MCO2;
9 NCO = mCO / MCO;
10 Mair = 29;
11 Nair = mair / Mair;
12 //carbon balance gives ,
13 F = (NCO2 + NCO)/3;
14 MC3H8 = 44.064;
15 mC3H8 = MC3H8 * F ;
16 disp("kg",mC3H8,"(a)mass of propane burnt = ")
17 //one mole of propane requres 5 moles of oxygen for
    combustion
18 NO2 = F * 5;
```

```

19 Nairt = NO2 * 100 / 21; //theoretical air required
20 Pexcess = (Nair - Nairt) * 100 / Nairt;
21 disp("%",Pexcess,"(b)The percent excess air = ")
22 //C3H8 + 7/2 * O2 = 3CO + 4H2O
23 NH2O = F * 4;
24 //Taking oxygen balance , unburned oxygen is
    calculated ,
25 //O2 supplied = O2 present in form of CO2, CO and
    H2O + unburned O2
26 Nunburnt = Nair * 21 / 100 - NCO2 - NCO/2 - NH2O/2;
27 NN2 = Nair * 79 / 100;
28 Ntotal = NCO2 + NCO + NH2O + NN2 + Nunburnt;
29 PCO2 = NCO2 * 100 / Ntotal;
30 PCO = NCO * 100 / Ntotal;
31 PH2O = NH2O * 100 / Ntotal;
32 PN2 = NN2 * 100 / Ntotal;
33 PO2 = Nunburnt * 100 / Ntotal;
34 disp("%",PCO2,"(c)Percent composition of CO2 = ")
35 disp("%",PCO,"Percent composition of CO = ")
36 disp("%",PH2O,"Percent composition of H2O = ")
37 disp("%",PN2,"Percent composition of N2 = ")
38 disp("%",PO2,"Percent composition of O2 = ")

```

Scilab code Exa 10.2 Combustion of hydrogen free coke

```

1 //clc ()
2 Nflue = 100; //kmol
3 NCO2 = 14.84;
4 NCO = 1.65;
5 NO2 = 5.16;
6 NN2 = 78.35;
7 PCF = 85; //PERCENT CARBON IN FEED
8 PIF = 15; //PERCENT INERT IN FEED
9 //F - amount of coke charged , W - mass of coke left ,
    W = 0.05F

```

```

10 NCflue = NCO2 + NCO ;
11 MC = 12;
12 mC = MC * NCflue ;
13 //carbon balance gives , F * PCF / 100 = W * PCF + mC
14 F = mC / ( PCF / 100 - 0.05*PCF / 100);
15 //let A kmol air supplied , taking N2 balance ,
16 Nair = NN2 * 100/79;
17 NO2supplied = Nair - NN2;
18 Ntheoretical = F * PCF / (100 * MC);
19 Pexcess = ( NO2supplied - Ntheoretical ) * 100 / (
    Ntheoretical );
20 disp("%",Pexcess,"(a)Percentage excess air = ")
21 mair = Nair * 29;
22 m = mair / F ;//air supplied per kg of coke charged
23 disp("kg",m,"(b)air supplied per kg of coke charged
    = ")
24 P = 100; //kPa
25 T = 500; //K
26 V = Nflue *22.4143*101.325 * T / (F * P * 273.15);
27 disp("m^3",V,"(c)volume of flue gas per kg of coke =
    ")
28 W = 0.05*F;
29 mCr = W * PCF/100; //carbon in refuse
30 mir = F * (1-PCF/100); //inert in refuse
31 mr = mCr + mir;
32 C = mCr * 100 / mr;
33 I = mir *100/ mr;
34 disp("%",C,"(d)Carbon = ")
35 disp("%",I,"Inert = ")

```

Scilab code Exa 10.3 Combustion of fuel oil

```

1 //clc ()
2 Nflue = 100; //kmol
3 NCO2 = 9;

```



```

4 NCO = 2;
5 NO2 = 3;
6 NN2 = 86;
7 NCflue = NCO2 + NCO ;
8 MC = 12;
9 mC = MC * NCflue ;
10 //let A kmol air supplied , taking N2 balance ,
11 Nair = NN2 * 100/79;
12 NO2supplied = Nair - NN2;
13 // 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
14 Noexcess = NO2 - NCO/2;
15 Pexcess = Noexcess * 100 / ( NO2supplied - Noexcess
    );
16 disp("%",Pexcess,"(a)Percentage excess air = ")
17 Nwater0 = NO2supplied - NCO2 - NCO/2 - NO2;
18 NH2 = Nwater0*2;
19 mH2 = NH2 * 2;
20 xCF = 0.7
21 R = mC / mH2;
22 disp(R,"(b)Ratio of carbon to hydrogen in the fuel =
    ")
23 //let x be the amount of moisture in the feed , n it
    is given that 70% is carbon ,therefore ,
24 //0.7 = 3.32 / ( 1 + 3.32 + x )
25 x = R / xCF - 1 - R;
26 mH = x * 2.016 / 18.016;
27 mHtotal = mH + mH2;
28 Rtotal = mC / mHtotal;
29 disp(Rtotal,"(c)Ratio of carbon to total hydrogen in
    the fuel = ")
30 ntotal = R + 1 +x;
31 PH2 = 1*100/ntotal;
32 PH2O = x * 100 / ntotal;
33 disp("%",PH2,"(d)percentage of combustible hydrogen
    in the fuel = ")
34 disp("%",PH2O,"percentage of moisture in the fuel =

```

```

    ")
35 nH2Ototal = (PH2O + PH2 * 18.016 / 2.016)/100;
36 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

```

1 //clc ()
2 Nflue = 100; //kmoles
3 NCO2 = 9.05;
4 NCO = 1.34;
5 NO2 = 9.98;
6 NN2 = 79.63;
7 PCO2F = 9.2; //% ( Feed )
8 PCOF = 21.3; //%
9 PH2F = 18; //%
10 PCH4F = 2.5; //%
11 PN2F = 49; //%
12 //Taking carbon balance ,
13 F = (NCO2 + NCO )/ ( (PCO2F + PCOF + PCH4F)/100);
14 //Nitrogen balance gives ,
15 Nair = (NN2 - F*PN2F/(100) ) * 100 / 79;
16 R = Nair/F;
17 disp(R,"(a)molar Ratio of air to fuel = ")
18 Oexcess = NO2 - NCO / 2;
19 Pexcess = Oexcess *100/ (Nair*21/100 - Oexcess);
20 disp("%",Pexcess,"(b)Percent excess of air = ")
21 NN2F = F * PN2F / 100;
22 PN2F = NN2F *100/ NN2;
23 disp("%",PN2F,"(c)Percent of nitrogen in the flue
    gas that came from fuel = ")

```

Scilab code Exa 10.5 Combustion of coal

```

1 //clc ()
2 Nflue = 100; //kmole
3 NCO2 = 16.4;
4 NCO = 0.4;
5 NO2 = 2.3;
6 NN2 = 80.9;
7 PCF = 80.5; //% ( Feed )
8 PO = 5.0; //%
9 PHF = 4.6; //%
10 PN = 1.1; //%
11 Pash = 8.8; //%
12 //Taking Carbon balance ,
13 W = (NCO2 + NCO)*12 / (PCF / 100);
14 mCO2 = NCO2 * 44;
15 mCO = NCO * 32;
16 mO2 = NO2 * 28;
17 mN2 = NN2 * 28.014;
18 mtotal = mCO2 + mCO + mO2 + mN2;
19 Mdryflue = mtotal * 100/ W;
20 disp("kg",Mdryflue,"(a)The weight of dry gaseous
    products formed per 100 kg of coal fired = ")
21 //taking nitrogen balance ,
22 x = (mN2 - W*PN/100)/28.014;
23 Noxygen = x * 21 / 79;
24 Nrequired = W * (PCF /12 + PHF/(2*2.016) - PO/32)
    /100;
25 Pexcess = (Noxygen - Nrequired)*100/Nrequired ;
26 disp("%",Pexcess,"(b)Percent excess air supplied for
    combustion = ")

```

Scilab code Exa 10.6 Stoichiometric analysis of combustion of coal

```

1 //clc ()
2 mcoal = 100; //kg
3 mC = 63; //kg

```

```

4 mH = 12; //kg
5 mO = 16; //kg
6 mash = 9; //kg
7 mfixC = 39; //kg
8 mH2O = 10; //kg
9 mCvolatile = mC - mfixC;
10 mHH2O = mH2O * 2.016/18.016; //(mass of hydrogen in
    moisture)
11 mHvolatile = mH - mHH2O;
12 mOH2O = mH2O - mHH2O;
13 mOvolatile = mO - mOH2O;
14 mtvolatile = mCvolatile + mHvolatile + mOvolatile;
15 PC = mCvolatile * 100 / mtvolatile;
16 PH = mHvolatile * 100 / mtvolatile;
17 PO = mOvolatile * 100 / mtvolatile;
18 disp("%",PC,"(a) percent carbon in volatile matter =
    ")
19 disp("%",PH,"    percent hydrogen in volatile matter
    = ")
20 disp("%",PO,"    percent oxygen in volatile matter =
    ")
21 PCflue = 10.8; //%
22 Pvflue = 9.0; //%
23 Pashflue = 80.2; //%
24 //taking ash balance, Wis the weight of the refuse,
25 W = mash * 100 / Pashflue;
26 mvflue = Pvflue * W / 100;
27 mCflue = W * PCflue / 100;
28 Ctflue = mCflue + mvflue * PC / 100; //total carbon
    in flue
29 Htflue = mvflue * PH / 100;
30 Otflue = mvflue * PO / 100;
31 PCflue = Ctflue * 100/W;
32 PHflue = Htflue * 100/W;
33 POflue = Otflue * 100/W;
34 disp("%",PCflue,"(b) percent Carbon in refuse = ")
35 disp("%",PHflue,"    percent Hydrogen in refuse = ")
36 disp("%",POflue,"    percent Oxygen in refuse = ")

```

```

37 disp("%",Pashflue," percent Ash in refuse = ")
38 Coalburnt = mcoal - W;
39 NCburnt = (mC - Ctflue)/12;
40 NHburnt = (mH - Htflue)/2.016;
41 NOburnt = (mO - Otflue)/32;
42 PCO2 = 80; //Percentage of carbon burnt
43 NCO2 = PCO2 * NCburnt / 100;
44 NCO = ( 1 - PCO2/100 ) * NCburnt;
45 Vair = 1000; //m^3
46 Nair = Vair / 22.4143;
47 NN2 = Nair * 79 / 100;
48 NO2 = Nair * 21 / 100;
49 Ocompounds = NCO2 + NCO/2 + NHburnt/2; //Oxygen
    present in CO2,CO and H2O
50 //Oxygen balance gives free oxygen as,
51 Ofree = NO2 + mO/32 - Otflue/32 - Ocompounds;
52 Ntotal = NN2 + Ofree + NCO2 + NCO; //dry basis
53 PCO21 = NCO2 *100/Ntotal;
54 PCO1 = NCO * 100/Ntotal;
55 PO21 = Ofree * 100/Ntotal;
56 PN21 = NN2 * 100/Ntotal;
57 disp("%",PCO21," (c)percent CO2 in flue = ")
58 disp("%",PCO1," percent CO in flue = ")
59 disp("%",PO21," percent O2 in flue = ")
60 disp("%",PN21," percent N2 in flue = ")
61 NOrequired = mC/12 + mH/(2.016*2) - mO/32;
62 Oexcess = NO2 - NOrequired;
63 Pexcess = Oexcess * 100 / NOrequired;
64 disp("%",Pexcess," (d)Percent excess air supplied = "
    )
65 NH2Oflue = NHburnt;
66 mH2O = NH2Oflue * 18.016;
67 m = mH2O * 100/Ntotal;
68 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

```
1 //clc ()
2 Pexcess = 20; // %
3 PS03 = 5; // % ( Percent of sulphur burnt to SO3 )
4 //S + O2 = SO2
5 N = 1; // kmol sulphur
6 Orequired = N; // kmol
7 Osupplied = Orequired * ( 1 + Pexcess/100);
8 Nsupplied = Osupplied * 79/21;
9 NS02 = (1-PS03/100)*N;
10 NS03 = PS03 * N /100;
11 Oconsumed = NS02 + 3/2 * PS03/100;
12 Oremaining = Osupplied - Oconsumed;
13 Ntotal = NS02 + NS03 + Oremaining + Nsupplied;
14 PS02 = NS02 * 100 / Ntotal;
15 PS03 = NS03 * 100 / Ntotal;
16 PO2 = Oremaining * 100 / Ntotal;
17 PN2 = Nsupplied * 100 / Ntotal;
18 disp("%",PS02,"Percent SO2 in burner gas = ")
19 disp("%",PS03,"Percent SO3 in burner gas = ")
20 disp("%",PO2,"Percent O2 in burner gas = ")
21 disp("%",PN2,"Percent N2 in burner gas = ")
```

Scilab code Exa 10.8 Burning of pyrites

```
1 //clc ()
2 Nburner = 100; // kmol
3 NS02b = 9.5; // kmol
4 NO2b = 7; // kmol
5 NN2 = Nburner - NS02b - NO2b;
6 NOsupplied = NN2 * 21 / 79; // Oxygen supplied
```

```

7 //4FeS2 + 11O2 = 2Fe2O3 + 8SO2
8 //4FeS2 + 15O2 = 2Fe2O3 + 8SO3
9 NOtotal = NO2b + NSO2b + NSO2b * 3 / 8;
10 NOunaccounted = NOsupplied - NOtotal;
11 NSO31 = NOunaccounted * 8 /15;
12 NStotal = NSO2b + NSO31;
13 mS = NStotal * 32.064;
14 Pburnt = 50; // % ( percentage of pyrites burnt )
15 mFeS2 = mS * 100 / Pburnt;
16 disp("kg",mFeS2,"(a)Total pyrites burnt = ")
17 NFeS2 = NStotal / 2;
18 MFeS2 = 119.975;
19 mFeS21 = MFeS2 * NFeS2;
20 mgangue = mFeS2 - mFeS21;
21 NFe2O3 = NFeS2 * Pburnt / 100;
22 MFe2O3 = 159.694;
23 mFe2O3 = MFe2O3 * NFe2O3;
24 PSO3c = 2.5; // % ( percentage sulphur as SO3 in
      cinder )
25 mc = 100; // kg ( basis )
26 NSO3 = PSO3c / 32.064;
27 mSO3 = NSO3 * 80.064;
28 mremaining = mc - mSO3; // ( Fe2O3 + gangue )
29 // x be the weight of the cinder
30 x = (mFe2O3 + mgangue)*100/mremaining ;
31 disp("kg",x,"(b)weight of cinder produced = ")
32 Slost = x * NSO3 / 100;
33 PSlost = Slost *100/ NStotal;
34 disp("%",PSlost,"(c)Percent of total S lost in the
      cinder = ")
35 mSO3c = mSO3 * x / 100;
36 NSO3b = NSO31 - Slost;
37 P = NSO3b * 100 / NStotal;
38 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

```
1 //clc ()
2 Ncgas = 100; //kmol ( basis - SO3 free converter gas
   )
3 NSO2 = 4.5; //kmol
4 NO2 = 7.5; //kmol
5 NN2 = 88.0; //kmol
6 NOsupplied = NN2 * 21 / 79;
7 NOconverter = NO2 + NSO2;
8 NOconsumed = NOsupplied - NOconverter; //(Oxygen
   consumed for SO3)
9 NSO3c = NOconsumed / 1.5;
10 NStotal = NSO3c + NSO2;
11 Nbgas = 100; //kmol ( basis - SO3 free burner gas )
12 NSO21 = 15; //%
13 NO21 = 5; //%
14 NN21 = 80; //%
15 NOburner = NO21 + NSO21;
16 NOsupplied1 = NN21 * 21 / 79;
17 NOconsumed1 = NOsupplied1 - NOburner; //(Oxygen
   consumed for SO3)
18 NSO3b = NOconsumed1 / 1.5;
19 NStotal1 = NSO3b + NSO21;
20 mS = 100; //kg ( basis - sulphur charged )
21 Pburned = 95; //%
22 mburned = mS * Pburned / 100;
23 Nburned = mburned / 32.064;
24 //let x be the SO3 free burner gas produced, then
   sulphur balance gives,
25 x = Nburned * Nbgas / NStotal1;
26 NSO2b = NSO21 * x / 100;
27 NO2b = NO21 * x / 100;
28 NN2b = NN21 * x / 100;
```



```

29 Ntotalb = NSO2b + NO2b + NN2b;
30 NSO3b1 = NSO3b * x / 100;
31 //let y be the no. of converter gas produced
32 y = Nburned * Ncgas / NStotal;
33 NSO2c = NSO2 * y / 100;
34 NO2c = NO2 * y / 100;
35 NN2c = NN2 * y / 100;
36 Ntotalc = NSO2c + NO2c + NN2c;
37 NSO3c1 = NSO3c * y / 100;
38 Nairsec = (NN2c - NN2b ) * 100 / 79;
39 P = 100; //kPa
40 T = 300; //K
41 V = Nairsec * 22.414 * 101.3 * T / (P * 273.15);
42 disp("m^3/h",V,"(a)The volume of secondary air at
      100kPa and 300K = ")
43 NSabsorbed = 95; //%
44 mSO3abs = NSabsorbed * NSO3c1 * 80.064 / 100;
45 //let z be the amount of 98% H2SO4, therefore , 100%
      H2SO4 produced = z + mSO3abs
46 // taking SO3 balance
47 z = (mSO3abs - mSO3abs * 80.064 / 98.08) / ( 80.064
      / 98.08 - 0.98 * 80.064/98.08);
48 disp("kg",z,"(b)98% H2SO4 required per hour = ")
49 w = z + mSO3abs;
50 disp("kg",w,"(c)100% H2SO4 produced per hour = ")

```

Scilab code Exa 10.10 Burning of limestone mixed with coke

```

1 //clc ()
2 mlime = 5; //kg
3 mcoke = 1; //kg
4 PCaCO3l = 84.5; //%
5 PMgCO3l = 11.5; //%
6 NCaCO3l = PCaCO3l * mlime / (100.09*100);
7 NMgCO3l = PMgCO3l * mlime / (84.312*100);

```

```

8 mInerts1 = mlime * ( 100 - PCaCO31 - PMgCO31 ) /
    100;
9 PCc = 76; %%
10 Pashc = 21; %%
11 Pwaterc = 3; %%
12 NCc = mcoke * PCc / (100*12);
13 Nwaterc = mcoke * Pwaterc / ( 100 * 18.016 );
14 mash = Pashc * mcoke / 100;
15 //CaCO3 + C + O2 = CaO + 2CO2
16 //MgCO3 + C + O2 = MgO + 2CO2
17 PCaCO3conv = 95; //(Percent calcination of CaCO3)
18 PMgCO3conv = 90; //(Percent calcination of MgCO3)
19 NCaO = PCaCO3conv * NCaCO31 / 100;
20 mCaO = NCaO * 56.08;
21 NMgO = PMgCO3conv * NMgCO31 / 100;
22 mMgO = NMgO * 40.312;
23 mCaCO3 = (NCaCO31 * (1-PCaCO3conv/100)*100.09);
24 mMgCO3 = (NMgCO31 * (1-PMgCO3conv/100)*84.312);
25 mtotal = mCaO + mMgO + mCaCO3 + mMgCO3 + mInerts1 +
    mash;
26 PCaO = mCaO * 100 / mtotal;
27 disp("%",PCaO,"The weight percent of CaO in the
    product leaving the kiln = ")

```

Scilab code Exa 10.11 treating limestone with aqueous H₂SO₄

```

1 //clc ()
2 R = 100; //kg ( basis - residue )
3 MCaSO4 = 136.144;
4 MMgSO4 = 120.376;
5 mCaSO4r = 9; //kg
6 mMgSO4r = 5; //kg
7 mH2SO4r = 1.2; //kg
8 minertr = 0.5; //kg
9 mCO2r = 0.2; //kg

```

```

10 mH2O = 84.10; //kg
11 NCaSO4 = mCaSO4r / MCaSO4;
12 NMgSO4 = mMgSO4r / MMgSO4;
13 //CaCO3 + H2SO4 = CaSO4 + H2O + CO2
14 //MgSO4 + H2SO4 = MgSO4 + H2O + CO2
15 mCaCO3 = NCaSO4 * 100.08;
16 mMgCO3 = NMgSO4 * 84.312;
17 mtotallime = minertr + mCaCO3 + mMgCO3;
18 PCaCO3 = mCaCO3 * 100/ mtotallime;
19 PMgCO3 = mMgCO3 *100/ mtotallime;
20 Pinerts = minertr *100/ mtotallime;
21 disp("%",PCaCO3,"(a)Percentage of CaCO3 in limestone
    = ")
22 disp("%",PMgCO3,"    Percentage of MgCO3 in limestone
    = ")
23 disp("%",Pinerts,"    Percentage of inerts in
    limestone = ")
24 NH2SO4 = NCaSO4 + NMgSO4;
25 mH2SO4 = NH2SO4 * 98.08;
26 Pexcess = mH2SO4r * 100 / ( mH2SO4);
27 disp("%",Pexcess,"(b)The percentage excess of acid
    used = ")
28 macidt = mH2SO4 + mH2SO4r;
29 Pacidic = 12; // %
30 mwaterin = macidt * (100 - Pacidic)/ Pacidic;
31 mwaterr = (NCaSO4 + NMgSO4)*18.016;
32 mwatert = mwaterin + mwaterr;
33 mvaporized = mwatert - mH2O;
34 m = mvaporized * 100/mtotallime; //water vaporized
    per 100kg of limestone
35 disp("kg",m,"(c)the mass of water vaporized per 100
    kg of limestone = ")
36 mCO2pr = (NCaSO4 + NMgSO4)*44;
37 mCO2rel = mCO2pr - mCO2r;
38 m1 = mCO2rel * 100 / mtotallime; //CO2 per 100kg of
    limestone
39 disp("kg",m1,"(d)the mass of CO2 per 100kg of
    limestone = ")

```

Scilab code Exa 10.12 Production of TSP

```
1 //clc()
2 macid = 1000;//kg ( basis - dilute phosphoric acid )
3 Mphacid = 97.998;
4 P = 1.25;//% ( dilute % )
5 mphacid = macid * P /100;
6 Nphacid = mphacid / Mphacid;
7 //1mole of phosphoric acid - 1mole of trisodium
  phosphate
8 NTSP = Nphacid;
9 MTSP = 380.166;
10 mTSP = NTSP * MTSP;
11 disp("kg",mTSP,"(a)Maximum weight of TSP obtained =
  ")
12 NCO2 = NTSP;
13 Pwater = 6.27//kPa
14 //since gas is saturated with water vapour, vapour
  pressure = partial pressure
15 Nwater = NCO2 * Pwater / ( 100 - Pwater );
16 Ntotal = Nwater + NCO2;
17 P = 100;//kPa
18 T = 310;//K
19 V = Ntotal * 101.3 * T *22.4143 / ( P * 273.15 );
20 disp("m^3",V,"(b)Volume of CO2 = ")
```

Scilab code Exa 10.13 Production of sodium phosphate

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

```

4 mTSP = mTSPd * P / 100;
5 NTSP = mTSP / 163.974;
6 msodaashd = NTSP * 106;
7 mphacidd = NTSP * 97.998;
8 mNaOHd = NTSP * 40.008;
9 Pphacid = 85;///  

10 PNaOH = 50;///  

11 ///  

12 ///  

13 x = (mTSPd - mTSP) - mNaOHd * PNaOH / (100 - PNaOH) -  

    mphacidd * (100 - Pphacid) / Pphacid;  

14 msodaash = msodaashd + x;  

15 C = msodaashd * 100 / msodaash;  

16 disp("%",C,"(a) Concentration of soda ash solution =  

    ")  

17 mphacid = mphacidd * 100 / Pphacid;  

18 R = msodaash / mphacid;  

19 disp(R,"(b) Weight ratio in which soda ash and  

    commercial phosphoric acid are mixed = ")

```

Scilab code Exa 10.14 Production of pig iron

```

1 //clc()
2 m = 1000;///  

3 ///  

4 PFepg = 95;///  

5 PCpg = 4;///  

6 PSipg = 1;///  

7 PFech = 85;///  

8 mcoke = 1000;///  

9 PCcoke = 90;///  

10 PSicoke = 10;///  

11 PSislag = 60;///  


```

```

12 PSiflux = 5; %%
13 PCaCO3fx = 90; %%
14 PMgCO3fx = 5; %%
15 PCMslag = 40; %%
16 //iron balance gives ,
17 x = PFepg * m *159.694 / ( PFech * 111.694);
18 //silicon balance gives ,
19 //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 )
20 //taking (CaO + MgO) balance
21 //y * ((PCaCO3fx)*56.88/(100*100.88)+(PMgCO3fx
    *40.312/(100*84.312))=z*PCMslag/100
22 //solving above 2 equations , we get
23 y = 403.31;
24 disp("kg",y,"the amount of flux required to produce
    1000kg of pig iron = ")

```

Scilab code Exa 10.15 Production of nitric acid

```

1 //clc ()
2 N = 100; %%mol(basis - scrubber)
3 NN0s = 2.4; %%mol
4 NN2s = 92; %%mol
5 NO2s = 5.6; %%mol
6 PNOs = 20; %% ( Percentage NO leaving scrubber)
7 NN0reac = NN0s * 100 / PNOs;
8 //let x mol of nitroge be produced in the reaction ,
    then the amount of N2 present in the air = NN2s -
    x mol - (1)
9 //4NH3 + 5O2 = 4NO + 6H2O
10 //4NH3 + 3O2 = 2N2 + 6H2O
11 //4moles of NO - 5 moles of O2, 2moles of N2 - 3
    moles of O2

```

```

12 //Total oxygen used up, O = NNOREac * 5/4 + x*3/2
13 //total oxygen supplied , NOtotal= (O) + NO2s
14 //Nitrogen associated with O2 supplied NN2 = NOtotal
    *79/21 - (2)
15 //comparing 1 and 2,
16 x = 2.1835;
17 //12moles NO requires 12moles ammonia, 1 mole N2
    requires 2 mole ammonia
18 Nammonia = x*2 + NNOREac;
19 Oreq = Nammonia * 5 / 4;
20 Osupp = NNOREac * 5/4 + x*3/2 + NO2s;
21 Pexcess = (Osupp - Oreq)*100/Oreq ;
22 disp("%",Pexcess,"(a)Percentage excess oxygen = ")
23 fr = x * 2 / Nammonia;
24 disp(fr,"Fraction of ammonia taking part in side
    reaction = ")

```

Scilab code Exa 10.16 Material balance in nitric acid production

```

1 //clc()
2 m = 100; //kg (basis sodium nitrate reacted)
3 NNaNO3 = m/85;
4 //2NaNO3 + H2SO4 = 2HNO3 + Na2SO4
5 mh2so4 = NNaNO3 * 98.08/2;
6 mhno3 = NNaNO3*63.008;
7 mna2so4 = NNaNO3 * 142.064 /2;
8 Phno3 = 2; //%(percent nitric acid remaining in the
    cake)
9 mhno3cake = mhno3 * Phno3 / 100;
10 Ph2so4 = 35; //%
11 Pwater = 1.5; //%
12 mtotal = (mna2so4 + mhno3cake)*100/(100 - Ph2so4 -
    Pwater);
13 mwater = Pwater * mtotal / 100;
14 mh2so4c = Ph2so4 * mtotal / 100;

```

```

15 Pna2so4 = mna2so4 *100/mtotal;
16 Phno3c = mhno3cake * 100 / mtotal;
17 disp("kg",mna2so4,"(a)Mass of Na2SO4 in the cake = "
    )
18 disp("kg",mhno3,"Mass of HNO3 in the cake = ")
19 disp("kg",mwater,"Mass of water in the cake = ")
20 disp("kg",mh2so4c,"Mass of H2SO4 in the cake = ")
21 disp("%",Pna2so4,"Percentage of Na2SO4 in the cake = "
    ")
22 disp("%",Phno3c,"Percentage of HNO3 in the cake = ")
23 disp("%",Pwater,"Percentage of water in the cake = "
    )
24 disp("%",Ph2so4,"Percentage of H2SO4 in the cake = "
    )
25 mh2so4req = mh2so4 + mh2so4c;
26 P = 95;///% (95% dilute sulphuric acid)
27 w = mh2so4req * 100 / P;
28 disp(mh2so4)
29 disp("kg",w,"(b)Weight of 95% sulphuric acid
    required = ")
30 mnitric = mhno3 - mhno3cake;
31 disp("kg",mnitric,"(c)weight of nitric acid product
    obtained = ")
32 mwaterd = w*(1-P/100)-mwater;
33 disp("kg",mwaterd,"(d)the water vapour tha tis
    distilled from the nitre cake = ")

```

Scilab code Exa 10.17 Electrolysis of brine

```

1 //clc()
2 m = 50;///kg ( basis - mass of brine charged )
3 //let x be the amount of NaCl in the brine
4 Pelect = 50;///% ( electrolyzed )
5 //2NaCl + 2H2O = 2NaOH + Cl2 + H2
6 //amount of NaCl reacted =x*Pelect/(100*58.45)kmol=x

```



```

    *Pelect/100kg    ( 1 )
7 //amount of water reacted = x * Pelect * 18.016 / (
    100 * 58.45 )kg ( 2 )
8 //Gases produced , Cl2 = x * Pelect / (100 * 58.45 *
    2 )kmol = x * Pelect *71/ (100 * 58.45 * 2 )kg
    ( 3 )
9 //H2 = x * Pelect / (100 * 58.45 * 2 )kmol = x *
    Pelect *2.016/ (100 * 58.45 * 2 )kg
    ( 4 )
10 Nwater = 0.03;//mol water vapour/mol of gas
11 //water vapour present = Nwater * 2*(Cl2 + H2)kmol =
    Nwater * 2*(Cl2 + H2)*18.016 kg
    ( 5 )
12 //NaOH = x * Pelect * 40.008/ (100 * 58.45 )kg
    ( 6 )
13 //water = water in brine - water reacted - water
    present in gas ( 7 )
14 // = (m - Pelect/100) - water reacted ( 2 ) - water
    present in the gas( 5 )
15 //Total weight of solution = NaCl ( 1 ) + NaOH ( 6 )
    + Water ( 7 )
16 //since NaOH is 10 percent of the total weight , we
    have NaOH = 0.1 * total weight , from these we get
    ,
17 x = 0.1 * 50 / (0.1* 0.3165 + 0.3422 );
18 NaOH = x * Pelect * 40.008/ (100 * 58.45 );
19 NaCl = x * Pelect / 100;
20 water = 34.5032;//kg
21 Pevap = 50;//NaOH percentage in solution leaving
    evaporator
22 //taking NaOH balance
23 mevap = NaOH * 100 / Pevap;
24 disp("kg",mevap,"(a)amount of 50% NaOH solution
    produced = ")
25 Cl2 = x * Pelect *71/ (100 * 58.45 * 2 );//kg
26 H2 = x * Pelect *2.016/ (100 * 58.45 * 2 );//kg

```

```

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

```

Scilab code Exa 10.18 Preparation of Formaldehyde

```

1 //clc()
2 m = 100; //mol ( basis reactore exit gas )
3 //CH3OH + O2 = HCOOH + H2O
4 //CH3OH + O2 / 2 = HCHO + H2O
5 Nn2 = 64.49; //mol
6 No2 = 13.88; //mol
7 Nh2o = 5.31; //mol
8 Nch3oh = 11.02; //mol
9 Nhcho = 4.08; //mol
10 Nhcooh = 1.22; //mol
11 //x be the moles of methanol reacted , taking C
    balance , we get ,
12 x = Nch3oh + Nhcho + Nhcooh;
13 Pconv = Nhcho * 100 / x ;
14 disp("%",Pconv,"(a) Percent conversion of
    formaldehyde = ")
15 Nair = Nn2 * 100 / 79;
16 R = Nair / x;
17 disp(R,"(b) Ratio of air to methanol in the feed = ")

```

Scilab code Exa 10.19 Recycle operation reactor and separator

```
1 //clc ()
2 NA = 100; //mol ( basi - 100 mol A in the fresh feed
   )
3 Pconv = 95; //%
4 NApro = NA * (100 - Pconv)/100;
5 //A = 2B + C
6 NB = NA * Pconv * 2 / 100;
7 NC = NA * Pconv/100;
8 PAent = 0.5; //%
9 NAent = NApro * 100 / PAent;
10 PBrec = 1; //%
11 NBent = NB * 100 / (100 - PBrec);
12 m = (NAent - NApro + NA);
13 conv = ((NAent - NApro + NA) - NAent)*100/(NAent -
   NApro + NA);
14 disp("%",conv,"(a) single pass conversion = ")
15 Nrecycled = (NAent - NApro) + (NBent - NB);
16 R = Nrecycled/NA;
17 disp(R,"(b) recycle ratio = ")
```

Scilab code Exa 10.20 Conversion of sugar to glucose and fructose

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

```

4 //z be the weight fraction of sucrose in the
   combined stream entering the reactor
5 Psfeed = 25; // % percent sucrose in fresh feed
6 //sucrose balance gives ,  $25 + R*x = (100+R)* z$ 
   (A)
7 //Glucose + fructose balance ,  $R * y = (100 + R )$ 
    $*0.04$  (B)
8 Sucrosecon = 71.7; // % sucrose consumed
9 //sucrose balance around the reactor ,  $(100+R)z$ 
    $=0.717*(100+R)z+(100+R)x$  (C)
10 //From (C) ,  $x = 0.283*z$  (D)
11 //Amount converted to Glucose + fructose =  $0.717 ($ 
    $100 + R ) * z$ 
12 // =  $0.717 ( 100 + R ) * z * 360.192 / 342.176$  kg
13 //Glucose and fructose balance around the reactor ,
14 //  $(100+R)*0.04 + 0.717(100+R)*z*360.192/342.176 =$ 
    $(100+R)*y$  (E)
15 //Solving (E) ,  $y = 0.04 + 0.7548*z$  (F)
16 //Solving , (A) , (B) , (C) and (F)
17 x = 0.06;
18 y = 0.2;
19 z = 0.212;
20 R = 25;
21 disp("kg",R,"(a) Recycle flow = ")
22 disp("%",y*100,"(b) Combined concentration of Glucose
   and Fructose in the recycle stream = ")

```

Scilab code Exa 10.21 Purging operation

```

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

```

```

5 Pconv = 60; %%
6 P1inert = 2; %%
7 NA1 = N * ( 1- P1inert/100 );
8 NA2 = NA1 * ( 1 - Pconv / 100 );
9 NB2 = NA1 - NA2;
10 N1inert = N * P1inert / 100;
11 N2inert = N1inert;
12 //Let R be the moles recycled and P be the moles
    purged
13 //W = R + P
14 W = NA2 + N2inert; //
    (A)
15 PWinert = N2inert * 100/ ( NA2 + N2inert);
16 //component A balance , A fresh feed = A purge stream
    + A recycle stream
17 //F * 0.9 = P * 0.9515 + 0.588
    (B)
18 //inert balance at the point where fresh feed is
    mixed with the recycle ,
19 //F*0.005 + R*0.0485 = 1* 0.02
    (C)
20 //Solving (A) ,(B) and (C)
21 F = 0.6552; //mol
22 P = 0.0671; //mol
23 R = 0.3448; //mol
24 disp("mol",R,"(a) moles of recycle stream = ")
25 disp("mol",P,"(b) moles of purge stream = ")
26 NAconv = NA1 - NA2;
27 NAf = F * (1 - Pinert / 100);
28 Conv = NAconv *100/ NAf;
29 disp("%",Conv,"(c) Overall conversion = ")

```

Scilab code Exa 10.22 Purging operation for production of methanol

```
1 //clc()
```

```

2 N = 100; //moles ( Basis - Fresh feed )
3 Pconv = 20; //%
4 xco = 0.33;
5 xh2 = 0.665;
6 xch4 = 0.005;
7 //R - recycle stream, P - purge stream
8 //x - mole fraction of CO in recycle stream ,
9 xch4r = 0.03;
10 //CO = x, H2 = 1 - xch4r - CO = 0.97 - x;
11 //methane balance over the entire system,
12 P = xch4 * N / xch4r;
13 //taking carbon balance, 33.5 = M + P ( 0.03 + x )
14 //Hydrogen balance, 66.5 + 2*0.5 = 2M + P(2*0.03 +
    0.97 - x)
15 //substituting P, M + 16.67x = 33.0 and 2M - 16.67x
    = 50.33
16 M = (33.0 + 50.33)/3;
17 x = ((xco + xch4)*N - M) / P - xch4r;
18 //methanol balance, (xco*N+Rx) * Pconv/100 = M
19 R = (M*100 / Pconv - (xco*N))/x;
20 disp("mol",R,"(a) moles of recycle stream = ")
21 disp("mol",P,"(b) moles of purge stream = ")
22 H2 = 1 - xch4r - x;
23 disp("%",xch4r*100,"(c)CH4 in purge stream = ")
24 disp("%",x*100,"CO in purge stream = ")
25 disp("%",H2*100,"hydrogen in purge stream = ")
26 disp("mol",M,"(d)Methanol produced = ")

```

Chapter 11

Energy Balance Thermophysics

Scilab code Exa 11.1 Power calculation

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

Scilab code Exa 11.2 Kinetic energy calculation

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

```

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

```

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

```

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

```

Scilab code Exa 11.4 Power requirement of the pump

```

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

```

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

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

Scilab code Exa 11.6 internal energy and enthalpy change calculation

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

Scilab code Exa 11.7 change in internal energy

```
1 // clc ()
```

```

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

```

Scilab code Exa 11.8 reaction of iron with HCl

```

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

```

Scilab code Exa 11.9 Thermic fluid

```

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

```

```

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

```

Scilab code Exa 11.10 Heat capacity

```

1 //clc()
2 //Cp = 26.54 + 42.454*10^-3 * T - 14.298 * 10^-6 * T
   ^2;
3 T1 = 300; //K
4 T2 = 1000; //K
5 m = 1; //kg
6 N = m/44; //kmol
7 x = integrate('26.54 + 42.454*10^-3 * T - 14.298 *
   10^-6 * T^2', 'T', T1, T2);
8 Q = N*x;
9 disp("kJ",Q,"(a)Heat required = ")
10 //for temperature in t degree celsius
11 //Cp = 26.54 + 42.454*10^-3 * (t + 273.15) - 14.298
   * 10^-6 * (t + 273.15)^2
12 //Cp = 37.068 + 34.643 * 10^-3*t - 14.298* 10^-6 * t
   ^2 (kJ/kmolC)
13 //Cp = 8.854 + 8.274*10^-3*t - 3.415*10^-6*t^2 ( Kcal
   /kmolC)
14 //For degree Fehreneit scale ,replacet by ( t1 - 32)
   /18, we get
15 //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

```

1 //clc()

```

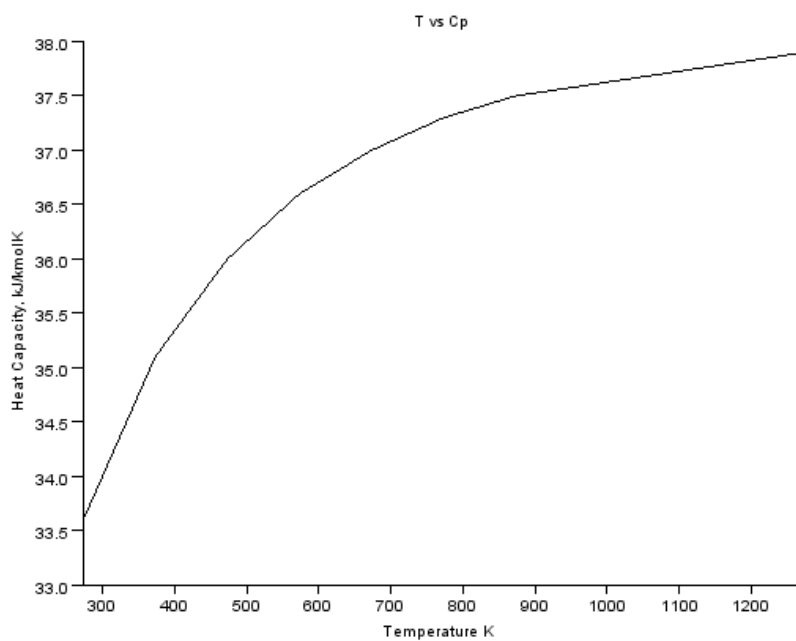


Figure 11.1: Enthalpy change when chlorine gas is heated

```

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

```

Scilab code Exa 11.12 Molal heat capacity

```

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

```

```

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

```

Scilab code Exa 11.13 Enthalpy change of a gas

```

1 //clc ()
2 T1 = 1500; //K
3 Tr = 273; //K
4 T2 = 400; //K
5 Cpm1 = 50; //kJ/kmol
6 Cpm2 = 35; //kJ/mol
7 H = Cpm1 * ( T1 - Tr ) - Cpm2 * ( T2 - Tr );
8 disp("kJ/kmol",H,"Enthalpy change = ")

```

Scilab code Exa 11.14 Combustion of solid waste

```

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

```

```

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

```

Scilab code Exa 11.15 Heat capacity calculation for Na₂SO₄ 10H₂O

```

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

```

Scilab code Exa 11.16 Heat of vaporization calculation

```

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

```

```

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

```

Scilab code Exa 11.17 Heat requirement

```

1 //clc ()
2 T1 = 250; //K
3 T = 273.15; //K
4 T2 = 400; //K
5 Cice = 2.037; //kJ/kgK
6 T3 = 373.15; //K
7 Cliq = 75.726; //kJ/kmolK
8 //Cp = 30.475 + 9.652*10-3*T + 1.189*10-6*T2
9 Hfusion = 6012; //kJ/kmol
10 Hvap = 40608; //kJ/kmol
11 //1 - Heat for raising the temperature of ice , H1
12 H1 = Cice * ( T - T1 );
13 //2 - Latent heat of fusion of ice , Hf
14 Hf = Hfusion / 18.016; //kJ
15 //3 - Sensible heat of raising the temperature of
    water , H2
16 H2 = Cliq * ( T3 - T ) / 18.016;
17 //4 - Latent heat of vaporization of water , Hv

```



```

18 Hv = Hvap / 18.016;
19 //5 - Sensible heat of raising the temperature of
    water vapour, H3
20 H3 = (integrate('30.475 + 9.652*10^-3*T +
    1.189*10^-6*T^2', 'T', T3, T2))/18.016;
21 Q = H1 + H2 + H3 + Hf + Hv;
22 disp("kJ", Q, "Heat required = ")

```

Scilab code Exa 11.18 Equilibrium temperature of mixture

```

1 //clc()
2 //Cp = 0.16 + 4.78 * (10^-3) * T ( organic liquid )
3 //Cp = 0.7935 + 1.298 * (10^-4) * T ( CCL4 )
4 Tb = 349.9; //K
5 Hv = 195; //kJ/kg
6 Cp = 0.4693; //kJ/kgK
7 //Let T be the final temperature
8 //integration(T - 650)(0.16 + 4.78 * (10^-3) * T)dt
    = integration(295 - T)(0.7935 + 1.298 * (10^-4) *
    T)dt
9 // the above equation yields , 2.4549*(10^-3)*T^2 +
    0.9535*T - 1353.51 = 0, from this we get
10 T = 573.3; //K
11 //since this temperature is above boiling point of
    CCL4,
12 //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
13 //solving above equation , we get ,
14 T1 = 540.1; //K
15 disp("K", T1, "equilibrium temperature of the mixture
    = ")

```

Scilab code Exa 11.19 Estimation of mean heat of vaporisation

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

Scilab code Exa 11.20 Heat of vaporization of methyl chloride

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

Scilab code Exa 11.21 Watson equation

```
1 //clc ()
2 Hv1 = 2256; //kJ/kg
3 T1 = 373; //K
4 T2 = 473; //K
5 Tc = 647; //K
```

```

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

```

Scilab code Exa 11.22 Kistyakowsky equation

```

1 //clc()
2 //Cp = a + b*T
3 T1 = 293.15; //K
4 Cp1 = 131.05; //J/molK
5 T2 = 323; //K
6 Cp2 = 138.04; //J/molK
7 //a + 293*b = 131.05
8 //a + 323*b = 138.04
9 b = (Cp1 - Cp2)/(T1 - T2);
10 a = Cp1 - b * T1;
11 //Cp = 62.781 + 0.233*T
12 // Hvb / Tb = 36.63 + 8.31 ln Tb
13 Tb = 273.15 + 80.1; //K
14 Hvb = (36.63 + 8.31*log(Tb)) * Tb;
15 m = 100; //kg
16 H = m*(10^3) * (integrate('62.781 + 0.233*T', 'T', T1,
      Tb))/78.048 + m*(10^3)*Hvb/78.048;
17 disp("J",H,"Heat required = ")

```

Scilab code Exa 11.23 Quality of steam

```

1 //clc()
2 P = 10; //kPa
3 T1 = 323.15; //K

```

```

4 T2 = 373.15; //K
5 T = 358.15; //K
6 H1 = 2592.6; //kJ/kg
7 H2 = 2687.5; //kJ/kg
8 //H by interpolation ,
9 H = H1 + ((H2 - H1)/(T2 - T1))*(T - T1);
10 Hl = 697.061; //kJ/kg
11 Hg = 2762; //kJ/kg
12 //H = x*Hl + ( 1 - x )* Hg
13 x = (H - Hg)/(Hl - Hg) ;
14 Pmois = x*100;
15 Psteam = ( 1 - x )*100;
16 disp("%",Pmois,"Percentage of moisture = ")
17 disp("%",Psteam,"Percentage of dry saturated steam =
    ")

```

Scilab code Exa 11.24 Heat calculation

```

1 //clc ()
2 P = 3500; //kPa
3 T = 673.15; //K
4 SV = 0.08453; //m^3/kg
5 Vcondensed = 1/2;
6 m = 100; //kg
7 V = m * SV / (m/2);
8 //m*(Vl+Vg)*Vcondensed = m * SV
9 //But Vl is negligible ,
10 Vg = m * SV / (m * Vcondensed);
11 //using steam table
12 T1 = 459.5; //K
13 P1 = 1158; //kPa
14 //internal energy of superheated steam from steam
    table
15 I = 2928.4; //kJ/kg
16 U1 = m * I;

```

```

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

```

Scilab code Exa 11.25 Enthalpy balance for evaporation process

```

1 //clc ()
2 m = 1000; //kg/h ( basis mass of 10% NaOH solution )
3 Pfeed = 10; //%
4 Ppro = 50; //(Percentage NaOH in product)
5 //Taking NaOH balance ,P being the weight of the
  product
6 P = Pfeed * m / Ppro;
7 //W be the weight of water evaporized
8 W = m - P;
9 //step1 - cooling 1000kg/h of 10% solution from 305K
  to 298K
10 T1 = 305; //K
11 T2 = 298; //K
12 Cliq = 3.67; //kJ/kgK
13 H1 = m*Cliq * (T2 - T1);
14 //step2 - separation into pure components
15 Hsolution = -42.85; //kJ/mol
16 H2 = -Pfeed * m *1000 *Hsolution/ (40*100);
17 //step3 - W kg water is converted to water vapour
18 Hvap = 2442.5; //kJ/kg
19 H3 = W * Hvap;
20 //step4 - water vapour at 298K is heated to 373.15K
21 Cvap = 1.884; //kJ/kgK
22 T3 = 373.15; //K
23 H4 = W * Cvap * ( T3 - T2 );
24 //step5 - formation of 200kg of 50% NaOH solution at

```

```

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

```

Scilab code Exa 11.26 Mean heat capacity of ethanol water solution

```

1 //clc()
2 Nwater = 0.8; //moles
3 Nethanol = 0.2; //moles
4 T = 323; //K
5 Cwater = 4.18*10^3; //J/kgK
6 Cethanol = 2.58*10^3; //J/kgK
7 Hmixing1 = -758; //J/mol ( at 298K )
8 Hmixing2 = -415; //J/mol ( at 323K )
9 T1 = 298; //K
10 T2 = 523; //K
11 //step1 - 0.8 mol of water is cooled from 323 K to
298K
12 H1 = Nwater * 18 * Cwater * ( T1 - T )/ 1000;
13 //step2 - 0.2 mol ethanol cooled from 323K to 298K
14 H2 = Nethanol * 46 * Cethanol * ( T1 - T )/1000;
15 //step3 - 0.8 mol water and 0.2 mol ethanol are
mixed together ,
16 H3 = Hmixing1;
17 //step4 solution is heated to 323K, H4 = Cpm * (T -
T1)
18 //Hmixing2 = H1 + H2 + H3 + H4
19 H4 = Hmixing2 - H1 - H2 - H3;

```

```

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

```

Scilab code Exa 11.27 Evaporation of NaOH solution

```

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

```

Scilab code Exa 11.28 Heat transfer to air

```

1 //clc ()
2 U2 = 0.35*10^3; //kJ
3 U1 = 0.25*10^3; //kJ
4 //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
5 Q = U2 - U1;
6 disp("kJ",Q,"Heat transferred to the air = ")

```

Scilab code Exa 11.29 change in internal energy

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

Scilab code Exa 11.30 Heat liberation in oxidation of iron fillings

```
1 // clc ()
2 //2Fe + 3/2O2 = Fe2O3
3 Hliberated = 831.08; //kJ
4 Q = -Hliberated*1000;
5 disp("J",Q,"Q = ")
6 //P(V) = (n)RT
7 //W = P(V) = (n)RT
8 n = -1.5;
9 R = 8.314;
10 T = 298; //K
11 W = (n) * R * T;
12 disp("J",W,"W = ")
13 U = Q - W;
14 disp("J",U,"U = ")
```

Scilab code Exa 11.31 Saturated steam and saturated water


```

1 //clc ()
2 Vgas = 0.09; //m^3
3 Vliq = 0.01; //m^3
4 SVliq = 1.061*10^-3; //m^3/kg
5 SVvap = 0.8857; //m^3/kg
6 mvap = Vgas / SVvap;
7 mliq = Vliq / SVliq;
8 U1 = 504.5; //kJ/kg
9 Ug = 2529.5; //kJ/kg
10 U1 = U1 * mliq + Ug * mvap;
11 SVtotal = (Vgas + Vliq)/(mvap + mliq);
12 //using steam table , these value of specific volume
    corresponds to pressure of 148.6bar and internal
    energy of 2464.6kJ/kg
13 U = 2464; //kJ/kg
14 Utotal = U * (mvap + mliq);
15 //Utotal - U1 = Q - W, but W = 0, hence ,
16 Q = Utotal - U1;
17 disp("kJ",Q,"Heat to be added = ")

```

Scilab code Exa 11.32 constant volume and constant pressure process

```

1 //clc ()
2 m = 10; //kg(air)
3 N = m / 29; //kmol
4 P1 = 100; //kPa
5 T1 = 300; //K
6 R = 8.314;
7 V1 = N * R * T1 / P1;
8 V2 = V1;
9 T2 = 600; //K
10 Cv = 20.785; //kJ/kmolK
11 Cp = 29.099; //kJ/kmolK
12 U = N * Cv * (T2 - T1);
13 Q = U;

```

```

14 W = Q - U;
15 H = U + N * R * ( T2 - T1 );
16 disp("kJ",U,"(a)Change in internal energy at
      constant volume = ")
17 disp("kJ",Q,"heat supplied at constant volume = ")
18 disp("kJ",W,"Work done at constant volume = ")
19 disp("kJ",H,"Change in Enthalpy at constant volume =
      ")
20 P2 = P1;
21 H2 = N * Cp * ( T2 - T1 );
22 Q2 = H2;
23 U2 = H2 - N * R * (T2 - T1);
24 W2 = Q2 - U2;
25 disp("kJ",U2,"(b)Change in internal energy at
      constant Pressure = ")
26 disp("kJ",Q2,"heat supplied at constant Pressure = "
      )
27 disp("kJ",W2,"Work done at constant Pressure = ")
28 disp("kJ",H2,"Change in Enthalpy at constant
      Pressure = ")

```

Scilab code Exa 11.33 series of operations

```

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

```

```

11 W1 = 0;
12 disp("kJ",W1,"Work done at constant volume = ")
13 disp("kJ",Q1,"Heat supplied at constant volume = ")
14 //step2 - Process is abdiabatic
15 Q2 = 0;
16 r = 1.4;
17 T3 = T2 * (( P1 / P2 )^((r - 1)/r));
18 W2 = Cv * ( T2 - T3 );
19 disp(T3)
20 disp("kJ",W2,"Work done in adiabatic process = ")
21 disp("kJ",Q2,"Heat supplied in adiabatic process = "
    )
22 //step3 - process is isobaric
23 Q3 = Cp * (T1 - T3);
24 U3 = Cv * (T1 - T3);
25 W3 = Q3 - U3;
26 disp("kJ",W3,"Work done at constant pressure = ")
27 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

```

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

```

```

13 R = 8.314;
14 W1 = R*T1*log(P1/P2);
15 Q1 = W1;
16 disp("kJ/kmol",U1,"(a)Change in the internal energy
    in isothermal condition = ")
17 disp("kJ/kmol",H1,"Change in the enthalpy energy in
    isothermal condition = ")
18 disp("kJ/kmol",W1,"Work done in isothermal condition
    = ")
19 disp("kJ/kmol",Q1,"Heat supplied in isothermal
    condition = ")
20 N = P * (1.01325 * 10^5) * V / ( R * T );
21 Cv = Cp - R;
22 U2 = Cv * (T2 - T)*N;
23 H2 = Cp * (T2 - T)*N;
24 W2 = 0;
25 Q2 = U2 + W2;
26 disp("kJ/kmol",U2,"(b)Change in the internal energy
    at constant volume condition = ")
27 disp("kJ/kmol",H2,"Change in the enthalpy energy at
    constant volume condition = ")
28 disp("kJ/kmol",W2,"Work done at constant volume
    condition = ")
29 disp("kJ/kmol",Q2,"Heat supplied at constant volume
    condition = ")

```

Scilab code Exa 11.35 Heat removed in condenser

```

1 //clc()
2 m = 1; //kg
3 u2 = 0.5; //m/s
4 u1 = 60; //m/s
5 H = -3000; //kJ/kg
6 //KE = (u^2)/2
7 KE = ((u2 ^ 2) - (u1^2))/2000;

```

```

8 g = 9.81; //m/s^2
9 Z1 = 7.5; //m
10 Z2 = 2; //m
11 //PE = g * (Z)
12 PE = g * (Z2 - Z1)/1000;
13 W = 800; //kJ/kg
14 Q = H + PE + KE + W;
15 disp("kJ/kg",Q,"Heat removed from the fluid = ")

```

Scilab code Exa 11.36 Throttling process

```

1 //clc()
2 PE = 0;
3 W = 0;
4 Q = 0;
5 //(H) + (u^2)/2 = 0
6 //according to the reation u1 * v1 = u2 * v2
7 //(u^2)/2 is negligible , change in enthalpy is 0
8 T1 = 623; //K
9 P1 = 6000; //kPa
10 H1 = 3045.8; //kJ/kg ( Enthalpy of the steam using
    steam table )
11 P2 = 1000; //kPa
12 T2 = 570; //K ( value of temperature corresponding to
    the enthalpy and pressure using the steam table
    )
13 disp("K",T2,"Temperature of superheated steam = ")

```

Scilab code Exa 11.37 water pumping and energy balances

```

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

```

```

4 PE = g * z;
5 KE = 0;
6 T2 = 288; //K
7 f = 1.5*10^-2; //m^3/min
8 D = 1000; //kg/m^3
9 m = f * D;
10 Qsupp = 500; //kJ/min
11 Qlost = 400; //kJ/min
12 Qnet = (Qsupp - Qlost) * D / m ;
13 W = 2*745.7; //W
14 Ws = -W * 0.6 / (m/60);
15 H = Qnet - Ws - PE - KE;
16 Cp = 4200;
17 T1 = H / Cp;
18 T = T1 + T2;
19 disp("K",T,"The temperature of exit water = ")

```

Scilab code Exa 11.38 Energy balance on rotary drier

```

1 //clc()
2 m = 1000; //kg/h (dried product)
3 // S be the amount of dry solid in the product
  stream
4 Pmoisture1 = 4; //%
5 Pmoisture2 = 0.2; //%
6 S = m *(1 - P/1000);
7 X1 = Pmoisture1/(100 - Pmoisture1);
8 X2 = Pmoisture2/(100 - Pmoisture2);
9 //let G be the weight of dry air in the air stream
10 Y1 = 0.01; //kg water/kg dry solid
11 Cp = 1.507;
12 Cw = 4.2;
13 T1 = 298; //K
14 T = 273; //K
15 T2 = 333; //K

```

```

16 Tg1 = 363; //K
17 Tg2 = 305; //K
18 Hs1 = (Cp + X1 * Cw) * (T1 - T);
19 Hs2 = (Cp + X2 * Cw) * (T2 - T);
20 //Hg = Cs(Tg - To) + Y*L
21 //Cs = 1.005 + 1.884*Y
22 L = 2502.3; //kJ/kg dry air
23 Hg1 = (1.005 + 1.884 * Y1)*(Tg1 - T) + Y1 * L;
24 Q = -40000; //kJ/h
25 //Calculating for T2, Hg2 = 32.16 + 2562.59*Y
26 //change in enthalpy = Q
27 //H1 = S * Hs1 + G * HG1 = 37814.22 + 117.17G
28 //H2 = 100728.14 + G* (32.16 + 2561.59*Y)
29 //change in enthalpy = Q
30 //62913.92 + G *(-85.01 + 2561.59*Y) + 40000 = 0
31 //102913.92 + G *(-85.01 + 2561.59*Y) = 0
      (1)
32 //moisture balance , S*X1 + G*Y1 = S*X2 + G*Y2
33 //G*(Y-0.01) = 39.62
      (2)
34 //solving simultaneously ( 1 ) and ( 2 ),
35 Gdry = 3443; //kg/h
36 G = Gdry*(1 + Y1);
37 disp("kg/h",G," Air requirement = ")

```

Scilab code Exa 11.39 Energy balance on the fractionator

```

1 //clc()
2 m = 1000; //kg/h ( feed solution )
3 //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.
4 //total balance , F = D + W
5 //Acetone balance , F*xf = D*xd + w*xw

```

```

6 F = 1000;
7 xf = 0.10;
8 xd = 0.9;
9 xw = 0.01;
10 //substituting in above equations ,
11 D = F * (xf - xw) / (xd - xw);
12 W = F - D;
13 R = 8;
14 L = R * D;
15 //material balance around the condenser ,G vapour
    reaching the condenser
16 G = L + D;
17 Td = 332; //K
18 T2 = 300; //K
19 Tw = 370; //K
20 Tf = 340; //K
21 Lacetone1 = 620; //kJ/kg
22 Lwater1 = 2500; //kJ/kg
23 Ld = xd * Lacetone1 + (1 - xd) * Lwater1;
24 Cpacetone = 2.2; //kJ/kgK
25 Cpwater = 4.2; //kJ/kgK
26 Cp = xd * Cpacetone + (1-xd)*Cpwater;
27 H = Ld + Cp * ( Td - T2 );
28 Cpc = 4.2; //kJ/kg
29 Tc = 30; //K ( change in temperature allowable for
    cooling water )
30 m = G * H / ( Cpc * Tc );
31 disp("kg/h",m,"(a)The circulation rate of cooling
    water = ")
32 Qc = G * H;
33 Hd = 0;
34 Hw = (xw * Cpacetone + (1-xw)*Cpwater)*(Tw - T2);
35 Hf = (xf * Cpacetone + (1-xf)*Cpwater)*(Tf - T2);
36 Qb = D * Hd + W * Hw + Qc - F * Hf;
37 Hcondensation = 2730; //kJ/kg
38 msteam = Qb/Hcondensation;
39 disp("kg/h",msteam,"(b)Amount of steam supplied = ")

```

Chapter 12

Energy Balance Thermochemistry

Scilab code Exa 12.1 Heat liberated calculation

```
1 //clc ()
2 N = 100; //mol gas mixture burned
3 //CO(g) + 1/2 O2(g) = CO2 -           Hr1 =
   - 282.91kJ/mol
4 //H2(g) + 1/2 O2(g) = H2O -         Hr2 =
   - 241.83kJ/mol
5 Hr1 = - 282.91; //kJ/mol
6 Hr2 = - 241.83; //kJ/mol
7 Nco1 = 20;
8 Nh21 = 30;
9 Nn21 = 50;
10 Htotal = Nco1*Hr1 + Nh21*Hr2;
11 disp("kJ",-Htotal,"the amount of heat liberated on
   the complete combustion of 100mol of the gas
   mixture = ")
12 Ncoreac = Nco1 * 0.9;
13 Nh2reac = Nh21 * 0.8;
14 Htotal1 = Ncoreac*Hr1 + Nh2reac*Hr2;
15 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

```
1 //clc ()
2 //C(s) + 2H2(g) = CH4(g)           Hf = ?
3 Hc = -393.51; //kJ/mol
4 Hh2 = -285.84; //kJ/mol
5 Hch4 = - 890.4; //kJ/mol
6 //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
7 Hf = 1 * Hc + 2 * Hh2 - 1 * Hch4;
8 disp("kJ",Hf,"Heat of formation of methane = ")
```

Scilab code Exa 12.3 Net heating value of coal

```
1 //clc ()
2 m = 1; //kg of coal burned
3 xc = 0.7;
4 xh2 = 0.055;
5 xn2 = 0.015;
6 xs = 0.03;
7 xo = 0.13;
8 xash = 0.07;
9 Hvap = 2370; //kJ/kg
```

```

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

```

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

```

1 //clc()
2 //C2H5OH(1) + CH3COOH(1) = C2H5COOCH3(1) + H2O(1) H
   = ?
3 Hc2h5oh = -1366.91; //kJ/mol
4 Hch3cooh = -871.69; //kJ/mol
5 Hc2h5cooch3 = -2274.48; //kJ/mol
6 //to calculate heat of reaction from the heat of
   combustion data ,
7 //Hreac = Hreac - Hprod
8 Hreac = Hc2h5oh + Hch3cooh - Hc2h5cooch3;
9 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

```

1 //clc()
2 //C2H4(g) + H2O(g) = C2H5OH(g)
3 //2CO2(g) + 3H2O(1) = C2H5OH(1) + 3O2(g)      H =
   1366.91kJ (A)
4 Hc2h4 = -1410.99; //kJ/mol
5 Hvap = 44.04; //kJ/mol
6 Hc2h5oh = 42.37; //kJ/mol

```

```

7 //C2H4(g) + 3H2O(l) = C2H5OH(l) + 3O2(g)      H =
      -1410.99kJ (B)
8 //H2O(l) = H2O(g)                              H =
      44.04kJ (C)
9 //C2H5OH(l) = C2H5OH(g)                        H =
      42.37kJ (D)
10 //A + B + D - C gives the required reaction
11 Ha = 1366.91; //kJ
12 Hb = -1410.99; //kJ
13 Hc = 44.04; //kJ
14 Hd = 42.37; //kJ
15 Hreac = Ha + Hb + Hd - Hc;
16 disp("kJ",Hreac,"The standard heat of reaction = ")

```

Scilab code Exa 12.6 Standard heat of formation of acetylene

```

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

```

Scilab code Exa 12.7 Standard heat of roasting of iron pyrites

```

1 //clc ()
2 m = 100; //kg of pyrites charged
3 xfes2in = 0.8;
4 xganguelin = 0.2;
5 xfes2out = 0.05;
6 //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
7 x = 0.05 * 73.24 / (1 - 0.05*0.3345);
8 mfes2reacted = m*xfes2in - x;
9 //4FeS2 + 11O2 = 2Fe2O3 + 8SO2
10 Hfes2 = -178.02; //kJ/mol
11 Hfe2o3 = -822.71; //kJ/mol
12 Hso2 = -296.9; //kJ/mol
13 Hreac = 2 * Hfe2o3 + 8 * Hso2 - 4 * Hfes2;
14 N = mfes2reacted *1000/ 119.98;
15 H = Hreac * N / 4;
16 H1 = H/m; //(heat of reaction per kg of coal burnt)
17 disp("kJ",H1,"Heat of reaction per 1 kg of coal
    burned = ")

```

Scilab code Exa 12.8 Standard heat of formation of liquid methanol

```

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

```

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

```
1 //clc()
2 N = 100; //mol fuel gas
3 Nco = 21;
4 Nh2 = 15.6;
5 Nco2 = 9.0;
6 Nch4 = 2;
7 Nc2h4 = 0.4;
8 Nn2 = 52;
9 Hco = 282.99; //kJ/mol ( heat of combustion )
10 Hh2 = 285.84; //kJ/mol ( heat of combustion )
11 Hch4 = 890.4; //kJ/mol ( heat of combustion )
12 Hc2h4 = 1410.99; //kJ/mol ( heat of combustion )
13 Hvap = 44.04; //kJ/mol
14 H = Nco * Hco + Nh2 * Hh2 + Nch4*Hch4 + Nc2h4*Hc2h4;
    //kJ
15 V = N * 22.4143/1000;
16 H1 = H / V; //kJ/m^3
17 //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
18 Nwater = Nh2 + 2 * Nch4 + 2 * Nc2h4;
19 Hvap1 = Hvap * Nwater;
20 Hnet = H1 - Hvap1;
21 disp("kJ",Hnet,"Net heating value of the fuel = ")
```

Scilab code Exa 12.10 Standard heat of reaction calculation

```
1 //clc()
2 // C5H12(g) + 8O2(g) = 5CO2(g) + 6H2O(l)
```

```

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

```

Scilab code Exa 12.11 Constant pressure heat of combustion

```

1 //clc ()
2 m = 1; //kg of oil burned
3 mc = 0.9; //kg
4 mh2 = 0.1; //kg
5 Mc = mc / 12; //kmol
6 //C(s) + O2(g) = CO2(g)
7 Nh2 = mh2 / 2.016; //kmol
8 //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
9 R = 8.314;
10 T = 298; //K
11 x = Nh2 * R * T / (-2);
12 Qv = -43000; //kJ/kg
13 Qp = Qv + x;
14 disp("kJ/kg",Qp,"the constant pressure heat of
   combustion = ")

```

Scilab code Exa 12.12 Heat of reaction for ammonia synthesis

```

1 //clc ()

```

```

2 //1 - N2, 2 - H2, 3 - NH3
3 a1 = 27.31;
4 a2 = 29.09;
5 a3 = 25.48;
6 b1 = 5.2335*10^-3;
7 b2 = -8.374*10^-4;
8 b3 = 36.89 * 10^-3;
9 c1 = -4.1868 * 10^-9;
10 c2 = 2.0139*10^-6;
11 c3 = -6.305*10^-6;
12 H1 = -46191; //J
13 T1 = 298; //K
14 //1/2 N2 + 3/2 H2 = NH3           H = -46.191kJ
15 //Ht = H + a*T + b*T^2 / 2+ c*T^3 / 3
16 //at 298,
17 a = a3 - a1 / 2 - 3 * a2 / 2;
18 b = b3 - b1 / 2 - 3 * b2 / 2;
19 c = c3 - c1 / 2 - 3 * c2 / 2;
20 H = H1 -a * T1 - b * (T1^2) / 2 - c * (T1^3) / 3;
21 T2 = 700; //K
22 H2 = H + a * T2 + b * (T2^2) / 2 + c * (T2^3) / 3;
23 disp(H);
24 disp("kJ",H2,"Heat of reaction at 700K = ")

```

Scilab code Exa 12.13 Standard heat of reaction of methanol synthesis

```

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

```



```

      10^4 * T^-2
8 //for reactants ,
9 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);
10 //for product ,
11 H2 = integrate('18.382 + 101.564 * 10^-3 * T -
      28.683 * 10^-6 * T^2', 'T', T1, T2);
12 //H298 = Hproducts - Hreactants;
13 //CO + 2H2 = CH3OH          Ha1 = -238.64kJ
14 Ha1 = -238.64; //kJ
15 //CH3OH(l) = CH3OH(g)      Hvap = 37.98kJ
16 Hvap = 37.98; //kJ
17 //CO(g) + 2H2(g) = CH3OH(g) Ha2 = -200.66kJ
18 Ha2 = Ha1 + Hvap; //kJ
19 Hco = -110.6; //kJ/mol
20 H298 = Ha2 - (Hco);
21 Htotal = H1/1000 + H298 + H2/1000;
22 disp("kJ/mol", Htotal, "The heat of reaction at 773K =
      ")

```

Scilab code Exa 12.14 Combustion of CO

```

1 //clc()
2 Nco = 1; //mol CO reacted
3 //CO + 1/2 O2 = CO2
4 No2 = Nco / 2;
5 Pexcess = 100;
6 Nosupp = No2 * ( 1 + Pexcess / 100 ); //oxygen
      supplied
7 Nn2 = Nosupp * 79 / 21;
8 Nco2 = Nco;
9 Noremain = Nosupp - No2;
10 T1 = 298; //K

```

```

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

```

Scilab code Exa 12.15 Heat added or removed calculation

```

1 //clc()
2 //CO(g) + H2O(g) = CO2(g) + H2(g)           H298 =
    -41.190
3 T1 = 298; //K
4 Pconv = 75; //%
5 T2 = 800; //K
6 H298 = -41.190; //kJ
7 Hco = 30.35; //J/molK
8 Hco2 = 45.64; //J/molK
9 Hwater = 36; //J/molK
10 Hh2 = 29.3; //J/molK
11 Nco = 1; //mol
12 Nh2o = 1; //mol
13 Ncofinal = Nco * (1 - Pconv/100);
14 Nwaterf = Ncofinal;
15 Nco2final = Nco - Ncofinal;
16 Nh2final = Nco2final;

```

```

17 H2 = (Nco2final * Hco2 + Nh2final * Hh2 + Ncofinal *
        Hco + Nwaterf * Hwater) * (T2 - T1);
18 Hr1 = H298 * (Nco - Ncofinal);
19 Hr2 = Hr1 * 1000 + H2;
20 mh2 = Nh2final * 2.016 * 10^-3; //kg
21 //therefore for 1000k H2,
22 Hr = Hr2 * 1000 / (mh2 * 1000); //kJ
23 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

```

1 //clc ()
2 //CO2(g) + C(s) = 2CO(g)           H1298 = 170
   kJ/mol
3 //O2(g) + 2C(s) = 2CO(g)         H2298 =
   -221.2kJ/mol
4 T2 = 1298; //K
5 T1 = 298; //K
6 Hc = 0.02; //kJ/molK
7 Ho = 0.03; //kJ/molK
8 Hco = 0.03; //kJ/molK
9 Hco2 = 0.05; //kJ/molK
10 //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
11 //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)
12 //H1 = (-70x - 70)kJ
13 //enthalpy of heating the product, H2 = 2 * ( 1 + x
    ) * Hco * (1298 - 298)
14 //H2 = 60 + 60x kJ
15 //Hr = 170x - 221.2
16 //Htotal = 0 = H1 + H2 + Hr

```

```

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

```

Scilab code Exa 12.17 Partial oxidation of natural gas

```

1 //clc ()
2 N = 100; //mol flue gas
3 //Carbon balance ,
4 //x is the feed of methane, w is water in flue gas, y
  is the oxygen supplied
5 xco2 = 0.019;
6 xch2o = 0.117;
7 xo2 = 0.038;
8 xch4 = 0.826;
9 xc = xco2 + xch2o + xch4;
10 Nc = xc * N;
11 Nch4i = Nc;
12 //Hydrogen balance ,
13 xh2 = xch2o + xch4*2;
14 w = 2 * (Nch4i) - xh2*N;
15 //oxygen balance
16 No2s = (xco2 + xch2o/2 + xo2)*N + w/2;
17 y = No2s;
18 T1 = 298; //K
19 T2 = 573; //K
20 T3 = 673; //K
21 //oxygen cooled from 573K and methane from 673 to
  298K
22 Ho573 = 30.5; //J/molK
23 Hch4673 = 45.9; //J/molK
24 H1 = y * Ho573 * (T1 - T2) + Nch4i * Hch4673 * (T1 -
  T3);
25 //CH4 + O2 = CH2O + H2O           Hr1 = -282.926kJ
26 //CH4 + 2O2 = CO2 + 2H2O         Hr2 = -802.372kJ

```

```

27 Hr1 = -282.926; //kJ
28 Hr2 = -802.372; //kJ
29 H2 = xch2o*N*Hr1 + xco2*N*Hr2;
30 T4 = 873; //K
31 Ho = 31.9
32 Hch4 = 51.4;
33 Hco2 = 46.3;
34 Hch2o = 47.1;
35 Hh2o = 36.3;
36 H3 = ((xco2 * Hco2 + xo2 * Ho + xch4 * Hch4 + Hch2o*
        xch2o)*N + w * Hh2o)*(T4 - T1);
37 Htotal = H1/1000 + H2 + H3/1000;
38 Nch2o = xch2o * N;
39 mch2o = Nch2o * 30.016/1000; //kg
40 //for 1000 kg of formaldehyde produced ,
41 H = Htotal * 1000 / mch2o;
42 disp("kJ",H,"The amount of heat to be removed per
        1000kg of formaldehyde produced = ")

```

Scilab code Exa 12.18 Maximum allowable conversion calculation

```

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

```

```

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

```

Scilab code Exa 12.19 Theoretical flame temperature calculation

```

1 //clc ()
2 Nco = 1; //mol CO
3 // CO + 1/2 O2 = CO2
4 O2r = 1; //mol
5 N2r = 3.76; //mol
6 CO2r = 1; //mol
7 O2p = 0.5; //mol
8 N2p = 3.76; //mol
9 CO2p = 1; //mol
10 Hco = 29.23; //J/molK
11 Ho2 = 34.83; //J/molK
12 Hn2 = 33.03; //J/molK
13 Hco2 = 53.59; //J/molK
14 Hcomb1 = -282.99; //kJ/mol
15 T1 = 298; //K
16 T2 = 373; //K
17 H1 = (O2r * Ho2 + N2r * Hn2 + CO2r * Hco) * (T1 - T2)
    ;
18 //For product at temp T, H2 = (O2p * Ho2 + N2p * Hn2
    + CO2p * Hco2) * (T - T1)
19 //For adiabatic condition , -(H1 + Hcomb1) = H2
20 T = -(H1 + Hcomb1 * 1000) / (O2p * Ho2 + N2p * Hn2 +
    CO2p * Hco2) + T1;

```

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

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

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