Scilab Textbook Companion for Stoichiometry by B. I. Bhatt And S. B. Thakore¹

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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 1

Dimensions and Units

Scilab code Exa 1.1 Mass flow rate

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 1
6 // Dimensions and Units
8
9 // Example 1.1
10 // Page 12
11 printf("Example 1.1, Page 12 n n);
12
13 // solution
14
15 // Using conversion factors from table 1.3 (Pg 9)
16 q1 = 75 // [gallon/min] (volumetric flow rate)
17 q2 = 75/(60*.219969) // [dm<sup>3</sup>/s]
18 row = 0.8 // [kg/dm^3]
19 q3 = q2*row // [kg/s] (mass flow rate)
20 printf("mass flow rate = "+string(q3)+" [kg/s] \ n")
```

Scilab code Exa 1.2 steam velocity in pipeline

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 1
6 // Dimensions and Units
7
9 // Example 1.2
10 // Page 12
11 printf("Example 1.2, Page 12 n n);
12
13 // solution
14
15 qm = 2000 // [kg/h] (mass flow rate)
16 d1 = 3.068 // [in] (internal dia of pipe)
17 // Using conversion factors from table 1.3 (Pg 9)
18 d2 = 3.068/.0393701 // [mm]
19 A = ((\%pi/4)*d2^2)/10^6 // [m<sup>2</sup>] (cross section area
20 // Using steam tables; Appendix IV.3
21 v = 0.46166 // [m^3/kg] (sp. vol. of steam at 440
     kPa)
22 qv = (qm*v)/3600 // [m^3/s]
23 vs = qv/A // [m/s]
24 printf("velocity of the steam in the pipeline is "+
     string(vs)+" m/s")
```

Scilab code Exa 1.3 conversion of TR

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 1
6 // Dimensions and Units
8
9 // Example 1.3
10 // Page 13
11 printf("Example 1.3, Page 13 n \n");
12
13 // solution
14
15 m = 2000 // [lb] (mass flow rate)
16 t = 24 //[hr]
17 lf = 144 // [Btu/lb] (latent heat of fusion)
18 // Using conversion factors from table 1.3 (Pg 9)
19 TR = (m*1f*.251996*4.184)/(3600*24)
20 printf("1 TR = "+string(TR)+" kW")
```

Scilab code Exa 1.4 conversion of equation into SI units

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 1
6 // Dimensions and Units
7
8
9 // Example 1.4
10 // Page 13
11 printf("Example 1.4, Page 13 \n \n");
12
```

```
13  // solution
14
15  // C = 89.2*A*(T/M^).5  [ft^3/s]
16  k = 89.2  //
17  C1 = 1  // [ft^3/s]
18  // Using conversion factors from table 1.3 (Pg 9)
19  C2 = 35.31467*C1
20  T1 = 1  // [dgree R]
21  T2 = 1.8*T1  // [K]
22  A1 = 1  // [ft^2]
23  A2 = 10.76391
24  k2 = (k*A2*(1.8)^.5)/35.34167
25  printf("eq in SI becomes \n C = "+string(k2)+"*(T/M)^.5  [m^3/s]")
```

Chapter 2

Basic Chemical Calculations

Scilab code Exa 2.1 gm of NH4Cl

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.1
10 // Page 17
11 printf("Example 2.1, Page 17 n \);
12
13 // solution
14
15 // NH4Cl
16 M = 14+4+35.5 // [g] (molar mass of NH4Cl)
17 n=5 // [mol]
18 \quad m = M*n // [g]
19 printf("5 mol of NH4Cl = "+string(m)+" [g]")
```

Scilab code Exa 2.2 equivalent moles of CuSO4

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
9 // Example 2.2
10 // Page 17
11 printf("Example 2.2, Page 17 n \n");
12
13 // solution
14
15 // CuSO4.5H2O
16 M1 = 159.5 // [g] (molar mass of CuSO4)
17 \text{ M2} = 159.5 + 5*(2+16) // \text{ (molar mass of CuSO}4.5 H2O)
18 m = 499
19 \quad n = m/M2 //[mol]
20 printf("In the formula CuSO4.5H2O, the moles of
     CuSO4 is one hence, \n the equivalent moles of
     CuSO4 in the crystal is "+string(n)+".")
```

Scilab code Exa 2.3 moles of K2CO3

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
```

```
6 // Basic Chemical Calculations
8
9 // Example 2.3
10 // Page 17
11 printf("Example 2.3, Page 17 n");
12
13 // solution
14
15 // K2CO3
16 m = 117 // [kg] (wt of K)
17 Mk = 39 // [g] (at wt of K)
18 a = m/Mk // [kg atoms]
19 // 1 mol of K2CO3 contains 2 atoms of K
20 n = a/2 // [kmol] (moles of K2CO3)
21 printf(" "+string(n)+" kmol of K2CO3 contains 117 kg
      of K.")
```

Scilab code Exa 2.4 no of atoms of BaCl2

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8
9 // Example 2.4
10 // Page 18
11 printf("Example 2.4, Page 18 \n \n");
12
13 // solution
14
15 // BaCl2
```

```
16 M = 137.3+2*35.5 // [g] (molar mass of BaCl2)
17 m = 416.6 // [g]
18 n = m/M // [mol]
19 N = n*6.022*10^23 // (no. of atoms)
20 printf("Atoms present in 416.6 g BaCl2 = "+string(N) +"")
```

Scilab code Exa 2.5 equivalent mass

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8
9 // Example 2.5
10 // Page 19
11 printf("Example 2.5, Page 19 n \n");
12
13 // solution
14
15 printf("(a) \n \n")
16 //PO4 radical
17 M = 31+4*16 //[g]
18 V = 3 // \text{ (valence of PO4)}
19 \text{ eqm} = M/V
20 printf("eq. mass of PO4 is "+string(eqm)+" [g] \setminus n \setminus n
       \n")
21 printf("(b) n n")
22 //Na3PO4
23 M = 3*23+95 //[g]
24 \ V = 3
25 \text{ eqm} = \text{M/V}
```

```
26 printf("eq. mass of Na3PO4 is "+string(eqm)+" [g] \n \n")
```

Scilab code Exa 2.6 equivalents

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.6
10 // Page 19
11 printf("Example 2.6, Page 19 n \n");
12
13 // solution
14
15 // AlCl3
16 v = 3 // valency of Al ion
17 eq = 3*3 // [mol]
18 printf("no. of equivalents in 3 kmol of AlCl3 is "+
     string(eq)+" keq.")
```

Scilab code Exa 2.7 composition of mixture

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
```

```
7
9 // Example 2.7
10 // Page 20
11 printf("Example 2.7, Page 20 n \n");
12
13 // solution
14
15 // (a)
16 printf("(a) \n \n")
17 // \text{ mass } \%
18 m1 = 600 //[kg] (NaCl)
19 m2 = 200 //[kg] (KCl)
20 m = m1+m2 // total mass
21 \text{ Wa} = (m1/m)*100
22 \text{ Wb} = (m2/m)*100
23 printf("mass percentage of NaCl is "+string(Wa)+" \
      nmass percentage of KCl is "+string(Wb)+" \n \n \
      n")
24 // (b)
25 printf("(b) \setminus n \setminus n")
26 // \text{mol } \%
27 \text{ M1} = 23+35.5 // \text{molar mass of NaCl}
28 n1 = m1/M1 // no. of moles of NaCl
29 M2 = 39+35.5 // molar mass of KCl
30 n2 = m2/M2 // no. of moles of KCl
31 n = n1 + n2
32 \text{ N1} = (n1/n)*100
33 \text{ N2} = (n2/n)*100
34 printf("mol percentage of NaCl is "+string(N1)+" \
      nmol percentage of KCl is "+string(N2)+" \n")
```

Scilab code Exa 2.8 composition and molar mass

```
1 clear;
```

```
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.8
10 // Page 21
11 printf("Example 2.8, Page 21 n n);
12
13 // solution
14 // CH.35O.35S.14
15 // mass %
16 \ C = 12.0107 \ // [kg]
17 \text{ H} = 1.00794*.35 // [kg]
18 \ 0 = 15.9994 * .35 // [kg]
19 S = 32.065*.14 / [kg]
20 \text{ m} = \text{C+H+O+S}
21 \text{ m1} = (C/m)*100
22 \text{ m2} = (H/m)*100
23 \text{ m3} = (0/\text{m})*100
24 \text{ m4} = (\text{S/m})*100
25 printf("mass percentage of C is "+string(m1)+" \
      nmass percentage of H is "+string(m2)+" \nmass
      percentage of O is "+string(m3)+" \nmass
      percentage of S is "+string(m4)+" \n \n")
26 M = m/(1+.35+.35+.14)
27 printf("molar mass = "+string(M)+" kg/kmol.")
```

Scilab code Exa 2.9 actual urea content

```
1 clear;
2 clc;
3
```

```
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.9
10 // Page 22
11 printf("Example 2.9, Page 22 n \n");
12
13 // solution
14
15 // basis 100kg urea
16 m1 = 45 //[kg] (mass of N present)
17 Mu = 60 // (molar mass of urea)
18 m2 = 14*2 / [kg] (mass of N in 1 kmol of urea)
19 \quad m = (Mu/m2)*m1
20 printf("The sample contains "+string(m)+" percent
     urea.")
```

Scilab code Exa 2.10 mass percent

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8
9 // Example 2.10
10 // Page 22
11 printf("Example 2.10, Page 22 \n \n");
12
13 // solution
14
```

```
15 // NaOH

16

17 Impurity = 60 // [ppm] SiO2

18 m = (60/1000000)*100

19 printf("Mass percent of SiO2 is "+string(m)+".")
```

Scilab code Exa 2.11 no of ions

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.11
10 // Page 22
11 printf("Example 2.11, Page 22 n \n");
12
13 // solution
14
15 Ca = 40.078 // at. wt of Ca
16 F = 18.9984032 // at wt of F
17 M1 = 3*Ca + 2*(30.97762+(4*15.9994)) // molar mass of
       Ca3PO4
18 M2 = Ca +12.0107+3*15.9994 // molar mass of CaCO3
19 M3 = Ca+2*F // molar mass of CaF2
20 \text{ m1} = 800 \text{ // [mg] Ca3PO4}
21 \text{ m2} = 200 \text{ } // \text{[mg]} \text{ CaCO3}
22 \text{ m3} = 5 //[\text{mg}] \text{ CaF2}
23 n1 = ((3*Ca)/M1)*m1+(Ca/M2)*m2+(Ca/M3)*m3 // [mg]
      total Ca ions
24 \text{ n2} = (F/M3)*2*5 //[mg] \text{ total } F \text{ ions}
25 printf("Total no. of Ca+ ions is "+string(n1)+" and
```

Scilab code Exa 2.12 composition of solution

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.12
10 // Page 23
11 printf("Example 2.12, Page 23 n n);
12
13 // solution
14
15 // (a)
16 printf("(a) \n \n")
17 // \text{ mass } \%
18 m1 = 100 //[kg] methanol (basis)
19 m2 = 64 //[kg] salicylic acid
20 m = m1+m2 // [kg] mass of solution
21 \text{ w1} = \text{m2/m}*100
22 	ext{ w2} = 100 - 	ext{w1}
23 printf("mass percent of salicylic acid is "+string(
      w1)+" and \nmass percent of methanol is "+string(
      24
25 //(b)
26 printf("(b) n n")
27 //mole %
28 M1 = 32 // molar mass of methanol
29 M2 = 138 //molar mass of salicylic acid
```

Scilab code Exa 2.13 composition of solution

```
1 clear;
2 clc;
 3
4 // Stoichiometry
5 // Chapter 2
 6 // Basic Chemical Calculations
8
9 // Example 2.13
10 // Page 24
11 printf("Example 2.13, Page 24 n n);
12
13 // solution
14
15
16 // \text{mass } \%
17 \text{ m1} = 13.70 \text{ // HCl}
18 \text{ m2} = 8.67 // \text{NaCl}
19 \text{ m3} = 100 // \text{H2O}
20 m = m1+m2+m3 // mass of solution
21 	 w1 = m1/m*100
22 w2 = m2/m*100
23 \text{ w3} = \text{m3/m} * 100
24
```

```
25 printf("mass percent of HCl is "+string(w1)+" , \
      nmass percent of NaCl is "+string(w2)+" and \nmass
       percent of H2O is "+string(w3)+". n n n")
26 \text{ M1} = 36.4609 //HCl
27 M2 = 58.4428 / NaCl
28 M3 = 18.0153 / H2O
29 \text{ n1=m1/M1} //\text{HCl}
30 \text{ n2=m2/M2} // \text{NaCl}
31 \text{ n3=m3/M3} //\text{H2O}
32 n=n1+n2+n3
33 N1 = n1/n * 100
34 N2=n2/n*100
35 N3=n3/n*100
36 printf("Mole percent of HCl is "+string(N1)+", \
      nMole percent of NaCl is "+string(N2)+" and \nMole
       percent of H2O is "+string(N3)+".")
```

Scilab code Exa 2.14 Na2O percentage

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8
9 // Example 2.14
10 // Page 24
11 printf("Example 2.14, Page 24 \n \n");
12
13 // solution
14
15 m = 100 //[kg] Lye (basis)
16 m1 = 73 //[kg] NaOH
```

```
17 M1 = 40 // NaOH

18 M2 = 62 // Na2O

19 p = (M2*m1)/(2*M1)

20 printf("percentage of Na2O in the solution is "+

string(p)+".")
```

Scilab code Exa 2.15 TOC and ThOD

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8
9 // Example 2.15
10 // Page 25
11 printf("Example 2.15, Page 25 n n);
12
13 // solution
14
15 // (CH2OH) 3
16 M = 92 // molar mass of glycerin
17 C = 600 //[mg/l] glycerin conc.
18 TOC = (3*12/92)*600 // [mg/1]
19 // by combustion reaction we see 3.5 O2 is required
     for 1 mol of (CH2OH)3
20 ThOD = (3.5*32*600)/92 / [mg/l]
21 printf("TOC = "+string(TOC) + "mg/l \nThOD = "+string(TOC))
     ThOD) + mg/l")
```

Scilab code Exa 2.16 conc of salts

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.16
10 // Page 25
11 printf("Example 2.16, Page 25 n n");
12
13 // solution
14
15 \text{ M1} = 100 // \text{CaCO3}
16 \text{ v1} = 2 \text{ // valence of CaCO3}
17 eqm1 = M1/v1 // equivalent mass of CaCO3
18 M2 = 162 // \text{Ca(HCO3)} 2
19 v2 = 2
20 \text{ eqm2} = M2/v2
21 \text{ m} = 500 \text{ // } [\text{mg/l}] \text{ CaCO3}
22 C1 = (eqm2/eqm1)*m*.6 // [mg/l] conc. of Ca(HCO3)2
23 \text{ M3} = 146.3 // Mg(HCO3) 2
24 v3 = 2
25 \text{ eqm3} = M3/v3
26 C2 = (eqm3/eqm1)*m*.4 //[mg/1] conc. of Mg(HCO3)2
27 printf ("Actual concentration of Ca(HCO3)2 in the
      sample water is "+string(C1)+" mg/l and of Mg(
      HCO3) 2 is "+string(C2)+" mg/l.")
```

Scilab code Exa 2.17 ppm unit

```
1 clear;
2 clc;
3
```

```
4  // Stoichiometry
5  // Chapter 2
6  // Basic Chemical Calculations
7
8
9  // Example 2.17
10  // Page 26
11 printf("Example 2.17, Page 26 \n \n");
12
13  // solution
14
15  S = .68  // sulphur content by mass
16  d = .85  // kg/l
17  s = (S*d*10^6)/100  // [mg/l] or [ppm]
18 printf("Sulphur content in LDO is "+string(s)+" ppm.")
```

Scilab code Exa 2.18 molarity normality and molality

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8 // Example 2.18
9
10 // Page 26
11 printf("Example 2.18, Page 26 \n \n");
12
13 // solution
14
15 m1 = 100 //[kg] solution (basis)
16 m2 = 20 //[kg] NaCl
```

Scilab code Exa 2.19 molarity of solution

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8 // Example 2.19
10 // Page 27
11 printf("Example 2.19, Page 27 n n);
12
13 // solution
14
15 m1 = 100 //[kg] TEA solution (basis)
16 \text{ m2} = 50 // [\text{kg}] \text{ TEA}
17 M1 = 149 // molar mass of TEA
18 d = 1.05 //[kg/l]
19 V = m1/d // volume of 100 kg sol.
20 n = (m2/M1)*100 // [mol] NaCl
21 \quad M = n/V //[M]
22 printf("Molarity of solution = "+string(M)+" M.")
```

Scilab code Exa 2.20 conc of CO2

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8 // Example 2.20
10 // Page 27
11 printf("Example 2.20, Page 27 n \n");
12
13 // solution
14
15 m1 = 100 //[kg] MEA solution (basis)
16 \text{ m2} = 20 // [kg] \text{ MEA}
17 M1 = 61 // molar mass of MEA
18 n1 = m2/M1 / [kmol]
19 \ C = .206
20 n2 = C*n1 //[kmol] dissolved CO2
21 \text{ m3} = n2*44 // [kg] \text{ mass of CO2}
22 \text{ n3} = (m1-m2-m3)/18 //[kmol] \text{ water}
23 n = (n2/(n1+n2+n3))*100
24 \text{ m} = (m3/100)*100
25 printf("Mass percent of CO2 = "+string(m)+" and Mol
      percent = "+string(n)+".")
```

Scilab code Exa 2.21 pH of HOCl

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8 // Example 2.21
10 // Page 27
11 printf("Example 2.21, Page 29 n \n");
12
13 // solution
14
15 //HOCl
16 Ma = .1 // molarity
17 \text{ Ka} = 9.6*10^-7
18 C = (Ma*Ka)^{.5} // conc. of H+ ions
19 pH = -\log 10 (C)
20 printf("pH of the sol is "+string(pH)+".")
```

Scilab code Exa 2.22 Mavg and composition of air

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8 // Example 2.22
9
10 // Page 39
11 printf("Example 2.22, Page 39 \n \n");
12
```

```
13  // solution
14
15  n = 100  // [mol] air (basis)
16  n1 = 21  // [mol] O2
17  n2 = 78  // [mol] N2
18  n3 = 1  // [mol] Ar
19  M1 = 31.9988  // O2
20  M2 = 28.0134  // N2
21  M3 = 39.948  // Ar
22  m1 = n1*M1
23  m2 = n2*M2
24  m3 = n3*M3
25  Ma = (m1+m2+m3)/n
26  printf("average molar mass of air is "+string(Ma)+" g.")
```

Scilab code Exa 2.23 Composition and specific gravity

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8 // Example 2.23
9
10 // Page 39
11 printf("Example 2.23, Page 39 \n \n");
12
13 // solution
14
15 // (a)
16 printf("(a) \n \n")
17 n = 100 // [kmol] cracked gas (basis)
```

```
18 n1 = 45 // methane
19 \quad n2 = 10 // ethane
20 \text{ n3} = 25 // \text{ethylene}
21 \quad n4 = 7 // propane
22 \text{ n5} = 8 // \text{propylene}
23 \quad n6 = 5 // n-butane
24 M1 = 16
25 \text{ M2} = 30
26 M3 = 28
27 \text{ M4} = 44
28 \text{ M5} = 42
29 \quad M6 = 58
30 \text{ m1} = \text{n1} * \text{M1}
31 \quad m2 = n2*M2
32 \text{ m3} = \text{n3} * \text{M3}
33 \quad m4 = n4 * M4
34 \text{ m5} = \text{n5}*\text{M5}
35 \text{ m6} = \text{n6} * \text{M6}
36 \text{ m} = \text{m1}+\text{m2}+\text{m3}+\text{m4}+\text{m5}+\text{m6}
37 M = m/n
38 printf("Average molar mass of gas is "+string(M)+" g
39 //(b)
40 printf("(b) \n \n")
41 // composition
42 p1 = (m1/m)*100
43 p2 = m2*100/m
44 p3 = m3*100/m
45 \text{ p4} = \text{m4}*100/\text{m}
46 p5 = m5*100/m
47 	 p6 = m6*100/m
48 printf("
                   GAS
                                        Mass Percent \n Methane
                          "+string(p1)+" \n Ethane
                          "+string(p2)+" \n Ethylene
                          "+string(p3)+" \n Propane
                          "+string(p4)+" \n Propylene
                          "+string(p5)+" \n n-Butane
                          "+string(p6)+" n n n"
```

```
49  // (c)
50  printf("(c) \n \n")
51  // specific gravity
52  g = M/28.97
53  printf("Specific gravity is "+string(g)+".")
```

Scilab code Exa 2.24 percentage error

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.24
10 // Page 40
11 printf("Example 2.24, Page 40 n \n");
12
13 // solution
14
15 p = 100 //[bar]
16 T = 623.15 / [K]
17 R = .083145
18 V = R*T/p // [l/mol] molar volume
19 v = V/18.0153 //
20 printf("Specific volume = "+string(v)+" m<sup>3</sup>/kg.")
```

Scilab code Exa 2.25 molar volume

```
1 clear;
2 clc;
```

```
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8
9 // Example 2.25
10 // Page 40
11 printf("Example 2.25, Page 40 n \n");
13 // solution
14
15 p = 4 //[bar]
16 T = 773.15 // [K]
17 R = .083145
18 V = R*T/p // [l/mol] molar volume
19 printf ("Molar volume = "+string(V)+" l/mol.\n \n \n"
    // using appendix III
20
    // calculating Tc and Pc of different gases
       according to their mass fractions
22 \text{ Tc1} = .352*32.20 // H2
23 \text{ Tc2} = .148*190.56 // \text{ methane}
24 \text{ Tc3} = .128*282.34 // ethylene
25 \text{ Tc4} = .339*132.91 // CO
26 \text{ Tc5} = .015*304.10 // CO2
27 \text{ Tc6} = .018*126.09 // N2
28 Tc = Tc1+Tc2+Tc3+Tc4+Tc5+Tc6 // Tc of gas
29 // similarly finding Pc
30 \text{ Pc1} = .352*12.97
31 \text{ Pc2} = .148 * 45.99
32 \text{ Pc3} = .128 * 50.41
33 \text{ Pc4} = .339 * 34.99
34 \text{ Pc5} = .015*73.75
35 \text{ Pc6} = .018*33.94
36 Pc=Pc1+Pc2+Pc3+Pc4+Pc5+Pc6 // Pc of gas
37 a = (27*R^2*Tc^2)/(64*Pc) // [bar/mol^2]
38 b = (R*Tc)/(8*Pc) // 1/mol
```

Scilab code Exa 2.26 ternary mix analysis

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
8
9 // Example 2.26
10 // Page 43
11 printf ("Example 2.26, Page 43 n n);
12
13 // solution
14 m = 6.5065 //[g] mixture (basis)
15 Pv = 2.175 / [kPa] V.P. of water over KOH
16 Pa = 102.5-2.175 / [kPa] Partial P of n-butane and 1
      butene
17 V = 415.1*10^{-3} //[1]
18 R = 8.314472
19 T = 296.4 / [K]
20 n = (Pa*V)/R*T // moles of butene and butane
21 \text{ n1} = n*.431 // n-butane
22 \text{ m1} = \text{n1*58} // [g]
23 n2 = n-n1 // 1 butene
24 \text{ m2} = n2*56 //[g]
25 m3 = m-m1 // [g] furfural
26 \text{ n3} = \text{m3/96}
```

Scilab code Exa 2.27 vapour mix composition

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
9 // Example 2.27
10 // Page 44
11 printf("Example 2.27, Page 44 n n");
12
13 // solution
14
15 P = 5.7+1.01 //[bar] absolute total P
16 // using Roult's law
17 vp = 3.293*.7737 //[kPa] vap P of furfural
18 // using Dalton's law of partial P
19 n1 = vp/(P*100) // mol fraction of furfural
20 n2 = 1-n1 // mol fraction of 1 -butene
21 printf("mol fraction of Furfural is "+string(n1)+"\
     nmol fraction of 1-Butene is "+string(n2)+".")
```

Scilab code Exa 2.28 absolute humidity

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
9 // Example 2.28
10 // Page 44
11 printf("Example 2.28, Page 44 n \n");
12
13 // solution
14
15 P = 100 //[kPa] total P
16 Pw = 2.5326 //[kPa] V.P> of water at dew point
17 //absolute humity = mass of water vapour/ mass of
     dry air
18 H = (Pw/(P-Pw))*(18.0153/28.9697) // absolute
     humidity
19 printf("absolute humidity = "+string(H)+".")
```

Scilab code Exa 2.29 nozzle outlet T

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 2
6 // Basic Chemical Calculations
7
8
9 // Example 2.29
10 // Page 45
11 printf("Example 2.29, Page 45 \n \n");
```

```
12
13  // solution
14
15  //Ti-Tf = mu*(Pi-Pf)
16  Pi = 20.7  //[bar]
17  Pf = 8.7  // [bar]
18  mu = 1.616  //[K/bar]
19  Ti = 355.15  //[K]
20  Tf = Ti-mu*(Pi-Pf)
21  printf("Outlet temperature is "+string(Tf)+" K")
```

Chapter 3

Material Balances without Chemical Reaction

Scilab code Exa 3.1 Lancashire boiler

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
9 // Example 3.1
10 // Page 60
11 printf("Example 3.1, Page 60 n n);
12
13 // solution
14
15 m = 1 //[kg] feed water
16 m1 = 1200 //[mg] dissolved solids in 1 kg feed water
17 m2 = 3500 //[mg] max dissolved solid content
18 x = (m*m1)/m2 // [kg] blown down water
19 printf ("Percentage of feed water to be blown down is
```

```
"+string(x)+".")
```

Scilab code Exa 3.2 Textile mill

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.2
10 // Page 61
11 printf("Example 3.2, Page 61 n \n");
12
13 // solution
14 m = 100 //[kg] weak liquor (feed)
15 m1 = 4 //[kg] NaOH
16 p = .25
17 x = 4/p // water left
18 y = 100-16 // [kg] evaporated water
19 printf("Amount of water that evaporated is "+string(
     y) + "kg.")
```

Scilab code Exa 3.3 recovered tannin

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
```

```
7
9 // Example 3.3
10 // Page 61
11 printf("Example 3.3, Page 61 n n);
12
13 // solution
14
15 m = 100 //[kg] babul bark (basis)
16 m1 = 5.8 / \lceil kg \rceil moisture
17 m2 = 12.6 //[kg] Tannin
18 m3 = 8.3 //[kg] soluble non tannin organic material
19 m4 = m-m1-m2-m3 // [kg] Lignin
20 // lignin content remains unaffected during leaching
21 m5 = 100 - .92 - .65 // [kg lignin/kg dry residue]
22 x = (m4*100)/m5 // [kg]
23 T1 = x*.0092 //[kg] Tannin present in residue
24 T2 = m2 - T1 // [kg] Tannin recovered
25 T = (T2/m2)*100
26 printf ("Percentage of Tannin recovered during
      leaching is "+string(T)+".")
```

Scilab code Exa 3.4 Extraction of dry neem leaves

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.4
10 // Page 62
11 printf("Example 3.4, Page 62 \n \n");
```

Scilab code Exa 3.5 Extraction of mix of Acetone and Chloroform

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.5
10 // Page 62
11 printf("Example 3.5, Page 62 n \n");
12
13 // solution
14
15 m = 100 //[kg] original mixture (basis)
16 A = 27.8 //[kg]
17 B = 72.2 / [kg]
18 // let x and y be uper and lower layer amounts
```

```
19 // \text{ total mixture} = (x+y) \text{ kg}
20 // balancing A and B
21 X = [.075 .203; .035 .673]
22 d = [27.8;72.2]
23 \times X = X \setminus d
24 M = X(1,1) + X(2,1) // [kg] total mixture
25 Ms = M - m //[kg] mixed solvent
26 Mr = Ms/m // mixed solvent/original mixture
27 \text{ S1} = x(1,1)*.574+x(2,1)*.028 //[kg] water balance
28 S2 = x(1,1)*.316+x(2,1)*.096 // [kg] acetic acid
      balance
29 \ Qs = S1 + S2
30 \text{ pS1} = (S1*100)/Qs
31 pS2 = 100 - pS1
32 printf("(a) \n \nUpper layer = "+string(x(1,1))+" kg
       and Lower layer = "+string(x(2,1))+"\n \n(b)
      \n \nmass ratio of the mixed solvent to the
      original mixture is "+string(Mr)+" \n \n \n (c) \
      n \setminus nwater mass percent = "+string(pS1)+" and
      acetic acid mass percent = "+string(pS2)+".")
```

Scilab code Exa 3.6 Pressure Swing Adsorption

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.6
10 // Page 63
11 printf("Example 3.6, Page 63 \n \n");
12
```

```
13  // solution
14
15  m = 170  // [Nm^3/h] air (basis)
16  m1 = 50*.99  // [Nm^3/h] N2 content of the stream
17  m2 = 50*.01  // [Nm^3/h]
18  N = m*.79-m1  // [Nm^3/h] N2
19  O = m*.21-m2  // [Nm^3/h] O2
20  V1 = N*100/(N+0)
21  V2 = 0*100/(N+0)
22  printf("Vol percent of N2 is "+string(V1)+" and Vol percent of O2 is "+string(V2)+".")
```

Scilab code Exa 3.7 Required Oleum strength

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
8
9 // Example 3.7
10 // Page 64
11 printf("Example 3.7, Page 64 n \n");
12
13 // solution
14
15 m = 100 //[kg] SO3 free mixed acid (basis)
16 m1 = 55 //[kg] HNO3
17 \text{ m2} = 45 / [\text{kg}] \text{ H2SO4}
18 // SO3 + H2O \longrightarrow H2SO4
19 m3 = (80/18)*3 //[kg] SO3 equivalent to 3 kg of
      water
20 Q = m2+m3 //[kg] oleum to be mixed
```

Scilab code Exa 3.8 Mixed acid formation

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.8
10 // Page 64
11 printf("Example 3.8, Page 64 n \n");
12
13 // solution
14
15 m = 1000 //[kg] mixed acid (basis)
16 // doing overall mass balance, H2SO4 balance and
     HNO3 balance
17 A = [1 1 1; .444 0 .98; .113 .9 0]
18 d = [1000;600;320]
19 \quad x = A \setminus d
20 printf ("quantities of acids required are :\n Spent
     = "+string(x(1,1))+"kg \n HNO3 = "+string(x(2,1))
     )+" kg n H2SO4 = "+string(x(3,1))+" kg."
```

Scilab code Exa 3.9 Actual analysis of borewell water

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.9
10 // Page 65
11 printf("Example 3.9, Page 65 n n");
12
13 // solution
14
15 l = 1 //[litre] water (basis)
16 \text{ Cl} = 475.6 // [\text{mg}]
17 m1 = (58.5/35.5)*C1 //[mg] NaCl present in water
18 \text{ SO4} = 102.9 // [mg] // SO4
19 m3 = (142/96)*S04 //[mg] Na2SO4 present in water
20 // carbonates are present due to Na2CO3
21 // \text{ eq mass of CaCO3} = 50
22 // eq mass of Na2CO3 = 53
23 m4 = (53/50)*65.9 // [mg] Na2CO3 present in water
24 // NaHCO3 in water = bicarbonates - temporary
      hardness
25 \text{ m5} = 390.6-384 \text{ // [mg] NaHCO3 present as CaCO3}
26 m6 = (84/50)*m5 // [mg] NaHCO3 present in water
27 // equivalent mass of Mg(HCO3)2 = 73.15
28 \text{ m7} = (\text{m6/50}) * 225
29 m8 = 384-225 // [mg] CaCO3 from Ca(HCO3)2
30 // equivalent mass of Ca(HCO3)2 is 81
31 m9 = (m8/50)*159 //[mg] Ca(HCO3)2 present in water
32 printf ("Component analysis of raw water: \n \n \
                          mg/l \setminus n \setminus nCa(HCO3) 2
      nCompound
      "+string(m7)+" \setminus
     nNaHCO3
                          "+string(m6)+" \nNa2CO3
                 "+string(m4)+" \nNaCl
                                         "+string(m3)+"")
```

Scilab code Exa 3.10 Matrix use

```
clear;
clc;

d // Stoichiometry
// Chapter 3
// Material Balances Without Chemical Reaction

// Balances Without Chemical Reaction
// Page 67
// Page 67
// Page 67
// Page 67
// Solution
// see examples 3.5 and 3.8
```

Scilab code Exa 3.11 Flowrate calculation

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.11
10 // Page 68
11 printf("Example 3.11, Page 68 \n \n");
```

```
12
13 // solution
14
15 // basis : 1000 \text{ kg/h} of feed
16 // balancing H2SO4, HNO3 and H2O in all the three
     product streams
0 0 1;1 0 0 0 0 0 0 0;0 1 0 0 0 0 0;0 0 1
     0 0 0 0 0;0 0 0 1 0 0 0;0 0 0 0 1 0 0 0;0
      0 0 0 0 1 0 0 0]
18 \quad v = [400;100;500;4;94;60;16;6;400]
19 s = M \ v
20 A = s(1)+s(2)+s(3)
21 B = s(4) + s(5) + s(6)
22 \ C = s(7) + s(8) + s(9)
23 printf("Flowrates are :\n A = "+string(A)+" kg/h \n
     B = "+string(B) + "kg/h n C = "+string(C) + "kg/h")
```

Scilab code Exa 3.12 solving eqs with graphical plot

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.12
10 // Page 70
11 printf("Example 3.12, Page 70 \n \n");
12
13 // solution
14 m = 100 // kg
15 x = linspace(70,110,5);
```

```
16 \text{ y} = linspace(100, 115, 4);
17 \text{ y1} = 27.8/.203 - .075*x/.203
18 \text{ y2} = 72.2/.673 - .035*x/.673
19 x = linspace(70, 110, 5);
20 \text{ plot}(x,y1,style=4)
21 \text{ plot}(x,y2,style=8)
22 // from graph its clear x = 93.4 kg and y = 102.4 kg
23 \times = 93.4;
24 y = 102.4;
25 M = x+y // [kg] total mixture
26 Ms = M - m //[kg] mixed solvent
27 Mr = Ms/m // mixed solvent/original mixture
28 S1 = x*.574+y*.028 //[kg] water balance
29 S2 = x*.316+y*.096 //[kg] acetic acid balance
30 \ Qs = S1+S2
31 \text{ pS1} = (S1*100)/Qs
32 pS2 = 100 - pS1
33 printf("(a) \n \nUpper layer = "+string(x)+" kg and
      Lower layer = "+string(y)+"\n\n(b)\n\nmass
      ratio of the mixed solvent to the original
      mixture is "+string(Mr)+" \n \n \n \c) \n \n
      mass percent = "+string(pS1)+" and acetic acid
      mass percent = "+string(pS2)+".")
```

Scilab code Exa 3.14 ion exclusion process

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
```

```
9 // Example 3.14
10 // Page 73
11 printf("Example 3.14, Page 73 n \n");
12
13 // solution
14
15 //using table 2.7 on page no 75
16 Rg = 8124*100/9448 // recovery of glycerine
17 Lg = (16+83)*100/9448 // loss of glycerine in waste
18 Reg = 100-Rg-Lg // recycle of glycerine
19 m1 = 238/8124 // NaCl in product
20 m2 = Rg*12/100 // glycerine in product
21 m3 = m1+m2 // total solute
22 n = m1*100/m3 // NaCl percent in total solute
23 printf("(a) \n \nrecovery percent of glycerine is "+
     string(Rg)+" \n \n \n \n \n
     glycerinr is "+string(Lg)+" \n \n(c) \n\
     nproduct contamination with respect to salt NaCl
     is "+string(n)+".")
```

Scilab code Exa 3.15 Air Conditioning plant

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.15
10 // Page 76
11 printf("Example 3.15, Page 76 \n \n");
12
13 // solution
```

```
14
15 f1 = 1.25 //[m^3/s] fresh ambient air as feed (basis
16 f2 = 5.806 //[m^{^{\prime}}/s] air entering auditorium
17 v1 = 8.314*290/101.3 //[m^3/kmol] sp. vol. of moist
      air at 101.3 kPa and 290 K
18 na1 = f2*1000/v1 // [mol/s] molar flow rate of air
     entering auditorium
19 nw1 = 243.95*.0163/1.0163 // [mol/s]
20 na2 = 243.95 - nw1 //[mol/s] dry air flow
21 nw2 = 240.04*.0225 //[mol/s] moisture enterin air
     conditioning plant
22 // using table 3.8
23 m1 = (nw2-nw1) // [kg/h] moisture removed in a c
     plant
24 m2 = na2-.0181 //[mol/s] moisture in air leaving
     auditorium
25 m3 = (m2-nw1)*18 // [kg/h] moisture added in
     auditorium
26 \text{ Vm2} = 8.314*308/101.3 // [m^3/kmol]
27 na3 = (f1/25.28)*1000 //[mol/s]
28 n4 = 5.40-1.925 //[mol/s] moisture in recycle stream
29 mr = 240.04-47.525 / [mol/s] molar flow rate of wet
     recycle stream
30 R = mr/na3
31 printf("(a) \setminus n \setminus nmoisture removed in AC plant = "+
     string(m1)+"\n \n \n \n \n
      auditorium = "+string(m3)+" \n \n \n \n \n
     nrecycle ratio of moles of air recycled per mole
     mole of fresh ambient air input = "+string(R)+"."
     )
```

Scilab code Exa 3.16 Overall efficiency of Pulp Mill

```
1 clear;
```

```
2 clc;
4 // Stoichiometry
5 // Chapter 3
  // Material Balances Without Chemical Reaction
8
9 // Example 3.16
10 // Page 78
11 printf("Example 3.16 Page 78 n \n");
12
13 // solution
14
15 // screen 1
16 // feed = N kg
17 // Oversize particle = NE1 kg
18 // Undersize particle = N-NE1
19
20 / screen 2
21 / feed = NE1+X kg
22 // Oversize particle = (NE1+X)*E2 kg
23 // Undersize particle = (NE1+X)(1-E2) kg
24
25
26 //screen 3
27 // \text{feed} = (NE1+X)*E2 \text{ kg}
28 // Oversize particle = (NE1+X)*E2*E3 kg
29 // Undersize particle = (NE1+X)*E2*(1-E3) kg
30 printf ("Overall Efficiency = (E1 E2 E3)*100/[(1-E1)]
     (1-E2)+E2 E3].")
```

Scilab code Exa 3.17 2 stage membrane CO separation

```
1 clear;
2 clc;
```

```
3
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
9 // Example 3.17
10 // Page 79
11 printf("Example 3.17, Page 79 n \n");
12
13 // solution
14
15 printf("(a) n n")
16 F = 5000 / [kmol/h] feed (basis)
17 m1 = F*.47 //[kmol/h] CO in F
18 m2 = F-m1 //[kmol/h] H2 in F
19 m3 = m1*.932 // CO in product stream
20 \text{ n2} = \text{m3/.98} //[\text{kmol/h}]
21 printf("Flow rate of product stream is "+string(n2)+
      " kmol/h. n n n(b) n n")
22 n2 = n2-m3 //[kmol/h] H2 in CO stream
23 printf(" Product H2 stream : \n H2 = "+string(m2)
      -n2)+" kmol/h \n CO = "+string(m1-m3)+" kmol/h \
      n \setminus n \setminus n(c) \setminus n \setminus n")
24 nH2 = 2697.39 / [kmol/h]
25 \text{ nCO} = 3000 - \text{nH2} // [\text{kmol/h}]
26 \quad n4 = m2 + nH2
27 	 n5 = m1+nC0
28 \quad n6 = n4 + n5
29
30 printf("
                 Composition of Mixed feed : \n H2 = "+
      string(n4*100/n6)+" \setminus n CO = "+string(n5*100/n6)+"
      "")
```

Scilab code Exa 3.18 2 stage reverse osmosis

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 3
6 // Material Balances Without Chemical Reaction
7
8
  // Example 3.18
10 // Page 79
11 printf ("Example 3.10, Page 79 n \n");
12
13 // solution
14
15 // Overall balance
16 // F = R1 + P2
17 // Balance across Module I
18 // F+R2 = R1+P1 \implies R1+P2+R2 = R1+P1
19 // balance across module II
20 // P1 = P2+R2
21 P2 = 5 //[m^3/h]
22 P1 = P2/.8 //[m^3/h]
23 R2 = P1-P2 //[m^3/h]
24 F = P1/.66 - R2//[m^3/h]
25 R1 = F-P2 //[\text{m}^3/\text{h}]
26
27 // Overall balance of DS in water
28 \text{ xR1} = (F*4200-P2*5)/R1 //[mg/1]
29 \text{ xP1} = (P2*5)/(.015*P1) // [mg/l]
30 \text{ xR2} = (P1*xP1-P2*5)/R2 // [mg/1]
31 m1 = F*4200+R2*xR2 //[g] DS mixed in MF
32 C1 = m1/(F+R2) // [mg/l]
33 m2 = R1*xR1 //[g] DS in R1
34 r = m2*100/m1 // rejection in module in I
35 \text{ m3} = \text{m1-m2} //[g] \text{ DS in P1}
36 \text{ C2} = \text{m3/P1} // [\text{mg/l}]
37 R = R2/F
38 R1 = P2*100/F
```

```
39 printf("F = "+string(F)+" m^3/h \nR1 = "+string(R1)+ " m^3/h \nP = "+string(P1+P2)+" m^3/h \nR2 = "+ string(R2)+" m^3/h \nrecycle ratio = "+string(R)+ " \nrejection percentage of salt in module I = "+ string(r)+"")
```

Scilab code Exa 3.20 Purging by atmospheric pressure method

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 3
  // Material Balances Without Chemical Reaction
8
9 // Example 3.20
10 // Page 86
11 printf("Example 3.20, Page 86 n \n");
12
13 // solution
14
15 // concetration of the component after n times
      introduction of v volume of inert gas:
16 // Cn = Co/(1+1/n)^n
17 // we know \lim n \longrightarrow \inf inity (1+1/n)^n = e
18 // therefore Cv = Co/e
```

Chapter 4

Material Balances Involving Chemical Reactions

Scilab code Exa 4.1 Manufacture of MCA

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
9 // Example 4.1
10 // Page 116
11 printf("Example 4.1, Page 116 n n);
12
13 // solution
14
15 // basis one day operation
16 // Cl2 is the limiting component
17 \text{ n1} = 4536/71 // [kmol] Cl2 charged
18 // 1mol MCA requires 1 mol Cl2, so
19 n2 = 5000/94.5 // [kmol] Cl2 used for MCA production
```

Scilab code Exa 4.2 Bechamp Process

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
8
9 // Example 4.2
10 // Page 117
11 printf("Example 4.2, Page 117 n \n");
12
13 // solution
14
15 m = 700 //[kg] ONT charged to reactor (basis)
16 \text{ m1} = 505*.99 // [kg] \text{ OT produced}
17 m2 = (4*137*500)/(4*107) // [kg] ONT required
18 m3 = m*.98 // [kg] ONT reacted
19 n1 = m1*100/m3 // yield of OT
20 \text{ m4} = (9*56*\text{m})/(4*137) // [kg] \text{ theoretical iron}
      regiurement
21 \text{ m5} = 800*.9 //[kg] \text{ iron charged}
22 E = (m5-m4)*100/m4 // excess iron
```

```
23 printf("(a) \setminus n \setminus nYield \text{ of } OT = "+string(n1)+" \setminus n \setminus n(b) \setminus n \setminus nExcess quantity of iron powder = "+string(E)+".")
```

Scilab code Exa 4.3 Pilot Plant Calculations

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
8
9 // Example 4.3
10 // Page 118
11 printf ("Example 4.3, Page 118 n n);
12
13 // solution
14
15 printf("(a) n n")
16 m = 100 //kg chlorobenzene (basis)
17 \text{ m1} = 106.5 * .655 // \text{kg HNO3}
18 \text{ m2} = 108 * .936 // \text{kg H2SO4}
19 m3 = 106.5*.345 + 108*.064 //kg water
20 \quad M = m1 + m2 + m3
21 printf(" Analysis of charge: \n Component
      mass percent \n Chlorobenzene
                                                "+string(m
      *100/M) + " \  \   HNO3
                                           "+string(m1
      *100/M)+" \n H2SO4
                                            "+string(m2
      *100/M)+" \n H2O
                                             "+string(m3
      *100/M)+" n n n(b) n n")
22 // (b)
23 // total charge mass is constant
24 m4 = 314.5*.02 //[kg] unreacted CB in the product
```

```
25 \text{ m5} = 100 \text{-m4} // \text{ [kg] CB that reacted}
26 c = m5*100/100 // conversion of CB
27 printf("Percent conversion of Chloro benzene is "+
      string(c) + " \setminus n \setminus n(c) \setminus n \setminus n"
28 // (c)
29 m6 = 63*c/112.5 // [kg] HNO3 consumed
30 \text{ m7} = \text{m1-m6} // \text{unreacted HNO3}
31 m7 = 157.5*c/112.5 // [kg] total NCB produced
32 m8 = m7*.66 / [kg] p-NCB
33 m9 = m7*.34 //[kg] o-NCB
34 \text{ m10} = 18*c/112.5 //[kg] \text{ water produced}
35 m11 = m10+m3 // total water in product
36 \text{ m}12 = \text{m}4+\text{m}8+\text{m}9+\text{m}7+\text{m}2+\text{m}11
37 printf(" Composition of product stream : \n
      Component
                               mass percent \n CB
                              "+string(m4*100/m12)+" \n p-
                               "+string(m8*100/m12)+" \n o-
      NCB
      NCB
                               "+string(m9*100/m12)+" \n
                                  "+string(m7*100/m12)+" \n
      HNO3
                                  "+string(m2*100/m12)+" \n
      H2SO4
      H2O
                                  "+string(m11*100/m12)+"")
```

Scilab code Exa 4.4 Manufacturing of Acetaldehyde

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.4
10 // Page 119
11 printf("Example 4.4, Page 119 \n \n");
```

```
12
13 // solution
14
15 n=100 //[kmol] outgoing gas from 2nd scrubber
16 n1 = .852*n // [kmol] N2
17 \text{ n} = 21 * \text{n} = 1/79 / [kmol] O2
18 n3=n2-2.1 // [kmol] reacted O2
19 // O2 balance
20 // O2 consumed in rxn (ii),(iii),(v) - O2 produced
      by rxn (iv) = 20.55 \text{ kmol}
21 // let a,b,c be ethanol reacted (ii),(iii),(iv) and
      d be H2 reacted in (v)
22
23 // CO balance
24 a=2.3/2 / kmol
25
26 //CO2 balance
27 b = .7/2
28
29 //CH4 balance
30 c = 2.6/2
31
32 //O2 balance
33 d = 41.1-a-3*b+c
34
35 //H2 balance
36 e = 7.1 + c + d //kmol (total H2 produced)
37 f = e - (3*b + 3*a) //kmol (H2 produced in (i) =
      ethanol reacted in (i))
38 \text{ g} = \text{f+a+b+c} // \text{total ethanol reacted}
39 h = 2*(n1+n2) // total ethanol entering
40 \text{ c1} = g*100/h
41 printf("(a) \setminus n \setminus n \text{ Conversion percent of ethanol} = "+
      string(c1) + " \setminus n \setminus n \setminus n")
42 y = f*100/g
43 printf("(b) \n Yield of acetaldehyde = "+string(y
      )+".")
```

Scilab code Exa 4.5 Lime Soda process

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
9 // Example 4.5
10 // Page 121
11 printf("Example 4.5, Page 121 n n");
12
13 // solution
14
15 v = 1 //[l] water (basis)
16 // 1 \text{ mol } (100 \text{mg}) \text{ CaCO3 gives } 1 \text{ mol } (56) \text{ Cao}
17 // use table 3.3 and eg 3.9
18 x = 56*390.6/100 // [mg/l] lime produced
19 printf("Amount of lime required = "+string(x)+" mg/l
      . ")
```

Scilab code Exa 4.6 Manufacture of Ammonia by Fertilizer plant

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
```

```
9 // Example 4.5
10 // Page 121
11 printf ("Example 4.5, Page 121 n n);
12
13 // solution
14
15 m=100 //[kmol] (basis) dry mixed gas
16 // x = kmol of water gas
17 // y = kmol of producer gas
18 // overall material balance :
19 // x+y = 100
                 ( i )
20
21 //r2 = .43x + .25y // H2 formed by shift rxn
22 //r2=.51x+.25y // H2 entering with water and
      producer gas
23 / r = r1 + r2 / taoal H2
24 //n = .02x + .63y // N2 entering
25 / N2 : H2 = 1:3
26 // = > x-1.807y = 0(ii)
27 //solving (i) and (ii)
28 A = [1 1; 1 -1.807]
29 d = [100;0]
30 x = A \setminus d
31 \text{ s} = .43*x(1) + .25*x(2) // \text{ steam req}.
32 printf("x = "+string(x(1))+" and y = "+string(x(2))+
      "\nAmount of steam required = "+string(s)+" kmol"
      )
```

Scilab code Exa 4.7 Saponification of Tallow

```
1 clear;
2 clc;
3
4 // Stoichiometry
```

```
5  // Chapter 4
6  // Material Balances involving Chemical Reaction
7
8
9  // Example 4.7
10  // Page 123
11 printf("Example 4.7, Page 123 \n \n");
12
13  // solution
14
15 m = 100//[kg] Tallow
16 m1 = 3*403*m/890 // [kg]
17 m2 = 92*m/890
18 printf("(a) \n \n NaOH required = "+string(m1)+" kg \n \n \n \n(b) \n \n amount of glycerine liberated = "+string(m2)+" kg.")
```

Scilab code Exa 4.8 Sulphur Burner

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.8
10 // Page 124
11 printf("Example 4.8, Page 124 \n \n");
12
13 // solution
14
15 n = 100//[kmol] SO3 free gas basis
16 n1 = 16.5 //[kmol] SO2
```

```
17 n2 = 3 //[kmol] O2
18 n3 = 80.5 //[kmol] N2
19 // S + O2 = SO2
20 // S + 3/2 O2 = SO3
21 n4 = (21/79)*80.5 / [kmol] O2 supplied
22 \text{ n5} = \text{n4-n1-n2} // \text{[kmol]} \text{Unaccounted } O2
23 // O2 used in 2nd eq is m5
24 n6 = (2/3)*n5 //[kmol] SO3 produced
25 \text{ n7} = \text{n1+n6} // \text{sulphur burnt}
26 \text{ m7} = \text{n7} * 32 // [\text{kg}]
27 f1 = n6/n7 // fraction of SO3 burnt
28 // O2 req. for complete combustion of S = n7
29 n8 = n4-n7 //[kmol] excess O2
30 p1 = n8*100/n7 // %age of excess air
31 n9 = n4+n3 //[kmol/s] air supplied
32 F1 = n9*.3/n7 // air supply rate
33 v = 22.414*(303.15/273.15)*(101.325/100) // [m^3/kmol]
      sp. vol of air
34 V1 = F1*v //[m^3/s] flow rate of fresh air
35 n10 = n+n7 //[kmol] total gas from burner
36 n11 = n10*.3/m7 // [kmol/s] gas req. for .3 kg/s S
37 \text{ V2} = 220414*1073.15*n11/273.15 // flowrate of burner
       gases
38 printf("(a) \n \n The fraction of S burnt = "+string
      (f1)+" \setminus n \setminus n(b) \setminus n \setminus n percentage of excess air
       over the amount req. for S oxidising to SO2 = "+
      = "+string(V1)+" m^3/s \setminus n \setminus n \setminus d) \n \n volume
      of burner gases = "+string(V2)+" m<sup>3</sup>/s.")
```

Scilab code Exa 4.9 Hydrogenation of Refined Soybean oil

```
1 clear;
2 clc;
3
```

```
4 // Stoichiometry
 5 // Chapter 4
  6 // Material Balances involving Chemical Reaction
  7
  8
  9 // Example 4.9
10 // Page 125
11 printf ("Example 4.9, Page 125 n n);
12
13 // solution
14
15 m = 100 //[kg] soya fatty acid (basis)
16 // use table 4.6
17 M1 = m/.3597 // M(avg) of soya fatty acid
18 //3 \text{ mol of fatty acid} + 1 \text{ mol of glycerol} = 1 \text{ mol}
                   triglyceride + 3 mol of water
19 \text{ M2} = \text{M1}*3+92.09-3*18.02 // Mavg of soyabean oil}
20 q1 = M2*m/(M1*3) // soyabean oil per 100 \text{kg} fatty
                  acid
21 // based on reactions occuring
22 \text{ q2} = .0967 + .1822 * 2 + .0241 * 3 // kmol H2 req. per 100
                  kg soya fatty acid
23 q3 = .5101 // kmol H2 req. per 100 kg soyabean oil
24 \text{ q4} = 11.434 // \text{Nm}^3 / 100 \text{kg soyabean oil}
25 // x = linoleic acid converted to oleic acid
26 // y = oleic acid converted to stearic acid
27 	ext{ q5} = 282.46*6.7/278.43 //
\frac{28}{9} = \frac{100717}{9} = \frac{282.46 \times x}{280.15} = \frac{1.00717}{100} = \frac{100717}{100} = \frac{10
                     linoleic acid
29 / q7 = 284.48*y/282.46 = 1.00715y [kg] stearic acid
                  by oleic acid
30 //98 = 100.097 + .00717x + .00715y total fatty acid
31 //stearic balance: -.00105x + 1.00611y = 10.8142
                           ( i )
        //linoleic balance : 1.0019x + .00019y = 48.4975
                               (ii)
33 // solving (i) and (ii) we get
34 x = 48.5 //kg
```

Scilab code Exa 4.10 Material Balance in Formox Process

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 4
  // Material Balances involving Chemical Reaction
9 // Example 4.10
10 // Page 128
11 printf("Example 4.10, Page 128 n \n");
12
13 // solution
14
15 F1 = 4000 //\text{kg/h} methanol (basis)
16 	ext{ F2} = 	ext{F1/32} // 	ext{kmol/h}
17 F3 = F2/.084 //\text{kmol/h} gaseous mix flowrate
18 F4 = F2-F3 //kmol/h flow of wet air
19 n1 = .011*29/18 // kmol/kmol dry air
```

```
20 F5 = F4/(1+n1) // kmol/h dry air flowrate
21 \ 02 = F5*.21 //kmol/h
22 N2 = F5-02 //kmol/h
23 Mreacted1 = F2*.99 / kmol/h
24 Munreacted1 = F2-Mreacted1 //\text{kmol/h}
25 // reaction (i)
26 Mreacted2 = Mreacted1*.9 //\text{kmol/h}
27 HCHOproduced1 = 111.375
28 \quad 02 \text{consumed1} = 111.375/2
29 \text{ H2Oproduced1} = 111.375
30 // for rxn ii to iv
31 Mconsumed = Mreacted1*.1
32 / rxn (ii)
33 CH30Hreacted1 = Mconsumed*.71
34 \quad 02 \text{consumed2} = 8.786 * 1.5
35 CO2produced = 8.786
36 \text{ H2Oproduced2} = 8.786*2
37 // rxn(iii)
38 \text{ CH3OHreacted2} = 12.375*.08
39 COproduced = .99
40 H2produced = 2*.99
41 // rxn(iv)
42 CH30Hreacted3 = 12.375*.05
43 CH4produced = .619
44 \ 02 \text{produced} = .619/2
45 / (rxn(v))
46 CH30Hreacted4 = 12.375-CH30Hreacted1-CH30Hreacted2-
      CH30Hreacted3
47 DMEproduced = 1.98/2
48 \text{ H2Oproduced3} = 1.98/2
49 \quad 02 = 281.27 - 02consumed1 - 02consumed2 + 02produced
50 H2O = 23.73+H2Oproduced1+H2Oproduced2+H2Oproduced3
51 printf ("Composition of exit gas stream : \n \n CH3OH
       = "+string(Munreacted1)+" \n HCHO = "+string(
      HCHOproduced1) + " \setminus n CO2 = "+string(CO2produced) + "

\ln CO = "+string(COproduced) +" \ln H2 = "+string(

      \text{H2produced})+" \n CH4 = "+string(CH4produced)+" \n
       (CH3)2O = "+string(DMEproduced) +" \setminus n O2 = "+
```

Scilab code Exa 4.11 Pyrites fines roasting

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
9 // Example 4.11
10 // Page 132
11 printf("Example 4.11, Page 132 n \n");
12
13 // solution
15 m = 100 //\text{kg} pyrites (basis)
16 //(a)
17 printf("(a) \n \n")
18 \text{ S1} = 42 //\text{kg}
19 i1 = 58 //kg inerts
20 // 8 moll S = 3 mol O2 in Fe2O3
21 m1 = 3*32*42/8*32 //kg O2 converted to Fe2O3
22 m2 = i1+m1 // mass of SO3 free cinder
23 //2.3 kg S is in 100kg cinder
24 \text{ m3} = 100 - (2.3*80/32)
25 \text{ m4} = (100/\text{m3})*\text{m2}
26 \text{ m5} = \text{m4}*.023 //\text{kg} \text{ S in cinder}
27 p1 = 1.8*100/42
28 printf("percentage of cinder remained in cinder = "+
      string(p1)+". n n n(b) n n")
29 //(b)
```

```
30 m6 = 100 //kmol SO3 free roaster gas (basis)
31 m7 = 7.12 / \text{kmol O2} as SO2
32 \text{ m8} = 10.6 //O2
33 \text{ m9} = 100 - \text{m8} - \text{m7} / \text{N2}
34 m10 = (21/79)*m9 // O2 entering roaster along N2
35 \text{ m}11 = \text{m}7 + \text{m}8 + (3*7.12/8) // accounted } O2
36 m12 = m10-m11 // unaccounted O2
37 \text{ m}13 = (8/15)*\text{m}12 // SO3 \text{ formed}
38 \text{ m}14 = \text{m}13 + \text{m}7 // \text{S burnt}
39 p2 = (m13/m14)*100
40 printf ("percentage of S burnt to form SO3 = "+string"
       (p2)+" n n n(c) n m")
41 // (c)
42 // basis 100kg pyrite
43 \text{ m}15 = 37.81/32 // SO2 \text{ formed}
44 \text{ m} 16 = (m9+m10)*1.181/m7 // air supplied
45 // 4 kg pyrite is roasted
46 m17 = m16*4/100 //\text{kmol/s} total air supplied
47 \text{ v1} = \text{m17} * 24.957
48 printf("volumetric flow rate of air = "+string(v1)+"
        m^3/s \setminus n \setminus n(d) \setminus n \setminus n
49 // (d)
50 \text{ m}18 = (100.455*\text{m}17)/(\text{m}9+\text{m}10) // \text{roaster gases}
51 v2 = m18*66.386
52 printf ("volumetric flow rate of roaster gases = "+
       string(v2)+" m^3/s \ln(n \ln(f) \ln(n))
53 //(f)
54 \text{ m19} = 4.838*10^-2*.98 // SO3 absorbed in absorber
55 // SO3 + H2O = H2SO4
56 \text{ m20} = (\text{m19}*98*24*3600)/(.98*1000) //[t/d]
57 printf ("Amount of 98 percent acid strength produced
      = "+string(m20)+" t/d.")
```

Scilab code Exa 4.12 Burning of Pyrites and ZnS

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.12
10 // Page 136
11 printf("Example 4.12, Page 136 n \n");
12
13 // solution
14
  // basis 100 \,\mathrm{kg} mixed charge = 75 kg pyrite + 25 \,\mathrm{kg}
      ZnS
16 // pyrites
17 \text{ m1} = 75*.92 // [kg]
18 G1 = 75-m1 // gangue
19 // 4 \text{FeS}2 + 1102 = 2 \text{Fe}203 + 8 \text{SO}2
20 // 4 \text{FeS}2 + 1502 = 2 \text{Fe}203 + 8 \text{SO}3
21 / Zn ore
22 \text{ m2} = 25*.68 // \text{ZnS}
23 I1 = 25-m2 // inerts
24 // 2ZnS + 3 O2 = 2 ZnO + 2 SO2
25 I2 = I1+6 // total inerts
26 // new basis : 100kg cinder
27 \text{ m3} = 3.5*.7 // S \text{ as SO3}
28 m4 = 3.5-m3 // S as FeS2
29 m5 = 100-m3-m4 // S free cinder
30 \text{ m6} = (81.4/97.4)*17 // ZnO
31 // \text{FeS2 reacted} = x
32 // (FeS2 in cinder/S free cinder) = (69-x)
      /(28.2 + .667x) = 1.969/91.906
33 // solving this we get
34 \times = 67.43 / kg
35 \text{ m7} = \text{m6} + .667*x + 14 // S \text{ free cinder}
36 m8 = 69-x // FeS2 in cinder
```

Scilab code Exa 4.13 Raising pH with NaOH

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.13
10 // Page 138
11 printf("Example 4.13, Page 138 \n \n");
12
13 // solution
14
15 m1 = 1200*1.2 //[kg] mass of reactants
16 pOH1 = 14-6 //pOH of reactants
17 pOH = 14-9 //pOH of final mass
```

```
18 // ROWs = 1/sigma(Wi/ROWsi)
19 / Ms = mass of .5\% NaOH required
20 / ROWs = density of final solution
21
22 / \text{ROWs} = 1 / \{ ((\text{m1}*10^3*1) / (((\text{m1}*10^3+\text{Ms})*1.2) + (\text{Ms}/((
      m1*10^3+Ms)*1.005)
                                  (i)
23 //balance of OH— ions
24 / (1200*10^{\circ} - 8 + Ms*10^{\circ} - 1.15/(1.005*10^{\circ} - 5) =
      (1200*1.2*10^3 + Ms)*10^-5/ROWs*10^-5
                                                      ( i i )
25 //solving (i) and (ii)
26 \text{ Ms} = 170.21 //g
27 ROWs = 1.2016 //[kg/l]
28 printf ("Mass of 0.5 percnt NaOH required to be added
        to raise the pH = "+string(Ms) + "g.")
```

Scilab code Exa 4.14 Solving eg 10 with Linear Model Method

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.14
10 // Page 140
11 printf ("Example 4.14, Page 140 n \);
12
13 // solution
14
15 // using equations of example 4.10
16
17 // soving 4.10 by linear model method
```

Scilab code Exa 4.15 Electrochemical cell

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.15
10 // Page 143
11 printf("Example 4.15, Page 143 n n);
12
13 // solution
14
15 // \text{ basis} = 1.12 \text{ M63 O2 at NTP}
16 \text{ m1} = 1.12*1000*32/22.4 //[g] O2
17 \text{ m2} = \text{m1/8} // \text{g eq } O2
18 //at \ cathode : Cu+++2e = Cu
```

Scilab code Exa 4.16 Hooker type Diaphragm Cell

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.16
10 // Page 144
11 printf("Example 4.16, Page 144 n n");
12
13 // solution
14
15 // basis : 1day operation
16 // NaCl = Na+ + Cl-
17 / H2O = H+ + OH-
18 / \text{Na} + \text{OH} = \text{NaOH}
19 / H + e = (1/2) H2
20 / Cl - e = (1/2) Cl2
21 E = (15000*3600*24)/96485 // faraday/day
                                                  Total
```

```
energy passed thrrough cell
22 NaOH = (15000*3600*24*40)/(96485*1000) //[kg/day]
                           theoretical NaOH
23 eff = (514.1/NaOH)*100 // current efficiency
24 \text{ Cl2} = (35.5/40)*514.1
25 \text{ H2} = (456.3*2)/(35.5*2)
\frac{26}{40} = \frac{1}{40} = \frac{58.5 \, \text{g}}{100} = \frac{58.5 \, \text{g}}{100} = \frac{1}{100} = \frac{1}{100}
27 \text{ consNaCl} = (58.5/40)*514.1 // NaCl consumed
28 Tliquor = 514.1/.11 / [kg/day] total cell liquor
29 \text{ remNaCl} = 514.1*1.4
30 totalNaCl = consNaCl+remNaCl
31 Fbrine = totalNaCl/.266 // feed rate of brine
32 \text{ consH2O} = (18/40)*514.1
33 lossH2O = Fbrine-Tliquor-consH2O
34 printf("(a) \n Current efficiency of the cell = "
                          produced = "+string(Cl2)+" kg/day \n H2 produced
                         = "+string(H2)+" kg/day n n n(c) n n cs of
                           water = "+string(lossH20)+" kg/day")
```

Scilab code Exa 4.17 Naptha Reforming to Ammonia

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.17
10 // Page 146
11 printf("Example 4.17, Page 146 \n \n");
12
13 // solution
```

```
14
15 / M = mix feed rate, F = fresh feed rate, R =
      recycle stream
16 // using fig 4.3
17 // N2 balance
18 / a = 24.75M/(.25M+7.5M)
                                   ( i )
19 // P = (4.15M + 17.75a)/M
                                     ( i i )
20 // .585M -1.775a + (4.15M+17.75a)/M = 100 (iii)
21 // solving (i,) (ii), (iii)
22 M = 438.589 / [kmol/s]
23 a = (24.75*M)/((.25*M)+7.5) //kmol/s
24 P = (4.15*438.589+17.75*92.662)/M //kmol/s
25 R = M-100 // kmol/s
26 r = R/100 // recycle ratio
27 \text{ NH3} = (.585*M-2.275*a)*17.0305 //kg/s
28 printf("(a) \setminus n \setminus n recycle feed rate = "+string(R)+"
      kmol/s \setminus n \setminus n \setminus n(b) \setminus n \setminus n  purge gas rate = "+
      string(P)+" kmol/s \setminus n \setminus n(c) \setminus n \setminus n mass rate of
       NH3 = "+string(NH3) + "kg/s"
```

Scilab code Exa 4.18 Additional membrane separator in eg 17

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.18
10 // Page 149
11 printf("Example 4.18, Page 149 \n \n");
12
13 // solution
```

```
14
15 // given
16
17 // (.1*M*R1) / (.415M+1.775a) + (.1125a*P) / (.415M + ...)
      1.775a) + 1 = .1M
18 / R1*(.315M-1.225a)/(.415M + 1.775a) = .9M-4a
19 // M = 100 + R1 + (2.25 a*p)/(.415M + 1.775 a)
20 // .1M*P/(.415M + 1.775a) - (.1125a*P)/(.415M1.775a)
21
22 //solving them
23 M = 457.011 // \text{ kmol/s}
24 R1 = 350.771 // \text{kmol/s}
25 P = 10.368 // kmol/s
26 = 96.608 / kmol/s
27 R2 = 2.25*96.608*10.369/(.415*457.011 +
      1.775*96.608) // kmol/s
28 	ext{ F} = 	ext{M} - 	ext{R1} - 	ext{R2}
29 printf("Mixed feed rate = "+string(M)+" kmol/s \setminus
      nRecycle stream = "+string(R1)+" kmol/s \setminus
      nRecovered H2 stream = "+string(R2)+" kmol/s \
      nFresh feed rate = "+string(F)+" kmol/s \nRecycle
       ratio = "+string((R1+R2)/F)+" kmol/kmol of fresh
       feed.")
```

Scilab code Exa 4.19 Partial Demineralisation Plant

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.19
```

```
10 // Page 153
11 printf("Example 4.19, Page 153 \n \n");
12
13 // solution
14
15 m1 = (50/35.5)*312 //[mg/l] Cl2 expressed as
     equivalent CaCO3
16 m2 = (50/48)*43.2 //[mg/1] Sulphates as equivalent
     CaCO3
17 A = m1+m2 // [mg/l as CaCO3] EMA in raw water
18 M1 = 550 // alkalinity of raw water
19 M2 = 50 // alkalinity of blend water
20 //let 100 l of raw water enters both ion exchangers
21 // balancing neutrilasion
22 \times = 100*(M1-M2)/(A+M1) // raw water inlet to H2 ion
     echanger
23 printf(""+string(x)+" percent of total raw water is
     passed through the H ion exchanger.")
```

Scilab code Exa 4.20 Capacity increment by Second Reactor

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 4
6 // Material Balances involving Chemical Reaction
7
8
9 // Example 4.20
10 // Page 155
11 printf("Example 4.20, Page 155 \n \n");
12
13 // solution
```

```
15 m1 = 1488.1 //\text{kmol/h} gas mix to reactor1 (basis)
16 \text{ m2} = \text{m1} * .0625 // \text{CH3OH}
17 m3 = m1-m2 // ambient air flow
18 \text{ m4} = \text{m3}/1.01772 // \text{dry air flow rate}
19 m5 = m3-m4 // moisture
20 m6 = m2*.99 // CH3OH conversion in R1
21 \text{ m7} = \text{m2-m6} // \text{unreacted CH3OH}
22 / rxn i
23 m8 = m7*.9 // CH3OH reacted = HCHO produced = H2O
       produced
24 m9 = m8/2 // O2 consumed
25 m10 = m6-m8 // CH3OH reacted in rxn ii to v
26 //rxn ii
27 m11 = m10*.71 // CH3OH reacted = CO2 produced
28 \text{ m}12 = \text{m}11*1.5 // O2 \text{ consumed}
29 m13 = 2*m11 // H2O produced
30 // rxn iii
31 m14 = m10*.08 // CH3OH reacted = CO produced
32 \text{ m15} = 2*\text{m14} // \text{H2} \text{ produced}
33 // rxn iv
34 m16 = m10*.05 // Ch3OH reacted = CH4 produced
35 \text{ m}17 = \text{m}16/2 // O2 \text{ produced}
36 //rxn v
37 \text{ m18} = \text{m10-m16-m14-m11} // \text{CH3OH reacted}
38 m19 = m18/2 // (CH3)2O = H2O produced
39
40 \text{ m} 20 = 287.87 - \text{m} 9 - \text{m} 12 + \text{m} 17 // O2 \text{ in } R1 \text{ exit stream}
41 \text{ m21} = \text{m5+m8+m13+m19} // \text{H2O in R1}
42 \text{ m} = \text{m7+m8+m11+m14+m15+m16+m19+m20+1082.93+m21}
43 // R2
44 // x kmol/h CH3OH is added b/w reactors
45 / (m7+x)/(m+x) = .084 \text{ solving it}
46 \times = 140.548 / [kmol/h]
47 m22 = x+m7 // CH3OH entering R2
48 \text{ m23} = \text{m22} \cdot .99 / \text{CH3OH reacted}
49 m24 = m22-m23 // CH3OH unreacted
50 //rxn i
51 m25 = m23*.9 // CH3OH reacted = HCHO produced = H2O
```

```
produced
52 \text{ m} 26 = \text{m} 25/2 // O2 \text{ consumed}
53 m27 = m23 - m25 // CH3OH reacted in rxn ii to v
54 // rxn ii
55 m28 = m27*.71 // CH3OH reacted = CO2 produced
56 \text{ m29} = \text{m28}*1.5 // O2 \text{ consumed}
57 \text{ m30} = \text{m28*2} // \text{H2O produced}
58 //rxn iii
59 m31 = m27*.08 // CH3OH reacted = CO produced
60 \text{ m32} = \text{m31*2} // \text{H2} \text{ produced}
61 // rxn iv
62 \text{ m33} = \text{m27} * .05 \text{ // Ch3OH reacted} = \text{CH4 produced}
63 \text{ m}34 = \text{m}33/2 // O2 \text{ produced}
64 // rxn v
65 m35 = m27-m28-m31-m33 // CH3OH reacted
66 \text{ m36} = \text{m35/2} // (\text{CH3}) 2\text{O} = \text{H2O produced}
67
68 m37 = m20 - m26-m29+m34 // O2 in R2 exit stream
69 \text{ m} 38 = \text{m} 21 + \text{m} 25 + \text{m} 36 // \text{H} 20 \text{ in } \text{R} 2
70 \text{ m}39 = 92.07 + \text{m}25 // \text{HCHO in } \text{R}2
71 \text{ m40} = \text{m24+m39+m28+m31+m32+m33+m36+m37+m38+1082.93}
72
73 m41 = m39*30 // \text{kg/h} HCHO produced
74 \text{ m42} = \text{m41/.37} // \text{bottom sol floe rate}
75 c = (m42-9030.4)*100/9030.4 // increase in capacity
76 printf("Increase in capacity = "+string(c)+" percent
        . ")
```

Scilab code Exa 4.21 Blast Furnace Calculations

```
1 clear;
2 clc;
3 
4 // Stoichiometry
5 // Chapter 4
```

```
6 // Material Balances involving Chemical Reaction
8
9 // Example 4.21
10 // Page 159
11 printf("Example 4.21, Page 159 n n);
12
13 // solution
14
15 // basis 1 tonne of pig iron
16 \text{ coke} = 1000 // \text{kg}
17 flux = 400 / kg
18 Fe1 = 1000*.95 // Fe in pig iron
19 Fe2 = (112/160)*.8 // Fe available per kg of ore
20 ore = Fe1/Fe2 // kg
21 Si = .014*1000 //kg //Si in pig iron
22 si1 = (60/28)*14 // silica present in pig iron
23 si2 = ore*.12 // silica in ore
24 si3 = .1*coke // silica in coke
25 \text{ si4} = \text{si2+si3-si1} // \text{silica in slag}
26 alumina = ore*.08 // Al2O3 in ore = Al2O3 in slag
27 \text{ CaO} = \text{flux}*(56/100)
28 \text{ slag} = \text{si4+alumina+Ca0}
29 printf("(a) \n \n Mass of slag made = "+string(slag)
      +" kg. n n n(b) n mass of ore required = "
      +string(ore)+" kg. \n \n \n \c) \n \n \composition
      "+string(alumina)+" kg \n CaO = "+string(CaO)+"
      kg. \setminus n \setminus n \setminus n(d) \setminus n \setminus n")
30 C = .9*coke+(12/100)*flux-36 // total C available
31 // CO:CO2 = 2:1
32 C1 = C/3 // C converted to CO2
33 C2 = 2*C/3 // C converted to CO
34 \ 021 = C1*(32/12)+C2*(16/12) // O2 required for CO
      and CO<sub>2</sub> formation
35 \ 022 = (32/28)*Si // O2 from SiO2
36 \ \text{O23} = \text{ore*(.8*48/160)} \ // \ \text{O2} \ \text{from} \ \text{Fe}2\text{O3}
37 \ 024 = flux*(32/100) // O2 from CaCO3
```

```
38  025 = 021-022-023-024 //kg O2 to be supplied

39  026 = 025/32 //kmol

40  air = 026/.21 //kmol

41  V = air*22.414 //m^3

42  printf(" Volume of air to be supplied = "+string(V)+" m^3.")
```

Chapter 5

Energy Balances

Scilab code Exa 5.1 Pumping of water

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.1
10 // Page 186
11 printf("Example 5.1, Page 186 n \n");
12
13 // solution
14
15 // basis pumping of 1 l/s of water
16 \text{ Hadd} = 52 // \text{ kW}
17 Hlost = 21 // kW
18 fi = Hadd - Hlost // kW
19 p1 = 101325 // Pa
20 p2 = p1
21 \ Z1 = -50 \ // m
```

```
22 Z2 = 10  // m
23 g = 9.80665  // m/s sq
24 gc = 1  // kg.m/(N.s sq)
25 row = 1  // kg/l
26 W = 1.5*.55  // kW
27  // energy balance b/w A and B
28  // dE = E2-E1 = W + Q + (Z1-Z2)*(g/gc)*qm
29 dE = 31.237  // kW
30 printf("Increase in internal energy between the storage tank and the bottom of the well = "+ string(dE)+" kW.")
```

Scilab code Exa 5.2 Heating of CH4

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.2
10 // Page 197
11 printf ("Example 5.2, Page 197 n \n");
12
13 // solution
14
15 // using table 5.1
16 // basis 1 kmol of methane
17 \quad T1 = 303.15
                // K
18 T2 = 523.15 // K
19 // using eq 5.17
20 H = 19.2494*(T2-T1) + 52.1135*10^{-3}*(T2^{2}-T1^{2})/2 +
      11.973*10^{-}6*(T2^{3}-T1^{3})/3 - 11.3173*(T2^{4}-T1^{4})
```

```
*10^-9/4 // kJ 21 printf(" Heat added = "+string(H)+" kJ/kmol methane. ")
```

Scilab code Exa 5.3 Calculation of heat added

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.3
10 // Page 198
11 printf("Example 5.3, Page 198 n \n");
12
13 // solution
14
15 // basis 1 kmol methane at 25 bar
                // bar
16 \text{ Pc} = 46.04
17 \text{ Tc} = 190.5
                // K
18 \text{ Pr} = 25/\text{Pc}
19 // H-Ho = intgr(from 303.15 to 523.15) \{CmpR dT\}
20 // solving it by simpson's rule
21 HE = 255.2 // kJ/kmol
22 \text{ H} = 9175.1 + \text{HE}
23 printf(" Heat added = "+string(H)+" kJ/kmol of
      methane.")
```

Scilab code Exa 5.4 Heating of Toulene

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
9 // Example 5.4
10 // Page 206
11 printf("Example 5.4, Page 206 n \n");
12
13 // solution
14
15 // using table 5.3
16 // .25 kg/s toulene heated from 290.15K to 350.15K
17 \text{ qm} = .25/92 // \text{kmol/s}
18 // reference 7
19 fi = 2.717*10^{-3}[1.8083*(350.15-290.15) +
      812.223*10^{-3}*(350.15^{2}-290.15^{2})/2 -
      1512.67*10^{-}6*(350.15^{3}-290.15^{3})/3 +
      1630.01*10^-9*(350.15^4-290.15^4)/4]
20 printf(" Heat required to be added to toulene = "+
      string(fi)+" kW.")
```

Scilab code Exa 5.5 Aq caustic soda heating

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
```

```
9  // Example 5.5
10  // Page 206
11  printf("Example 5.5, Page 206 \n \n");
12
13  // solution
14
15  // basis 1kg of 20% NaOH sol
16  // referring to fig 5.4
17  C11 = 3.56  // kJ/kg.K at 280.15K
18  C12 = 3.71  // kJ/kg.K at 360.15K
19  C1m = (C11+C12)/2
20  H = 1*C1m*(360.15-280.15)  // kJ
21  printf(" Heat required to be added = "+string(H)+"kJ
.")
```

Scilab code Exa 5.6 Heating Chlorinated diphenyl

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.6
10 // Page 207
11 printf("Example 5.6, Page 207 n \n");
12
13 // solution
14
15 // basis 1kg Diphyl A-30
16 Q = .7511*(553.15-313.15) +
      1.465*10^{-3}*(553.15^{2}-313.15^{2})/2 // kJ/kg
17 fi = Q*4000 // kJ/h for mass flowrate 4000 \text{ kg/h}
```

Scilab code Exa 5.7 Roasting of pyrites fine

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.7
10 // Page 208
11 printf("Example 5.7, Page 208 n \n");
12
13 // solution
14
15 \text{ T1} = 298.15 // \text{ K}
16 	ext{ T2} = 775.15 	ext{ //K}
17 // using eq 5.17
18 \ Q = 28.839*(T2-T1)+2.0395*10^-3*(T2^2-T1^2)/2 +
      6.9907*10^{-}6*(T2^{3}-T1^{3})/3 - 3.2304*10^{-}9*(T2^{4}-
      T1^4)/4 // kJ/kmol
19 printf(" Heat content of 1 kmol of gas mixture at
      298K = "+string(Q)+" kJ/kmol.")
```

Scilab code Exa 5.8 Anniline and water mix subcooled

```
1 clear;
    2 clc;
  4 // Stoichiometry
  5 // Chapter 5
    6 // Energy Balances
   8
  9 // Example 5.8
10 // Page 210
11 printf("Example 5.8, Page 210 n \n");
12
13 // solution
14
15 // basis 8000 kg/h mixture is to be cooled
                                                                                                                              // kg/h
16 \text{ qn1m} = .118*8000
17 qn1 = qn1m/93.1242 \frac{1}{k} \frac{1}{k
                                                                                                                                  // kg/h
18 \quad qn2m = 8000 - qn1m
19 \quad qn2 = qn2m/18
                                                                                                                                          // kmol/h
20 \text{ T1} = 373.15
                                                                                                 //K
21 \quad T2 = 313.15
                                                                                                 //K
22 fi = qn1*[206.27*(T1-T2)-211.5065*10^-3*(T1^2-T2^2)]
                                /2+564.2902*10^{-}6*(T1^{3}-T2^{3})/3 + qn2*[50.845*(
                                T1-T2)+213.08*10^-3*(T1^2-T2^2)/2-631.398*10^-6*(
                                T1^3-T2^3)/3+648.746*10^-9*(T1^4-T2^4)/4]
23 printf(" Heat removal rate of subcooling zone of the
                                      condenser = "+string(fi)+" kJ/h.")
```

Scilab code Exa 5.9 Vapor Pressure calculations

```
1 clear;
2 clc;
3
4 // Stoichiometry
```

```
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.9
10 // Page 220
11 printf("Example 5.9, Page 220 n \n");
12
13 // solution
14
15 // (a)
16 T = 305.15 / K
17 \text{ Pv1} = 10^{(4.0026 - (1171.530/(305.15 - 48.784)))} // \text{bar}
18 // (b)
19 T = 395.15
20 \text{ Pv2} = 10^{(3.559-(643.748/(395.15-198.043)))}
21 printf(" (a) n V.P. of n-hexane at 305.15K = "+
      string(Pv1)+" bar. \n \n \n \n \N (b) \n \N V.P. of
      water at 395.15K = "+string(Pv2)+" bar.")
```

Scilab code Exa 5.10 Calculations on O zylene

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.10
10 // Page 225
11 printf("Example 5.10, Page 225 \n \n");
12
13 // solution
```

```
14
15 // (a)
16 \text{ Pc} = 3732 \text{ // kPa}
17 Tc = 630.3 // K
18 Tb = 417.6
               //K
19 	ext{ TBr} = 	ext{Tb/Tc}
20 lambdav = 8.314472*417.6*(1.092*(log(3732)-5.6182)
      /(.930-.6625))
21 // (b)
22 T1 = 298.15
23 \ lambdav1 = 36240*[(630.3-298.15)/(630.3-417.6)]^{.38}
24 printf(" (a) \n \n Latent heat of vaporization at Tb
       using Riedel eq is "+string(lambdav)+" kJ/kmol.
      \n \n \n (b) \n \n Latent heat of vaporization
      at 298.15 K using Watson eq is "+string(lambdav1)
      +" kJ/kmol.")
```

Scilab code Exa 5.11 latent heat of vaporization of ethanol

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.11
10 // Page 225
11 printf("Example 5.11, Page 225 \n \n");
12
13 // solution
14
15 // (a)
16 Pc = 61.37 // bar
```

```
17 Tc = 514 / K
18 Tb = 351.4
19 P = 1 // atm
20 \text{ TBr} = \text{Tb/Tc}
21 // Riedel eq
22 \quad lambdav1 = 8.314472*Tb*1.092*(log(6137)-5.6182)
      /(.930-TBr)
23 // NIST eq
24 \ lambdav2 = 50430*exp(-(-.4475*TBr))*(1-TBr)^.4989
25 // (b)
26 \text{ T1} = 298.15
27 \text{ TBr1} = \text{T1/Tc}
28 // Watson eq
29 \ lambdav21 = 38563*[(514-298.15)/(514-351.4)]^.38
30 // NIST eq
31 \quad lambdav22 = 50430*exp(-(-.4475*TBr1))*(1-TBr1)^.4969
32 printf(" (a) \n \n Latent heat of vaporization at Tb
       using \n Riedel eq is "+string(lambdav1)+" kJ/
      kmol \n NIST eq is "+string(lambdav2)+" kJ/kmol \
      n \n \n (b) \n \n Latent heat of vaporization at
      298.15 K using \n Watson eq is "+string(lambdav21
      )+" kJ/kmol \ n \ NIST \ eq \ is "+string(lambdav22)+"
      kJ/kmol")
```

Scilab code Exa 5.12 Saturation P of steam

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.12
```

```
10  // Page 227
11  printf("Example 5.12, Page 227 \n \n");
12
13  // solution
14
15  // using Appendix IV.2
16  Ps1 = 75
17  Ps2 = 80
18  T1 = 563.65
19  T2 = 568.12
20  T = 565.15
21  Ps = 75*exp((T2*(T-T1)*log(80/75)/(T*(T2-T1))))
22  printf(" Saturation Pressure of steam at 565.15K is "+string(Ps)+" bar.")
```

Scilab code Exa 5.13 Bubble and Dew pt calculations

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.13
10 // Page 236
11 printf("Example 5.13, Page 236 n \n");
12
13 // solution
14
15 // basis 1 kmol equimolar mix
16 npent = .5 // \text{kmol}
17 nhex = .5 // kmol
18 P = 101.325 // kPa
```

Scilab code Exa 5.14 Hot air drying machine

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
9 // Example 5.14
10 // Page 237
11 printf("Example 5.14, Page 237 n \n");
12
13 // solution
14
15 // basis 1000 kg/h of condensate at the saturation
     temperature corresponding to 8 bar a
16 // using Appendix IV.2
17 H = 720.94 // kJ/kg
18 Hm = 419.06 // kJ/kg
19 x = poly(0, 'x')
20 condensate = 1000-x
21 Hcondensate1 = 1000*H
```

Scilab code Exa 5.15 Flow of saturated vapors of R134

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.15
10 // Page 238
11 printf("Example 5.15, Page 238 n \n");
12
13 // solution
14
15 \text{ qv1} = 50 // l/s
16 qm = qv1*1.08 // kg/s
17 fi = qm*3.08*(263.15-258.15) // kW
18 lv = 384.19-168.7 // kJ/kg
19 \text{ qm2} = \text{fi/lv}
20 \text{ H} = 256.35 // kJ/kg
21 x = poly(0, 'x')
22 p = H*(qm2+x) - 168.7*qm2-x*384.19
23 = qm2 + roots(p)
24 printf(" Flow of vapor from he chiller = "+string(a)
      +" kg/s.")
```

Scilab code Exa 5.16 Liquifaction of Cl2

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.16
10 // Page 238
11 printf("Example 5.16, Page 238 n \n");
12
13 // solution
14
15 // basis liquifaction capacity = 0.116 \text{ kg/s}
16 p1 = 101 // kPa
17 \text{ Ts1} = 239.15
18 \text{ lv1} = 288.13 \text{ // kJ/kg}
19 p2 = 530 // kPa
20 \text{ Ts2} = 290.75 // \text{ K}
21 \text{ lv2} = 252.93 \text{ // kJ/kg}
22 // referring to table 5.3 and using eq 5.21
23 \text{ H1} = -39.246*(Ts2-Ts1)+1401.223*10^-3*(Ts2^2-Ts1^2)
      /2-6047.226*10^-6*(Ts2^3-Ts1^3)/3+8591.4*10^-9*(
      Ts2^4-Ts1^4)/4 // kJ/kmol
24 \quad T3 = 313.15
25 \text{ H2} = [28.5463*(T3-Ts1)+23.8795*10^-3*(T3^2-Ts1^2)]
      /2-21.3631*10^{-}6*(T3^{3}-Ts1^{3})/3+6.4726*10^{-}9*(T3^{3}-Ts1^{3})
      ^4-Ts1^4)/4]/70.903 // kJ/kg
26 \text{ fi2} = .116*H2
27 Cl2evp = fi2/lv1 // kg/s
28 \text{ Cl2recy} = \text{Cl2evp}/(1-.185)
```

```
29 R = Cl2recy/.116 // kg/kg fresh feed
30 / T4/T1 = (p2/p1)^{(gamma-1)/gamma}
31 \text{ gm} = 1.355
32 p22 = 326.3
33 p21 = 101
34 T4 = Ts1*(p2/p1)^[(gm-1)/gm]
35 	ext{ T5} = 313.15
36 \text{ fi3} = 1.88*10^{-3}*(343.1+91.6-26.2+2.5) // kW
37 Fwater1 = fi3/(8*4.1868) // kg/s
38 // similarly
39 \quad T6 = 379.9
40 \text{ fi4} = 1.88*10^{-3}*[28.5463*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.8795*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23.879*10^{-3}*(T6-T5)+23
                                ^2-T5^2)/2-21.3631*10^-6*(T6^3-T5^3)
                                /3+6.4726*10^-9*(T6^4-T5^4)/4] // kW
41 Fwater2 = fi4/(8*4.1868) // kg/s
42 \text{ Wreq} = \text{Fwater1} + \text{Fwater2}
43 fi5 = 1.88*10^{-3}*[28.5463*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.8795*10^{-3}*(T5-Ts2)+23.879*10^{-3}*(T5-Ts2)+23.879*10^{-3}*(T5-Ts2)+23.879*10^{-3}*(T5-Ts2)+23.879*
                                ^2-Ts2^2)/2-21.3631*10^-6*(T5^3-Ts2^3)
                               /3+6.4726*10<sup>-9</sup>*(T5<sup>4</sup>-Ts2<sup>4</sup>)/4] +.1333*252.93 //
                             kW
Cl2/kg fresh feed \n \n \n (b) \n \n Cooling
                                water required at \n interface = "+string(Fwater1
                               )+" kg/s \setminus n after cooler = "+string(Wreq)+" kg/s
                              \n \n \n (c) \n Refrigiration load of chiller
                              = "+string(fi5)+" kW.")
```

Scilab code Exa 5.17 Melting of Tin

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
```

```
7
9 // Example 5.17
10 // Page 242
11 printf("Example 5.17, Page 242 n \n");
12
13 // solution
14
15 // basis 100 kg of tin
16 T1 = 303.15
17 T2 = 505.15
18 n = 100/118.7 // kmol
19 // Q1 = n*[intgr from T1 to T2 (Cms dT)]
20 \ Q1 = 4973.3 \ // \ kJ
21 lf = 7201
              // kJ
22 \quad Q2 = n*1f
23 \ Q = Q1+Q2
24 \text{ lv} = 278 // \text{kJ/kg}
25 \text{ vp} = Q/lv // kg
26 printf(" Quantity of eutectic mixture condensed = "+
      string(vp)+" kg per 100 kg of tin melted at its
      melting point.")
```

Scilab code Exa 5.18 steam fluctuation calculations

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.18
10 // Page 243
```

```
11 printf("Example 5.18, Page 243 n \n");
12
13 // solution
14
15 \text{ Ts1} = (438.2+436)/2
16 Ta = 300
17 \text{ fil} = .045*(Ts1-Ta)*3600
18 theta1 = 307293/fi1 //h
19 \text{ Ts2} = (436+434)/2
20 \text{ fi2} = .045*(Ts2-Ta)*3600
21 \text{ theta2} = 302415/fi2
22 \text{ Ts3} = (434+432.1)/2
23 \text{ fi3} = .045*(Ts3-Ta)*3600
24 \text{ theta3} = 313859/fi3
25 theta = theta1+theta2+theta3
26 printf(" total time required = "+string(theta)+" hrs
      . ")
```

Scilab code Exa 5.19 Manufacture of dry ice

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.19
10 // Page 245
11 printf("Example 5.19, Page 245 \n \n");
12
13 // solution
14
15 H1 = 482.9 // kJ/kg
```

```
16 \text{ H2} = 273.4
17 \text{ fil} = 100*(H1-H2) // kJ/h
18 \text{ T1} = 313.15
19 T2 = 403.15
20 \text{ fill} = 21.3655*(T2-T1)+64.2841*10^-3*(T2^2-T1^2)
      /2-41.0506*10^-6*(T2^3-T1^3)/3+9.7999*10^-9*(T2
      ^4-T1^4)/4 // kJ/h
21 // at 20 MPa
22 h1 = 211.1
23 Ts = 277.6
24 \text{ H11} = 427.8
25 x = poly(0, 'x')
26 p = x*h1+(100-x)*H11-100*H2
27 a = roots(p)
28 fi2 = (100-a)*(H11-h1) // kJ/h
29 \text{ h2} = -148.39
30 \text{ H3} = 422.61
31 y = poly(0, 'y')
32 p1 = 100*176.18-(100-y)*H3+h2*y
33 b = roots(p1)
34 \text{ fi3} = 100*(h1-176.8)
35 \text{ H} = \text{fi3} + 24021
36 \text{ H4} = \text{H/}(100-43.16)
37 // from ref 23
38 T = 262.15
39 printf(" (a) \n Yield of dry ice = "+string(b)+"
      string(a)+". \n \n \n (c) \n \n Temp of vented
      gas = "+string(T)+" K.")
```

Scilab code Exa 5.20 Steam produced in S burner

```
1 clear;
2 clc;
3
```

```
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.20
10 // Page 247
11 printf("Example 5.20, Page 247 n \);
12
13 // solution
14
15 // basis 200 kg/h of Sulphur firing
16 	ext{ F} = 200/32 	ext{ // kmol/h}
17 	 02req = 6.25*1.1
18 \text{ airin} = 02\text{req}/.21
19 \text{ N2in} = airin-02req}
20 \text{ T1} = 1144.15
21 \quad T2 = 463.15
22 fi = 788852.2 // kJ/h
23 \text{ H} = 15*4.1868+1945.2
24 \text{ qm} = \text{fi} * .9/2008 // \text{kg/h}
25 printf(" Amount of steam produced = "+string(qm)+"
      kg/h.")
```

Scilab code Exa 5.21 Equimoar pentane and hexane mix

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.21
```

```
10 // Page 248
11 printf("Example 5.21, Page 248 n n");
12
13 // solution
14
15 // enthalpy at Tbb
16 \text{ Tbb} = 321.6
17 T1 = 298.15
18 \text{ H1} = 65.4961*(\text{Tbb-T1})+628.628*10^{-3}*(\text{Tbb^2-T1^2})
      /2-1898.8*10^{-}6*(Tbb^{3}-T1^{3})/3+3186.51*10^{-}9*(Tbb
      ^4-T1^4)/4 // kJ/kmol
19 \text{ H2} = 31.421*(\text{Tbb-T1})+976.058*10^-3*(\text{Tbb^2-T1^2})
      /2-2353.68*10^-6*(Tbb^3-T1^3)/3+3092.73*10^-9*(
      Tbb^4-T1^4)/4 // kJ/kmol
20 Hsol = (H1+H2)/2 // kJ/kmol
21 // enthalpy at Tdp
22 \text{ lv1} = 25790*((469.7-329.9)/(469.7-309.2))^{.38}
23 \text{ lv2} = 28850*((507.6-329.9)/(507.6-341.9))^.38
24 \text{ Tdp} = 329.9
25 H21ig = 65.4961*(Tdp-T1)+628.628*10^-3*(Tdp^2-T1^2)
      /2-1898.8*10^-6*(Tdp^3-T1^3)/3+3186.51*10^-9*(Tdp
      ^4-T1^4)/4 + lv1 // kJ/kmol
26 \text{ H}22ig = 31.421*(Tdp-T1)+976.058*10^-3*(Tdp^2-T1^2)
      /2-2353.68*10^-6*(Tdp^3-T1^3)/3+3092.73*10^-9*(
      Tdp^4-T1^4)/4 + lv2 // kJ/kmol
27 \text{ Hmixig} = (H21ig+H22ig)/2
28 printf(" (a) n = "+string(Hsol) + "kJ/kmol n
      n \setminus n (b) \setminus n \setminus n H = "+string(Hmixig) + "kJ/kmol")
```

Scilab code Exa 5.22 Flashing of saturated liq mix

```
1 clear;
2 clc;
3
4 // Stoichiometry
```

```
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.22
10 // Page 252
11 printf("Example 5.22, Page 252 \n \n");
12
13 // solution
14
15 H1 = 23549 //kJ/kmol
16 H2 = 16325
17 H3 = 28332
18 H4 = .4*H2+.6*H3
19 printf("Enthalpy of vapor-liquid mixture after flashing = "+string(H4)+" kJ/mol.")
```

Scilab code Exa 5.23 H2 recovery from Refinery off gases

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.23
10 // Page 253
11 printf("Example 5.23, Page 253 \n \n");
12
13 // solution
14
15 // basis feed gas = 12000 Nm^3 = 535.4 kmol/h
16 T1 = 147.65 // K
```

Scilab code Exa 5.24 Refrigiration calculations

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
9 // Example 5.24
10 // Page 256
11 printf("Example 5.24, Page 256 n \n");
12
13 // solution
14
15 // \text{ fil} = \text{integr (from } 304.15 \text{ to } 313.15)
      \{11831.6+24997.4*10T^{-3}-5979.8*10^{-6}T
      ^2 - 31.7*10^ - 9T3 dt
16 fi1 = 170787.7 // kJ/h
17 \text{ fi2} = 535.4*12086 -
      [344.36*8743.2+168.97*18036+22.07*15892]
                                                       // kJ/h
18 printf(" (a) \n Refrigiration requirement = "+
      string(fi1)+" kJ/h \setminus n \setminus n \setminus n \setminus n
      Refrigiration requirement based on real
      enthalpies = "+string(fi2)+" kJ/h.")
```

Scilab code Exa 5.25 Chlorination of benzene

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
9 // Example 5.25
10 // Page 257
11 printf("Example 5.25, Page 257 n n);
12
13 // solution
14
15 // basis 100 kmol/h of benzene feed rate
16 \text{ Cl2} = .4*100
17 \text{ HClp} = 40
18 Benzenecon = 37
19 \text{ MCBp} = 100*.37*.9189
20 DCBp = Benzenecon-MCBp
21 unreactBenzene = 100-Benzenecon
22 Nt = HClp + MCBp + DCBp + unreactBenzene
23 // using eq xi = Ni/(L(1-K1)+NtKi) and sigma
      xi = 1
              // kmol/h
24 L = 89.669
25 V = Nt - L
26 printf(" Liquid product stream = "+string(L)+" kmol/
     h \n Vapor product stream = "+string(V)+" kmol/h"
     )
```

Scilab code Exa 5.26 Heat of formation of ethylene

```
1 clear;
2 clc;
3
  // Stoichiometry
  // Chapter 5
  // Energy Balances
8
9 // Example 5.26
10 // Page 260
11 printf("Example 5.26, Page 260 n \n");
12
13 // solution
14
15 // 2C + 2O2 = 2CO2
                                          A
16 // 2H2 + O2 = 2H2O
                                          В
17 // C2H4 + 3O2 = 2CO2 + 2H2O
                                          \mathbf{C}
18 // A+B-C gives
19 // 2C(g) + 2H2 = C2H4(g)
                                         D
20 \text{ H} = -2*393.51-2*241.82+1323.1} // kJ/mol
21 printf(" Heat of formation of Ethylene is "+string(H
      )+" kJ/mol.")
```

Scilab code Exa 5.27 Heat of combustion of ethyl mercaptan

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
```

Scilab code Exa 5.28 Std heat of formation of gaseous di ethyl ether

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
  // Energy Balances
7
9 // Example 5.28
10 // Page 261
11 printf("Example 5.28, Page 261 n n");
12
13 // solution
14
15 \text{ lv1} = 26694
                  // kj/kmol
16 \text{ Tc} = 466.74
17 \text{ lv2} = \text{lv1}*((\text{Tc}-298.15)/(\text{Tc}-307.7))^{.38/1000} // \text{kJ/}
      mol
18 \text{ Hf} = -252
                  // kJ/mol
19 Hf1 = Hf-lv2 // kJ/kmol
20 printf("Heat of formation of liquid di ethyl ether =
       "+string(Hf1)+" kJ/mol.")
```

Scilab code Exa 5.29 Heat of formation of motor spirit

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.29
10 // Page 261
11 printf("Example 5.29, Page 261 n n);
12
13 // solution
14
15 // basis 1 kg motor spirit
16 G = 141.5/(131.5+64)
17 // r = C/H
18 r = (74+15*G)/(26-15*G)
19 C = r/6.605 // C content of motor spirit
20 \text{ H2} = 1-C
21 O2req = C+H2
22 Hf = 44050-27829-18306 // kJ/kg
23 printf(" Heat of formation of motor spirit = "+
      string (Hf) + ^{\circ} kJ/kg.^{\circ})
```

Scilab code Exa 5.30 Mean heat capacity

```
1 clear;
2 clc;
```

```
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.30
10 // Page 267
11 printf("Example 5.30, Page 267 n \n");
12
13 // solution
14
15 // basis 1 kmol of styrene
16 \text{ dH} = 241749 - 189398 // kJ/mol
17 Cmpn = dH/(600-298.15) // kJ/kmol K
18 printf(" Mean heat capacity between 600K and 298.15
     K is "+string(Cmpn)+" kJ/kmol K.")
```

Scilab code Exa 5.31 Heat of reaction

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.31
10 // Page 269
11 printf("Example 5.31, Page 269 \n \n");
12
13 // solution
14
15 // basis 1 mol of SiO2 reacted
```

```
16 Hf = [-2879+3*(-296.81)+3*0/2]-[3*(-1432.7)
+1*(-903.5)] // kJ/mol SiO2
17 printf(" Heat of reaction = "+string(Hf)+" kJ/mol SiO2.")
```

Scilab code Exa 5.32 Std heat of reaction

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
9 // Example 5.32
10 // Page 269
11 printf("Example 5.32, Page 269 n \n");
12
13 // solution
14
15 // basis 100 kg of 2% ammonia solution
16 \text{ NH3} = 2 // \text{kg}
17 \text{ H2O} = 98 // \text{kg}
18 Hr = -361.2-(-45.94-285.83) // kJ/mol NH3 dissolved
19 Hd = -(Hr*2*1000/17.0305) // kJ/100 kg sol.
20 printf(" heat of reaction = "+string(Hd)+" kJ/100 kg
       solution.")
```

Scilab code Exa 5.33 Burning of SO2

```
1 clear;
2 clc;
```

```
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.33
10 // Page 272
11 printf("Example 5.33, Page 272 n \n");
12
13 // solution
14
15 // basis 1 kmol of SO2 reacted
16 \quad a = 22.036-24.771-.5*(26.026)
17 b = (121.624-62.948-.5*11.755)
18 c = (-91.876+44.258-.5*(-2.343))
19 \quad d = (24.369 - 11.122 - .5*(-.562))
20 \text{ Hr} = -395720 + 296810 // kJ/kmol
21 Hro = Hr-a*298.15-b*10^-3*298.15^2/2-c
      *10^-6*298.15^3/3-d*10^-9*298.15^4/4
22 T = 778.15
23 Hrt = -\text{Hro}-15.748*T+26.4*10^-3*T^2-15.48*10^-6*T
      ^3+3.382*10^-9*T^4
24 printf(" Heat of reaction at 775K is "+string(Hrt)+"
      kJ/kmol.")
```

Scilab code Exa 5.34 Esterification of acetic acid

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
```

```
9 // Example 5.34
10 // Page 272
11 printf("Example 5.34, Page 272 n \n");
12
13 // solution
14
15 Hr = -480-285.83+277.2+484.2 // kJ/mol
16 Hrt1 = Hr*1000 + [146.89+75.76-119.55-129.70]*75
      kJ/kmol
17 a = 4.2905+50.845-100.92-155.48
18 b = 934.378+213.08+111.8386+326.5951
19 c = -2640 - 631.398 - 498.54 - 744.199
20 d = 3342.58+648.746
21 Hro = Hr*1000+a*(-298.15)+b*10^-3*(-298.15^2)/2+c
     *10^{-}6*(-298.15^{3})/3+d*10^{-}9*(-298.15^{4})/4
22 T = 373.15
23 Hrt = Hro+a*T+792.949*10^{-3}*T^{2}-1504.712*10^{-6}*T
      ^3+997.832*10^-9*T^4
24 printf(" Heat of reaction at 373 K is "+string(Hrt)+
     " kJ/kmol reactant.")
```

Scilab code Exa 5.35 Heat transfer in intercoolers

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.35
10 // Page 273
11 printf("Example 5.35, Page 273 \n \n");
```

```
12
13 // solution
14
15 T2 = 800
16 \text{ T1} = 298.15
17 \text{ fil} = 3614.577*(T2-T1)+305.561*10^-3*(T2^2-T2^2)
      /2+836.881*10^-6*(T2^3-T1^3)/3-393.707*10^-9*(T2
      ^4-T1^4)/4 // kW
18 T3 = 875
19 fi2 = 3480.737*(T3-T1)+754.347*10^-3*(T3^2-T2^2)
      /2+442.159*10^-6*(T3^3-T1^3)/3-278.735*10^-9*(T3
      ^4-T1^4)/4 // kW
20 Hr = -98910 // kJ/kmol SO2 reacted
                                           by eg 5.33
21 \text{ fi3} = (8.8511 - .351) * Hr/3600
22 	 dH = fi2/3600+fi3-fi1/3600
23 printf(" Net enthalpy change = "+string(dH)+" kW.")
```

Scilab code Exa 5.36 Enthalpy balance in the reactor

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.36
10 // Page 275
11 printf("Example 5.36, Page 275 \n \n");
12
13 // solution
14
15 // basis 100 kmol outgoing gas mixture from scrubber
16 moistin = 3127.7*.015/18 // kmol
```

```
17 waterin = 40.2+moistin // kmol
18 // using tables 5.29 and 5.30
19 Hr = -27002658-(-26853359)
20 Hr1 = Hr/246.4493 // kJ/kmol total reactants
21 printf(" Heat of reaction = "+string(Hr1)+" kJ/kmol total reactants.")
```

Scilab code Exa 5.37 Calculation of circulation rate

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
9 // Example 5.37
10 // Page 276
11 printf("Example 5.37, Page 276 n \n");
12
13 // solution
14
15 fi3 = 15505407 // kJ/h
16 lv = 296.2 // from table 5.6
17 Ht = 17131551 // kJ/h
18 r = Ht/lv // kg/h
19 printf(" Downtherm circulation rate = "+string(r)+"
     kg/h.")
```

Scilab code Exa 5.38 Loop reactor for EDC manufacture

```
1 clear;
```

```
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.38
10 // Page 279
11 printf("Example 5.38, Page 279 n \n");
12
13 // solution
14
15 F = 100 // \text{kmol/h} feed rate of ethylene
16 \text{ Econ} = .99 * F
17 \text{ Econ1} = \text{Econ} * .998
18 \quad \text{Econ2} = \text{Econ-Econ1}
19 \quad \text{Cl2con} = \text{Econ1} + 2 \times \text{Econ2}
20 \text{ Cl2in} = F*1.1
21 Cl2s3 = Cl2in-Cl2con
22 HCls3 = Econ2
23 TCEp = Econ2
24 \text{ EDCp} = \text{Econ1}
25 \text{ nC2H4} = 1
26 T = 328.15
27 \text{ pv1} = \exp(4.58518-1521.789/(T-24.67)) // bar
28 pv2 = \exp(4.06974-1310.297/(T-64.41)) // bar
29 \text{ xEDC} = \text{Econ1/(Econ1+Econ2)}
30 \text{ xTEC} = 1 - \text{xEDC}
31 \text{ pEDC} = 37.2 \times \text{xEDC}
32 \text{ pTEC} = 12.64*xTEC
33 \text{ pCl2HClC2H4} = 1.6*100-\text{pEDC-pTEC}
34 \text{ yEDC} = \text{pEDC}/160
35 \text{ yTEC} = \text{pTEC}/160
36 \text{ nt} = (C12s3+Econ2+1)*160/pC12HC1C2H4
37 \text{ nEDC} = \text{yEDC*nt}
38 \text{ nTEC} = \text{yTEC*nt}
39 printf(" Compositions of gas streams : \n \n
```

```
Component Stream 3 Stream 5
              Stream 4 Stream 6 \n Cl2
                "+string(Cl2s3)+"
s3)+" \n HCl
                                         "+string(
     string(C12s3)+" \n HCl
     HCls3)+"
                         "+string(HCls3)+" \n C2H4
                    "+string(nC2H4)+"
     "+string(nC2H4)+" \n EDC
                                             "+string
     (nEDC)+"
                     0.2355
                                      3.3947
                98.5665 \setminus n TEC
     string(nTEC)+" Nil
                                              "+string
     (nTEC)+"
                      "+string(TCEp)+" n n")
40 \, \text{fil} =
     (10.802*33.9+.198*29.1+1*43.6+3.6302*17.4+.0025*85.3)
     *(328.15-273.15)
41 \text{ fi2} = 35.053*1000*3.3947+39.58*1000*.0025
42 \text{ fi3} = (3.3947*129.4+.0025*144.4)*55/2
43 fi = fi1+ fi2+ fi3 // kJ/h
44 printf(" Heavy duty of Overhead condenser = "+string
     (fi)+"kJ/h. \n \n ")
45 \text{ fi5} = (100*43.6+110*33.9)*(328.15-273.15)
46 fi6 = 3.6302*1000*33.6+.0025*1000*38.166
47 \text{ fi7} = (98.5665*129.4+.1988*144.4)*(328.15-273.15)
48 fi8 = 216845.5*98.802+392394.5*.198
49 ficol = fi5+fi8-fi1-fi6-fi7
50 printf(" Heavy duty of external cooler = "+string(
     ficol) + "kJ/h.")
```

Scilab code Exa 5.39 Calculations in adiabatic converter

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
```

```
7
9 // Example 5.39
10 // Page 284
11 printf("Example 5.39, Page 284 n n");
12
13 // solution
14
15 To = 298.15
16 \text{ T1} = 483.15
17 // fil = intgr (from To to T1) \{12199.5+2241.4*10^{-3} + 3*T\}
      +1557.7*10^{-}-6*T^{2}-671.3*10^{-}-9*T^{3}dT
18 fi1 = 2455874.6 // kJ/h
19 dHr = 2*(-45.94) // kJ/mol N2 reacted
20 \text{ fi2} = 91.88*1000*23.168
21 fi3 = fi1+fi2
\frac{1}{2} // fi3 = intgr (from To to T2) \{10713.9+3841*10^{-}-3*T\}
      +1278.8*10^{-}-6*T^{2}-752.6*10^{-}-9*T^{3}dT
23 // solving it
24 \text{ T2} = 657.41 \text{ // K}
25 printf("Temperature of the gas mixture leaving the
      reactor = "+string(T2)+" K.")
```

Scilab code Exa 5.40 Burning of HCl

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.40
10 // Page 292
```

```
11 printf("Example 5.40, Page 292 n n);
12
13 // solution
14
15 // basis 4 kmol of HCl gas
16 O2req = 1 // \text{kmol}
17 \ \text{O2spply} = 1.35*1
18 N2 = 1.35*79/21
19 \text{ air} = 02\text{spply} + N2
20 HClbrnt = .8*4
21 HCl = 4-HClbrnt
22 \ 02 = 02spply - .8
23 \text{ C12} = .8*2
24 \text{ H2O} = .8*2
25 printf(" (a) \n \n Composition of dry product gas
      stream: \n Component
                                        Dry product gas
                                            "+string(HCl)+
      stream, kmol \n HCl
      "\n O2
                                 "+string(02)+" \n Cl2
                       "+string(Cl2)+" \n H2O
                       "+string(H2O)+" \n N2
                        n ")
26 \text{ H2} = 114.4*1000*.8
27 // H2 = intgr (from 298.15 to T)
      \{286.554+12.596*10^{-3}*T+63.246*10^{-6}*T
      ^2 - 25.933*10^{-9}T^3dT
28 // solving it
29 T = 599.5 // K
30 printf(" Adiabatic reaction temperature of product
      gas stream = "+string(T)+" K.")
```

Scilab code Exa 5.41 Dehydrogenation of EB

```
1 clear;
2 clc;
```

```
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.41
10 // Page 294
11 printf("Example 5.41, Page 294 n n");
12
13 // solution
14
15 // 1 kmol of EB vapors entering the reactor at
      811.15 K
16 // (from 811.15 to T1) intgr\{-36.72+671.12*10^{-3}*T
      -422.02*10^{\circ}-6*T^{\circ}2+101.15*10^{\circ}-9*T^{\circ}3dT = (from T1
      to 978.15) intgr\{487.38+1.19*10^{-3}*T+198.16*10^{-6}*
      T^2-68.21*10^-9*T^3dT
17 // \text{ we get}
18 \text{ T1} = 929.72
                 // K
19 To = 298.15
20 \text{ H1} = 493405
21 \text{ EBr} = .35
22 Styrenep = EBr*.9
23 Benzeneb = EBr*.03
24 Ethyleneb = Benzeneb
25 \text{ Cb} = EBr*.01
26 Toulened = EBr*.06
27 \text{ Hr1} = 147.36-29.92
                         // kJ/mol EB
28 \text{ Hr2} = 82.93+52.5-29.92
29 \text{ Hr3} = -29.92
30 Hr4 = 50.17-74.52-147.36 // kJ/mol styrene
31 dHr = 1000*(Hr1*(Styrenep+Toulened)+Hr2*Benzeneb+Hr3
      *Cb+Hr4*Toulened)
32 \text{ H2} = \text{H1-dHr}
33 // H2 = (from To t0 T2) intgr{Comp2dT
34 // we get
35 T2 = 798.79 // K
```

```
36 printf(" Adiabatic reaction T at the outlet of the reactor is "+string(T2)+" K.")
```

Scilab code Exa 5.42 Heat of crystallization

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.42
10 // Page 297
11 printf("Example 5.42, Page 297 n \n");
12
13 // solution
14
15 Hsol = 62.86 // kJ/mol solute
16 \text{ Mcrystal} = 286.1414
17 Hcry = Hsol*1000/Mcrystal // kJ/kg solute
18 printf(" Heat of crystallization of 1 kg crystal is
     "+string(Hcry)+" kJ.")
```

Scilab code Exa 5.43 Heat of crystallization

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
```

```
7
8
9  // Example 5.43
10  // Page 297
11 printf("Example 5.43, Page 297 \n \n");
12
13  // solution
14
15  Hf = -285.82  // kJ/mol of H2O
16  Hcryst = -4327.26-(-1387.08+10*Hf)
17 printf(" Heat of crystallization = "+string(Hcryst)+" kJ/mol.")
```

Scilab code Exa 5.44 Heat of sol of Boric acid

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.44
10 // Page 297
11 printf("Example 5.44, Page 297 n \n");
12
13 // solution
14
15 \text{ Hfs} = -1094.33
16 \text{ Hfao} = -1072.32
17 \text{ Hsol} = \text{Hfao-Hfs}
18 printf(" Heat of solution of Boric acid = "+string(
      Hsol)+"kJ/mol."
```

Scilab code Exa 5.45 Heat of dissolution

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
9 // Example 5.45
10 // Page 297
11 printf("Example 5.45, Page 297 n n);
12
13 // solution
14
15 // (a)
16 \text{ Hf} = -982.8
17 \text{ Hfcryst} = -1053.904
18 Hdis = Hfcryst-Hf
19 // (b)
20 \text{ Hfcr} = -3077.75
21 \text{ Hsol} = \text{Hfcryst} + 7*(-285.83) - (-3077.75)
22 printf(" (a) \n H dissolulition = "+string(Hdis)+"
      string(Hsol)+" kJ/kmol.")
```

Scilab code Exa 5.46 T change in dissolution

```
1 clear;
2 clc;
3
```

```
4  // Stoichiometry
5  // Chapter 5
6  // Energy Balances
7
8
9  // Example 5.46
10  // Page 300
11 printf("Example 5.46, Page 300 \n \n");
12
13  // solution
14
15  // using chart 5.16 we get
16 T = 329.5  // K
17 printf(" T = "+string(T)+" K.")
```

Scilab code Exa 5.47 Using std heat of formations

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
9 // Example 5.47
10 // Page 300
11 printf("Example 5.47, Page 300 n \n");
12
13 // solution
14 \ // \ basis \ 100(m1) \ kg \ 46\% \ sol
15 NaOH = 46 // kg
16 \text{ H2O} = 54 // \text{kg}
17 m2 = NaOH/.25
18 NaOHo = 25 // kg
```

```
19 H2Oo = 75  // kg
20 Hf1 = -453.138  // kJ/mol
21 Hf2 = -467.678  // kJ/mol
22 Hs = Hf2-Hf1
23 Hg = -Hs*1000*1.501
24  // using Appendix IV.1
25 Hw1 = 146.65
26 Hw2 = 104.9
27 Hadd = 84*(Hw1-Hw2)
28 H = Hg+Hadd
29 C1 = 3.55
30 T2 = 298.15+H/(184*C1)  // K
31 printf(" Final sol T = "+string(T2)+" K.")
```

Scilab code Exa 5.48 Heat effect of the solution

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
9 // Example 5.48
10 // Page 301
11 printf("Example 5.48, Page 301 n \n");
12
13 // solution
14 // basis 100 kg of sol with 32\% N
15 \text{ MNH4NO3} = 80.0434
16 \text{ MNH2CONO2} = 60.0553
17 \text{ MN2} = 28.0134
18 \text{ na} = 32/(60.9516)
19 Ureadis = 1.1758*na*MNH2CONO2 // kg
```

```
20 water = 100-(na*MNH4NO3+Ureadis)
21 ndis = 525
22 m = ndis/water
23 HE1 = 40.3044-2.5962*m+.1582*m^2-3.4782*10^-3*m^3
24 HE = HE1*ndis
25 printf("Heat effect of the sol = "+string(HE)+" kJ."
)
```

Scilab code Exa 5.49 Integral heats of solution

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
9 // Example 5.49
10 // Page 302
11 printf("Example 5.49, Page 302 n \n");
12
13 // solution
14 \text{ Hmix} = 896
15 M1 = 88 // molar mass of n-amyl alcohol
16 M2 = 78 // molar mass of benzene
17 B = .473*M2
18 A = .527*M1
19 Ha = Hmix/A
20 \text{ Hb} = \text{Hmix/B}
21 printf(" Integral heat of sol of n-amyl alcohol = "+
      string(Ha)+" kJ/kg n-amyl alcohol and of benzene
     = "+string(Hb)+" kJ/kg benzene.")
```

Scilab code Exa 5.50 Hx for H2SO4

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
9 // Example 5.50
10 // Page 302
11 printf("Example 5.50, Page 302 n n");
12
13 // solution
14 // from fig 5.18
15 Ta = 379.5 // K
16 dH = -274-(-106.5) // kJ/kg sol
17 Cm = 2.05 // kJ/kg K
18 dHc = Cm*(Ta-298.15)
19 // basis 100 kg of 93 % acid
20 // acid balance
21 x = poly(0, 'x')
22 p = .93*100+x*.15-(100+x)*.77
23 y = roots(p)
24 //from fig
25 \text{ y1} = 25.3
26 printf(" (a) \n Resultant T of 77 percent sol = "
     +string(Ta)+" K. \n \n \n \b) \n \n Heat to be
     removed to cool it to 298.15 \text{ K} = "+string(dH)+"
     kJ/kg sol \n \n \n (c) \n \n By mean heat
     capacity method : "+string(dHc)+" kJ/kg sol \n \n
      \n (d) \n \n Quantity of 15 percent acid to be
```

```
fig : "+string(y1)+" kg.")
```

Scilab code Exa 5.51 Using heat of formations of H2SO4

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.51
10 // Page 304
11 printf("Example 5.51, Page 304 n \n");
12
13 // solution
14 // basis 100 kg of 93% acid and 25.8 kg of 15% acid
15 \text{ Hfp} = -814
16 \text{ Hf1} = -830
17 \text{ HE1} = \text{Hf1-Hfp}
18 \text{ Hf2} = -886.2
19 \text{ HE2} = \text{Hf2-Hfp}
20 \text{ Hf3} = -851
21 HE3 = Hf3-Hfp
22 \text{ Hsol} = .9876*1000*(-37)-[.9482*1000*(-16)]
      +.0394*1000*(-72.2)]
23 \text{ Hev} = 100*(30-25)*1.6
24 \text{ Hcon} = 25.8*25*3.7
25 netHev = -Hsol-Hcon+Hev
26 T = 298.15 + netHev/(125.8*2.05)
27 printf(" Temp of sol = "+string(T)+" K.")
```

Scilab code Exa 5.52 Heat to be removed for cooling it to 308K

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.52
10 // Page 306
11 printf("Example 5.52, Page 306 \n \n");
12
13 // solution
14
15 // basis 1000 kg of mixed acid
16 \text{ C11} = 2.45
17 \text{ H1} = -296.7 + \text{C11} * (308.15 - 273.15)
18 \text{ C12} = 2.2
19 \text{ H2} = -87.8 + \text{C12} * (308.15 - 273.15)
20 \text{ C13} = 1.45
21 \text{ H3} = -35.5 + \text{C13} * (308.15 - 273.15)
22 \text{ C14} = 1.8
23 \text{ H4} = -148.9 + \text{C14} * (308.15 - 273.15)
24 \text{ Hmix} = 1000*H4-[76.3*H1+345.9*H2+577.7*H3]
25 printf(" Heat of mixing = "+string(Hmix)+" kJ.")
```

Scilab code Exa 5.53 Heat changes in formation of MNB

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
```

```
6 // Energy Balances
8
9 // Example 5.53
10 // Page 308
11 printf("Example 5.53, Page 308 n n");
12
13 // solution
14
15 F = 1135
16 \text{ Benzenef} = 400*.993
17 \text{ HNO3con} = \text{Benzenef} *63/78
18 \text{ H1} = -186.5
19 \text{ C11} = 1.88
20 \text{ H11} = \text{H1}+\text{C11}*(298.15-273.15)
21 \text{ H2} = -288.9
22 \text{ C12} = 1.96
23 \text{ H}22 = \text{H}2+\text{C}12*(298.15-273.15)
24 H3 = 0
25 \text{ C13} = 1.98
26 \text{ H33} = \text{C13}*(298.15-273.15)
27 \text{ Hr} = -285.83+12.5-(-174.1+49.08)
28 Benzener = Benzenef/78.1118
29 fi = 903.84*H22+HN03con*H33-F*H11+Benzener*Hr*1000
       // kJ/h
30 printf(" Total heat exchanged = "+string(fi)+" kJ/h.
       ")
```

Scilab code Exa 5.54 Final T of solution in absorption of NH3

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
```

```
// Energy Balances
8
9 // Example 5.54
10 // Page 311
11 printf("Example 5.54, Page 311 n n);
12
13 // solution
14
15 // from ref 24
16 \text{ H} = 1600.83
17 \text{ To} = 273.15
18 h = 200
19 \text{ Hf1} = -79.3
                 // table 5.59
20 \text{ Hf2} = -46.11
21 Hsol = Hf1-Hf2
22 \text{ Hg} = \text{Hsol}*1000*140/17.0305
23 Raq = 140/.15 // kg/h
24 \ dT = Hg/(4.145*Raq)
25 T = -dT + 303
26 printf(" Temp of resultant sol = "+string(T)+" K.")
```

Scilab code Exa 5.55 Using table 5 60

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.55
10 // Page 311
11 printf("Example 5.55, Page 311 \n \n");
```

```
12
13  // solution
14
15  Hf1 = -80.14
16  Hf2 = -46.11
17  Hsol = Hf1-Hf2
18  Hg = Hsol*1000*2/17.0305
19  printf(" Heat generated for making 2 percent solution = "+string(Hg)+" kJ/100 kg sol.")
```

Scilab code Exa 5.56 Heat removed in cooler

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.56
10 // Page 312
11 printf("Example 5.56, Page 312 n \n");
12
13 // solution
14
15 \text{ fi3} = 15505407
16 \text{ fi4} = 11395056
17 fi5 = fi3-fi4 // kJ/h
18 \text{ fi6} = 111.375*62.75*1000
19 \text{ fi7} = 1063379
20 \text{ fi8} = 5532.15*4.1868*(303.15-298.15)
21 \text{ fi9} = 9030.4*3.45*(323.15-298.15)
22 fi = fi5+fi6+fi8-fi7-fi9
23 printf(" Heat removal in the cooler = "+string(fi)+"
```

Scilab code Exa 5.57 Hx vs x1

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.57
10 // Page 314
11 printf("Example 5.57, Page 314 n \n");
12
13 // solution
14
15 To = 273.15
16 \text{ T1} = 308.15
17 \text{ H1} = 124.8*(T1-To)
                            // kJ/kmol
                           // kJ/kmol
18 \text{ H2} = 134.9*(T1-To)
19 HE1 = .1*.9*[542.4+55.4*(.9-.1)-132.8*(.9-.1)
       ^2-168.9*(.9-.1)^3] // kJ/kmol of mix
20 \text{ Ha} = \text{HE1} + \text{H1} * .1 + \text{H2} * .9
21 \text{ HE2} = .2*.8*[542.4+55.4*(.8-.2)-132.8*(.8-.2)
       ^2-168.9*(.8-.2)^3] // kJ/kmol of mix
22 \text{ Hb} = \text{HE2+H1}*.2+\text{H2}*.8
23 HE3 = .3*.7*[542.4+55.4*(.7-.3)-132.8*(.7-.3)
       ^2-168.9*(.7-.3)^3] // kJ/kmol of mix
24 \text{ Hc} = \text{HE3} + \text{H1} * .3 + \text{H2} * .7
25 \text{ HE4} = .4*.6*[542.4+55.4*(.6-.4)-132.8*(.6-.4)
       ^2-168.9*(.6-.4)^3] // kJ/kmol of mix
26 \text{ Hd} = \text{HE4+H1}*.4+\text{H2}*.6
27 \text{ HE5} = .5*.5*[542.4+55.4*(.5-.5)-132.8*(.5-.5)
```

```
^2-168.9*(.5-.5)^3] // kJ/kmol of mix
28 \text{ He} = \text{HE5+H1}*.5+\text{H2}*.5
29 \text{ HE6} = .6*.4*[542.4+55.4*(.4-.6)-132.8*(.4-.6)]
       ^2-168.9*(.4-.6)^3] // kJ/kmol of mix
30 \text{ Hf} = \text{HE}6 + \text{H1} * .6 + \text{H2} * .4
31 HE7 = .7*.3*[542.4+55.4*(.3-.7)-132.8*(.3-.7)
       ^2-168.9*(.3-.7)^3] // kJ/kmol of mix
32 \text{ Hg} = \text{HE7} + \text{H1} * .7 + \text{H2} * .3
33 HE8 = .8*.2*[542.4+55.4*(.2-.8)-132.8*(.2-.8)
       ^2-168.9*(.2-.8)^3] // kJ/kmol of mix
34 \text{ Hh} = \text{HE8+H1}*.8+\text{H2}*.2
35 \text{ HE9} = .9*.1*[542.4+55.4*(.1-.9)-132.8*(.1-.9)
       ^2-168.9*(.1-.9)^3] // kJ/kmol of mix
36 \text{ Hi} = \text{HE9} + \text{H1} * .9 + \text{H2} * .1
37 \text{ HE10} = .0*1.*[542.4+55.4*(.0-1.)-132.8*(.0-1.)
       ^2-168.9*(.0-1.)^3] // kJ/kmol of mix
38 \text{ Hj} = \text{HE10} + \text{H1} + \text{H2} * 0
39 x = linspace(0,1,100)
40 y = linspace(4300,5000,100)
41 \quad y = 4721.5-57.4*x+1137.7*x^2-3993.6*x^3+3909.2*x
      ^4-1351.2*x^5
42 \, plot(x,y)
43 title("H vs x1")
44 xlabel("x1")
45 ylabel("H (kJ/kg sol.)")
46 printf("
                                            Enthalpy, kJ/kmol
      mix \n
               x1
                                HE
                                                        H \setminus n = 0
                                            "+string(H2)+" \n
       0.1
                       "+string(HE1)+"
                                                     "+string(Ha
      "+string(HE2)+"
                                           "+string(HE3)+"
       string(Hb) + " \setminus n = 0.3
                  "+string(Hc)+" \setminusn 0.4
       string(HE4)+"
                                   "+string(Hd)+" n 0.5
                 "+string(HE5)+"
                                                     "+string(He
      )+" n 0.6
                                "+string(HE6)+"
      string(Hf)+" \ n \ 0.7
                                           "+string(HE7)+"
                 "+string(Hg)+" n 0.8
                                                         "+string
       (HE8) + "
                           "+string(Hh)+" \setminusn 0.9
```

```
"+string(HE9)+" "+string(Hi)+" \n 1.0
"+string(HE10)+" "+
string(Hj)+"")
```

Scilab code Exa 5.58 repat of 5 57 using heat capacities

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.58
10 // Page 316
11 printf("Example 5.58, Page 316 \n \n");
12
13 // solution
14
15 // see eg 5.57
16 printf(" refer to eg 5.57")
```

Scilab code Exa 5.59 He vs x1 of acetone and ethylacetate

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
```

```
9  // Example 5.59
10  // Page 318
11  printf("Example 5.59, Page 318 \n \n");
12
13  // solution
14
15  // from graph drawn in 5.57 we can see
16  H1E1 = 300
17  H1E2 = 63
18  H2E1 = 30
19  H2E2 = 214
20  printf(" H1 at x1=0.3 is "+string(H1E1)+" kJ/kg sol \n H2 at x1=0.6 is "+string(H1E2)+" kJ/kg sol \n H1 at x1=0.6 is "+string(H1E2)+" kJ/kg sol \n H2 at x1=0.6 is "+string(H2E2)+" kJ/kg sol.")
```

Scilab code Exa 5.60 Heat of dilution

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
8
9 // Example 5.60
10 // Page 320
11 printf("Example 5.60, Page 320 n \n");
12
13 // solution
14
15 // basis 100 kg 96.1% H2SO4
16 // from table 5.64
17 \text{ m}1S03 = 78.4 // kg
```

```
18 \text{ m1H2O} = 21.6
19 \text{ n1SO3} = \text{m1SO3}/80.063
20 \text{ n1H2O} = \text{m1H2O}/18.015
21 // resultant sol has 23.2% H2SO4
22 \text{ m}2SO3 = 19
23 \text{ m}2\text{H}2\text{O} = 81
24 \text{ Mrsol} = m1S03*100/m2S03
25 \text{ Mw} = \text{Mrsol} - 100
26 \text{ w} = \text{Mrsol} - \text{m1SO3} / 18.015 / / \text{kmol}
27 \text{ HEosol} = n1S03*(-56940)+n1H20*(-32657) // kJ
28 \text{ HErsol} = n1SO3*(-156168)+w-(-335)
29 HE = HErsol-HEosol // kJ/kg original acid
30 \text{ C} = 3.43 \text{ // kJ/kg K}
31 	ext{ dT} = -HE/(Mrsol*C)
32 T = 291.15 + dT / K
33 printf(" Heat of dilution = "+string(HE)+" kJ/kg
       original solution \n \n Final T of resultant
       solution = "+string(T)+" K.")
```

Scilab code Exa 5.61 eg 5 60 with use of ice at 273K

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 5
6 // Energy Balances
7
8
9 // Example 5.61
10 // Page 321
11 printf("Example 5.61, Page 321 \n \n");
12
13 // solution
```

```
15 // basis 100 kg of original acid

16 lv = 333.7 // kJ/kg

17 H = -lv-18*4.1868

18 HE = (-64277-H*312.63)/100 // kJ/kg

19 printf(" Heat of dilution = "+string(HE)+" kJ/kg.")
```

Chapter 6

Stoichiometry and Unit Operations

Scilab code Exa 6.1 Overall material and energy balance

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
9 // Example 6.1
10 // Page 346
11 printf("Example 6.1, Page 346 n n");
12
13 // solution
14
15 // basis = 100 kmol of feed
16 Benzene = 100*.72// kmol
17 Toulene = 100-Benzene //\text{kmol}
18 // use fig 6.1
19 // D = distillate, B = bottom
```

```
(i) overall material balance
20 // F = B + D
21 \text{ xd} = .995
22 \text{ xb} = .03
23 \text{ xf} = .72
24 // xd*D + xb*B = F*xf (ii) benzene balance
25 // solving (i) and (ii)
26 D = 71.5 //kmol
27 B = 28.5 //kmol
28 printf("(a) \n \n performing overall material
      balance for 100 kmol of feed we get "+string(D)+"
      kmol as distillate and "+string(B)+"kml as bottom
       product. n \setminus n \setminus n (b) \setminus n \setminus n")
29 // enthalpy balance
30 // use fig 6.2
31 R = 1.95
32 v = D*(1+R) //kmol total overhead vapours
33 To = 273.15 / K
34 // using fig 6.2
35 Ev = 42170 //kJ/kmol enthalpy of vapours overhead 36 El = 11370 //kJ/kmol enthalpy of liquid
37 E1 = Ev-El // enthalpy removed in condenser
38 Hc = E1*v // heat load of condenser
39 \text{ Hd} = \text{El} * 71.5
40 Hb = 18780*28.5
41 \text{ Hf} = 44500*100
42 Hn = Hd+Hc+Hb-Hf // kJ heat load of reboiler
43 printf(" performing overall enthalpy balance we get
      Heat load of condenser = "+string(Hc)+"kJ/kmol
      and Heat load of reboiler = "+string(Hn)+"kJ/kmol
      . ")
```

Scilab code Exa 6.2 Cryogenic Separation of Nitrogen

```
1 clear;
2 clc;
```

```
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.2
10 // Page 349
11 printf("Example 6.2, Page 349 n \n");
12
13 // solution
14
15 // \text{ basis} = 2000 \text{kg/h} \text{ liquid feed rate}
16 \text{ F} = 2000/28.84 //\text{kmol/h}
17 /D = distillate, W = residue flow rate
18 //N2 balance
19 / F * .79 = .999D + .422W
                                    ( i )
20 // 54.840 = D + .4224W
                                   ( i i )
21 // solving it
22 W = 25.118 / \frac{kmol}{h}
23 D = 44.230 //kmol/h
24 //using fig 6.4 and 6.5
25 // trial method is used for flash calculations
26 // Trial I
27 x = .75
28 // from fig 6.4
29 y = .8833
30 // from fig 6.5
31 H1 = 1083.65
32 \text{ Hv} = 6071.7
33 \text{ Hf} = .3*Hv+Hv*.7
34 // calculating we get Emix is not close to 2592.2kJ/
      kmol
35 // Trial II
36 \times = .71
37 y = .859
38 \text{ H1} = 1085.6
39 \text{ Hv} = 6118.6
```

```
40 Hf = .3*Hv+.7*Hl //kJ/kmol
41 // which is aproox equal to 2595.2kJ/kmol, so
        flashing will occur
42 printf("composition of vapour liquid mix : \n mol
        fraction N2 = "+string(x)+" in liquid phase and "
        +string(y)+" in vapour phase.")
```

Scilab code Exa 6.3 Azeotropic distillation of IPA and water

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
  // Stoichiometry and Unit Operations
7
8
9 // Example 6.3
10 // Page 353
11 printf("Example 6.3, Page 353 n n");
12
13 // solution
14 // material balance
15
16 // V2 vapour mix is a ternary azeotrope in which all
       cyclohexane of D1 is recycled
17 // V2 stream
18 // Cyclohexane balance
19 // D1 = (.488/.024) *V2
20 // IPA in V2 = .206V2
21 // water in V2 = (1 - .488 - .206) *V2
22 // W2 stream
23 // IPA in W2 = (.23D1 - .206V2)
24 // water in W2 = (1 - .024 - .23) *D1 - .306 V2
25 / W2 \text{ stream} = 4.471 V2 + 14.862 V2
```

```
26 // D3 is an azeotrope containing 67.5 mol% IPA
27 // \text{ water in W3 stream} = (1 - .675) F
28 // basis = 100 kmol/h fresh feed
29 / W1+W3 = 100
30 // .998W1 + .001W3 = 67.5
                                 ( i i )
31 // solving it
32 \text{ W1} = 67.603 //\text{kmol/h}
33 \text{ W3} = 32.397 //\text{kmol/h}
34 \text{ IPA1} = W3*.001 // IPA in W3
35 //IPA2 = 4.471*V2 - .032
                                IPA in D3
36 //C-1 = F+D3 = F1
37 // \text{ water in } D3 = 6.624 V2 - .047 - 4.471 V2 + .032
38 // water in W3 = 14.862V2-2.153V2+.015
39 // solving them
40 \text{ V2} = 2.624 //\text{kmol/h}
41 \quad D3 = 2.153 * V2 - .015
42 D1 = 20.333*V2
43 \text{ F1} = 6.624 * V2 + 99.953
44 R = 1.75*D1 // = V1+V2-D1
45 \text{ V1} = 144.1
46 r = D3/100 // recycle ratio
47 printf ("After performing overall material balance we
       get Reflux, R = "+string(R) + "kmol/h and \n
      recycle ratio = "+string(r)+" kmol/kmol fresh
      feed.")
```

Scilab code Exa 6.4 CO2 absorption in aq MEA solution

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
```

```
9 // Example 6.4
10 // Page 355
11 printf ("Example 6.4, Page 355 n n");
12
13 // solution
14
15 // basis 0.625 l/s of MEA solution
16 c = 3.2 / M conc of MEA
17 M = 61 // molar mass of MEA
18 C = M*c //g/l conc of MEA in sol
19 MEAin = c*.625*3600/1000 // \text{kmol/h}
20 CO2diss = .166*7.2 //kmol/h CO2 dissolved in lean
       MEA
21 v = 26.107 //\text{m}^3 sp. vol of gas at 318K and 101.3
      kPa (table 7.8)
22 \text{ qv} = 1000/\text{v} //\text{kmol/h}
23 CO2in = qv*.104 // moles of CO2 in inlet gas
24 CO2freegas = qv - CO2in
25 //outgoing has 4.5\% CO2
26 GASout = CO2freegas/(1-.0455) //\text{kmol/h}
27 CO2abs = qv-GASout
28 \text{ CO2} = \text{CO2diss} + \text{CO2abs}
29 CO2conc = CO2/MEAin //\text{kmol/kmol MEA}
30 printf ("Concentration of dissolved CO2 in the
      solution leaving the tower = "+string(CO2conc)+"
      kmol/kmol of MEA.")
```

Scilab code Exa 6.5 Heat effect of Scrubbing

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
```

```
6 // Stoichiometry and Unit Operations
8
9 // Example 6.5
10 // Page 356
11 printf("Example 6.5, Page 356 n n");
12
13 // solution
14
15 //(a)
16 printf("(a) n n")
17 // basis 50000 m<sup>3</sup>/h of gas mix at 295.5K 100kPa
18 v = 24.57 //\text{m}^3/\text{kmol sp vol of gas at } 295.5\text{K} and 100
       kPa
19 n1 = 50000/v // kmol/h flow of incoming gas
20 \text{ NO2in} = \text{n1} * .0546
21 \quad N204in = n1*.0214
22 \text{ N2in} = \text{n1} - \text{N02in} - \text{N204in}
23 //N2 is unaffected
24 \text{ n2} = 1880.34/.95 //\text{kmol/h} outgoing gas flow
25 // using tables 6.3 and 6.4 on page 357
26 \text{ NO2rem} = \text{NO2in} - (n2*.0393)
27 \text{ N2O4rem} = \text{N2O4in} - (\text{n2}*.0082)
28 // rxn (ii)
29 NaOHreac2 = 2*40*N2O4rem
30 \text{ NaNO2pro2} = 69*N2O4rem
31 \text{ NaNO3pro2} = 85*N2O4rem
32 \text{ H2Opro2} = 18*\text{N2O4rem}
33 // rxn (iii)
34 \text{ NO2reac3} = 3*n2*.0025
35 \text{ NaOHreac3} = 2*4.95*40
36 \text{ NaNO3pro3} = 2*4.95*85
37 \text{ H2Opro3} = 4.95*18
38 \ \text{NO2abs2} = 33.33 - \text{NO2reac3}
39 \text{ NaOHreac1} = 18.48*40
40 \quad \text{NaNO2pro1} = 69*\text{NO2abs2/2}
41 \text{ NaNO3pro1} = 85*\text{NO2abs2/2}
42 \text{ H2Opro1} = 18*N02abs2/2
```

```
43 \text{ NaNO2t} = \text{NaNO2pro2} + \text{NaNO2pro1}
44 \text{ NaNO3t} = \text{NaNO3pro2} + \text{NaNO3pro3}
45 \text{ H2Ot} = \text{H2Opro1} + \text{H2Opro2} + \text{H2Opro3}
46 NaOHt = NaOHreac1+NaOHreac2+NaOHreac3
47 liq = 37500 / kg/h
48 NaOHin = liq*.236
49 NaOHout = NaOHin-NaOHt
50 \text{ moist} = n2*.045*18
51 water = liq-NaOHin-H2Ot-moist //kg/h
52 printf("Composition of final liquor: \n Component
                  mi (kg/h) \n NaOH
      string(NaOHout)+" \setminus n NaNO2
      string(NaNO2t)+" \n NaNO3
      string(NaNO3t)+" \n H2O
      53 //(b)
54 //heat effect of scrubbing
55 //using tables 6.6 and 6.7
56 / fi1 = integ \{59865.7 + 4545.8 + 10^{-3} *T +
      15266.3*10^{-} - 6*T^{2} - 705.11*10^{-} - 9*T^{3}
57 \text{ fil} = -155941.3/3600 //kW
58 //similarly
59 \text{ fi2} = 75.778 / \text{kW}
60 	ext{ dH1} = (-346.303-450.1-285.83-(2*(-468.257)+2*33.18))
      /2 //kJ/mol NO2
61 \text{ dH2} = -346.303-450.1-285.83-(2*(-468.257)+9.16) //kJ
      / \text{mol N2O4}
62 \text{ dH3} = (2*(-450.1) - 285.83 + 90.25 - (2*(-468.257))
      +3*33.18))/3 // kJ/mol NO2
63 dHdil = -469.837 - (-468.257) //kJ/mol NaOH
64 \text{ fi3} = (dH1*1000*18.48+dH2*1000*27.32+dH3*1000*14.85+
      dHdil*1000*138.23)/3600 //kW
65 \text{ fi4} = -\text{fi1}+\text{fi2}+\text{fi3}
66 printf("Heat efect of scrubbing system = "+string(
      fi4)+" kW.")
```

Scilab code Exa 6.6 Extraction of Acetic Acid

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
9 // Example 6.6
10 // Page 361
11 printf("Example 6.6, Page 361 n n");
12
13 // solution
14
15 //(a)
16 // basis 100 kg feed mix
17 // F = E + R = 100
                                 (i)
18 \text{ xf} = .475
19 \text{ xe} = .82
20 \text{ xr} = .14
21 //acetic acid balance
22 // xf*F = xe*E + xr*R
                                (ii)
23 //solving (i) & (ii)
24 E = 49.2 //kg
25 R = 50.8 / kg
26 a = R*xr //kg acetic acid leftover
27 b = (a/(xf*100))*100
28 printf(" Acetic acid that remained unextracted = "+
      string(b)+" percent.")
```

Scilab code Exa 6.7 Multiple contact counter current Extractor

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
8
9 // Example 6.7
10 // Page 361
11 printf("Example 6.7, Page 361 n \n");
12
13 // solution
14
15 // referring to fig 6.9
16 //basis 1000kg/h halibut livers
17 F = 1000 // kg/h
18 OILin = F*.257
19 Sin = F-OILin // solid in the charge
20 \ U = .23*Sin
21 \text{ OILu} = U*.128
22 Eu = U-OILu // ether in underflow
23 R = OILin-OILu //kg/h
                           recovery of oil
24 p = R*100/OILin
25 \ 0 = R/.7
26 \text{ Eo} = \text{O-R}
27 Et = Eu+Eo
28 printf(" Flow rate of ether to the system = "+string
      (Et)+" kg/h \n and percentage of recovery oil = "
      +string(p)+".")
```

Scilab code Exa 6.8 Recovery of Acetic Acid by Ethyl Acetate Extraction

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
8
9 // Example 6.8
10 // Page 362
11 printf("Example 6.8, Page 362 n \n");
12
13 // solution
14
15 F = 1000 // kg/h
                       Basis feed rate
16 // using fig 6.11
17 // W/A = 15.77/5.87
18 // A+F+W = 1000
19 // solving it
20 W = 15.77*F/21.64 //kg/h
21 A = F-W //kg/h
22 // material balance across C3
23 // R+R1 = D+W
24 // W/D = 19.31/1.81
25 // solving it
26 D = 1.81*W/19.31 //kg/h
27 \text{ M1} = D+W
28 / R1/R = 4.63/6.57
29 R1 = 4.63*793/11.2
30 \quad R = M1 - R1
31 // material balance across C2
32 \text{ m} = .89 // = E1/R1
33 // E = A+E1+R1 = A+M11
34 / M11/A = 15.6/3.97
35 \text{ M11} = 15.6 * \text{A} / 3.97
36 E = M11 + A
37 E1 = M11 - R1
38 // material balance across C1
```

```
39 // F+S = M = E+R
40 \quad M = E + R
41 S = D + E1
42 AAloss = W*.4*100/(100*.3)
43 AArec = 100-AAloss
44 printf(" Summary : \n Stream
     Flow rate (kg/h) \n Feed
                                "+string(F)+" \n Solvent
                              "+string(S)+" \n Extract
                             "+string(E)+" \n Raffinate
                           "+string(R)+" \n Acetic acid
                        "+string(A)+" \n Top layer from
                      "+string(E1)+" \n Bottom layer
      D1
                       "+string(R1)+" \n Feed to C3
      from D1
                          "+string(M1)+" \n Overhead
                            "+string(D)+" \n Water waste
     from C3
                         "+string(W)+" \n Stream
                              "+string(M)+"")
```

Scilab code Exa 6.9 Yield of Glauber salt

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.9
10 // Page 367
11 printf("Example 6.9, Page 367 \n \n");
12
13 // solution
```

```
15 // basis 100 kg free water
16 Na2SO4in = 32 //kg
17 Win = 68 // kg
18 W1 = (180/142)*32 //kg water with Na2SO4
19 \text{ Wfree1} = \text{Win-W1}
20 GS1 = ((Na2SO4in+W1)*100)/Wfree1 //kg
                                                    glauber
      salt present in 100 kg free water
21 W2 = (180*19.4)/142 // water associated with Na2SO4
      in final mother liquor
22 \text{ Wfree2} = 100 - W2
23 \text{ GS2} = ((19.4+W2)/Wfree2)*100
24 \text{ Y} = \text{GS1} - \text{GS2} //\text{kg}
25 p = Y*100/GS1
26 printf("Percent yield of glauber salt = "+string(p)+
      " . " )
```

Scilab code Exa 6.10 Cooling in a Crystallizer

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
8
9 // Example 6.10
10 // Page 368
11 printf("Example 6.10, Page 368 n n");
12
13 // solution
14
15 // basis 100kg free water in original sol
16 // initial T = 353K
17 \text{ W1} = (126/120.3)*64.2
                            //kg
```

```
18 \text{ Wfree1} = 100 - \text{W1}
19 MS1 = ((64.20+W1)*100)/32.76 // MgSO4.7H2O in 100 \text{kg}
      free water
20 // 4\% of original sol evaporates
21 E = (MS1 + 100) *.04
22 Wfree2 = 100-E // free water in mother liquor
23 // at 303.15 K
24 \text{ W2} = (126/120.3)*40.8
25 \text{ Wfree3} = 100 - W2
26 MS2 = (W2+40.80)*Wfree2/Wfree3 // crystals of MgSO4
      .7H2O
27 \quad y = MS1 - MS2 / kg
28 \ q = 501.2*1000/284.6 // quantity of original sol to
      be fed
29 printf (" Quantity if original solution to be fed to
      the crystallizer per 1000kg crystals of MgSO4.7
      H2O = "+string(q) + "kg."
```

Scilab code Exa 6.11 Recovery of p DCB

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.11
10 // Page 370
11 printf("Example 6.11, Page 370 \n \n");
12
13 // solution
14
15 // (a)
```

```
16 printf("(a) \n \n ")
17 // using fig 6.12
18 // peforming material balance at 290K
19 \text{ a1} = 5.76
20 \text{ b1} = 4.91
21 DCBs = b1*100/(a1+b1) // % of solid separated p-DCB
22 DCBr1 = DCBs*100/70 // recovery of p-DCB
23 printf("Percentage recovery of p-DCB = "+string(
      DCBr1)+". n n n (b) n n ")
24
25 //(b)
26 / at 255K
27 	 a2 = 5.76
28 b2 = 10.22
29 DCBs = b2*100/(a2+b2)
30 \text{ DCBr2} = (DCBs*100)/70
31 \text{ Ar} = DCBr2-DCBr1
32 printf("Additional recovery of p-DCB = "+string(Ar)+
```

Scilab code Exa ${\bf 6.12}\,$ Extractive Crystallization of o and p nitrochlorobenzenes

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.12
10 // Page 371
11 printf("Example 6.12, Page 371 \n \n");
12
```

```
13 // solution
14 F = 5000 //kg/h solvent free mix fed to simple
      crystallization unit
15 B1 = 4000/157.5 / \text{kmol/h} p-NCB in feed
16 \text{ A1} = 1000/157.5 \text{ // kmol/h} \text{ o-NCB in feed}
17 // after crstallization mother liquor has 33.1 mol \%
       B, A doesn't crstallizes
18 m = A1/(1-.331) // mother liquor entering
      extractive crytallization unit
19 B2 = m - A1
20 // optimizing solid flux
21 // dCt/dR = 1 - 2/R^3 = 0
22 R = 2^{(1/3)}
23 // referring fig 6.14
24 // overall material balance
25 // p-isomer (B)
26 / / .98D + xT = 4000
                              ( i )
27 // o-isomer (A)
28 // .02D + (1 - .05 - x)T = 1000
                                  ( i i )
29 // material balance around solvent recovery unit
30 // B
                                 (iii)
31 // 2.26 \text{Tx} = .198 \text{G} = \text{xH}
32 // A
33 // 2.26T(.95-x) = .531G
                                        (iv)
34 // solving above eq
35 T = 1337.6 // kg/h
36 D = 3729 // kg/h
37 \text{ G} = 3939 // \text{kg/h}
38 x = .258
39 //putting these values we get composition of various
       streams
40 printf(" Composition of various streams : \n
                            T kg/h
                                                  D kg/h n
      Component
                                                   74.6 \ n
          Α
                            925.6
          В
                                                   3654.9 \ n
                            345.1
           \mathbf{C}
                              66.9
                                                    nil \n \
      n")
41 printf(" Purity of top product = 69.2 percent A \n
```

```
Purity of bottom product = 98.0 percent \n Make-
up solvent = 66.9 kg/h.")
```

Scilab code Exa 6.13 Calculation of Dew Point

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
8
9 // Example 6.13
10 // Page 383
11 printf("Example 6.13, Page 383 n n");
12
13 // solution
14
15 Pw1 = 12.84 //Pa v.p. of ice at 233.15K (table
      6.12)
16 \text{ P1} = 101325 //Pa
17 Hm = (Pw1/(P1-Pw1)) // kmol/kmol dry air
18 P2 = 801325 //Pa
19 \text{ Pw2} = \text{P2} * .0001267 / (1 + .0001267)
20 \text{ dp} = -20.18 + 273.15 \text{ //K}  from table 6.12
21 printf("Dew Point = "+string(dp)+"K.")
```

Scilab code Exa 6.14 Calculations on Ambient Air

```
1 clear;
2 clc;
3
```

```
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.14
10 // Page 384
11 printf("Example 6.14, Page 383 n n");
12
13 // solution
14
15 / Pa = v.p. at DP
16 \text{ Pw} = 2.0624 //\text{kPa}
17 P = 100 //kPa
18 Hm = Pw/(P-Pw) // kmol water vapour / kmol dry air
19 H = .622*Hm // kg moisture/kg dry air
20 // at saturation, DB = WB = DP
21 \text{ Ps} = 4.004 //\text{kPa}
22 \text{ RH} = Pw*100/Ps
23 Hs = (Ps/(P-Ps))*.622
24 s = H*100/Hs
25 Ch = 1.006+1.84*H //kJ/kg dry air K
26 Vh = (.00073 + .03448) *22.414 *1.1062 *1.0133 //m<sup>3</sup>/kg
      dry air
27 // using fig 6.15
28 \text{ WB} = 294.55 / \text{K}
29 ias = 62.3 // kJ/kg dry air
30 d = -.28 // kJ/kg dry air
31 ia = ias + d
32 printf("The absolute molar humidity = "+string(Hm)+"
       kmol water vapour/kg dry air \nAbsolute humidity
       = "+string(H)+" kg moisture/kg dry air \npercent
      RH = "+string(RH)+" \npercent saturation = "+
      string(s)+" \nHumid heat = "+string(Ch)+" kJ/kg
      dry air K \setminus nHumid volume = "+string(Vh)+" m^3/kg
      dry air.")
```

Scilab code Exa 6.15 Humidification of Air in a Textile Industry

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
9 // Example 6.15
10 // Page 385
11 printf("Example 6.15, Page 385 n n");
12
13 // solution
14
15 // basis 1kg of dry air entering the air washer
16 //from fig 6.15
17 H1 = 11.8 //g/kg dry air
18 H2 = 17.76 //g/kg \, dry \, air
19 H = H2-H1 // moisture added during saturation
20 \text{ DB} = 300.95 \text{ //K}
21 \text{ WB} = 298.15 / \text{K}
22 \text{ DP} = 297.15 / \text{K}
23 Ch = 1.006+1.84*.01776 //kJ/kg dry air K
24 \text{ dT} = DB - DP
25 \text{ Hs} = \text{Ch} * 3.8
26 A = 25000 //\text{m}^3/\text{h} actual air at 41 and 24 degree
       celcius
27 // again from fig 6.15
28 Vh = .9067 / \text{m}^3/\text{kg} \, \text{dry air}
29 qm = A/Vh //kg dry air/h
30 fi = qm*Hs //kJ/h
31 P = 300 //kPa
```

Scilab code Exa 6.16 Induced draft cooling tower

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
8
9 // Example 6.16
10 // Page 387
11 printf ("Example 6.16, Page 387 n \n");
12
13 // solution
14
15 // M = E+B+W
16 Tav = (45+32)/2 + 273.15 / K avg cooling water T
17 // using steam tables (Appendix A IV.1)
18 \; lamda = 2410.5
                  //kJ/kg
                  //kg/s
19 E = 530/lamda
20 \text{ Cl} = 4.1868
21 Ti = 45+273.15 //K
22 To = 32+273.15 //K
23 fi = 530 // = mc*Cl*(Ti-To)
```

```
//kg/s
24 \text{ mc} = 530/(Cl*(Ti-To))
25 \text{ W} = .3*\text{mc}/100 //\text{kg/s}
26 // dissolved solid balance
27 / M*xm = (B+W)*xc
28 // 500*10^{-} - 6*M = (B+.0292)*2000*10^{-} - 6
29 // solving above eqs
30 B = .0441 //kg/s
31 \text{ M} = .2932 //\text{kg/s}
32 //energy balance on cooling tower
33 // fi = ma*(i2-i1)
34 \ // \ i2-i1 = 11.042 \ kJ/kg \ dry \ air
35 // moisture balance
36 / E = ma(H2-H1)
37 \text{ H2} = .2199/48 + .0196
38 iws = 2546.2 // Appendix IV
39 \text{ Ch1} = 1.006 + 1.84 * .0196
40 \text{ i1} = 1.006*(297.45-273.15)+.0196*iws
      +1.042*(308.15-297.5) // kJ/kg dry air
41 \quad i2 = i1 + 11.04
42 Tdb = ((i2 - 1.006*(301.25-273.15)-iws*H2)/1.05)
      +301.25 // K
43 printf("Air leaves th induced draft fan at "+string(
      Tdb)+" K.")
```

Scilab code Exa 6.17 Waste Heat recovery unit

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.17
```

```
10 // Page 389
11 printf("Example 6.17, Page 389 \n \n");
12
13 // solution
14
15 // basis 1 kg dry air fed to tower
16 // from fig 6.16 we get
17 // \text{ at WB=}330 \text{ K and DB=}393 \text{ K}
18 H1 = .0972 // kg/kg dry air
19 DP = 325.15 / K
20 // at 313 K
21 H2 = .0492 // kg/kg dry air
22 H = H1-H2 // moisture condensed in tower
23 Ch1 = 1.006 + 1.84*H1 // kJ/kg dry air
24 \text{ Ch2} = 1.006 + 1.84*H2
25 \text{ ia1} = 1.006*(325-273) + H1*2596 + 1.185*(393-325) //
       enthalpy of entering air
26 \text{ ia2} = 1.006*(313-273) + \text{H2}*2574.4 // enthalpy of
      outgoing air
27 \quad i = ia1-ia2
28 \text{ qm} = 2000/(1+\text{H1})
29 fi1 = qm*i // heat loss rate
30 fi2 = 1.167*3600*4.1868*(323-305) // heat gained by
      water
31 r = fi2*100/fi1
32 printf("(a) \setminus n \setminus n \text{ The heat loss rate rate from the}]
      hot air in the bed = "+string(fi1)+" kW \n \n \n(
      b) \n \n The percentage heat recovery in hot
      water = "+string(r)+" percent.")
```

Scilab code Exa 6.18 Recovery of CS2 by adsorption

```
1 clear;
2 clc;
3
```

```
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
8
9 // Example 6.18
10 // Page 390
11 printf("Example 6.18, Page 390 n \n");
12
13 // solution
14
15 // basis 800 kmol of inlet CS2-H2 mix
16 Pi = 106.7 //kPa Total Pressure
17 Pcs2i = 16.93 // kPa
18 \, n = 800 \, // \, kmol
19 ncs2i = Pcs2i*n/Pi // kmol
20 \text{ nh2i} = \text{n-ncs2i}
21 \text{ Po} = 101.325 // \text{kPa}
22 \text{ Pcs2o} = 6.19 // \text{ kPa}
23 \text{ nh2o} = 673.1 // \text{kmol}
24 \text{ ncs2o} = \text{Pcs2o*nh2o/(Po-Pcs2o)}
25 \text{ ncs}2a = \text{ncs}2i-\text{ncs}2o
26 \text{ mcs} 2a = \text{ncs} 2a * 76.1407 // kg
27 r = 600 // kg/h design adsorption rate
28 Mi = n*r/mcs2a // kmol/h
29 Vi = Mi*22.843 // m^3/h
30 mcs2ac = .32-.04 // kg CS2 absorbed per kg BD
      activated carbon
31 qm = r*1.04/mcs2ac // kg/h
32 C = ncs2o/nh2o // kmol CS2/kmol H2 = Pcs2/(P-Pcs2)
33 Pcs2 = 24.763 // kPa
34 T = 281.5 //K by eq 5.24
35 printf("(a) \n \n Volumetric flowrate of entering
      mixture = "+string(Vi)+" m^3/h \ n \ n \ n \ n
      Mass flowrate of activated carbon = "+string(qm)+
      " kg/h \mid n \mid n(c) \mid n \mid n Original mixture must be
       coole to "+string(T)+" K at 405 kPa for
      achieving same concentration of the outlet
```

Scilab code Exa 6.19 Hooker type diaphragm cell

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
8
9 // Example 6.19
10 // Page 391
11 printf("Example 6.19, Page 391 n \n");
12
13 // solution
14
15 // basis 4000 kg/h of NaOH produced
16 Cl2p = 35.5*2*4000/80 // kg/h
17 \text{ Mcl2} = \text{Cl2p}/71 // \text{kmol/h}
18 P = 101.325 // kPa
19 Pw = 2.0624 // kPa
20 moist = (Pw/(P-Pw))*(18.0154/70.906) //
21 Tmoist = Cl2p*moist // kg/h
22 // for 90\% onc of acid
23 n = (10/18.0153)/(90/98.0776) /// kmol H2O/kmol acid
24 Q = 134477/(18*(n+1.7983)^2) //kJ/kg H2O by eq (ii)
25 lambdav = 2459 // kJ/kg (Appendix IV)
26 heatload = Q+lambdav
27 fi = heatload*18.74 //kJ/h
28 printf(" The heat liberation rate in the tower = "+
      string(fi) + kJ/h.")
```

Scilab code Exa 6.20 Absorption of NH3 from pure gas

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.20
10 // Page 393
11 printf("Example 6.20, Page 393 \setminus n \setminus n");
12
13 // solution
14
15 // basis 100 kmol of feed gas
16 // using table 5.1
17 Sniai =
      20.6*29.5909+62*28.6105+4.1*20.7723+11.1*19.2494+2.2*25.6503
18 Snibi = [20.6*(-5.141)]
      +62*1.0194+11.1*52.1135+2.2*33.4806]/1000
19 Snici = [20.6*13.1829+62*(-.1476)]
      +11.1*11.973+2.2*.3518]/10^6
20 Snidi = [20.6*(-4.968)+62*.769+11.1*(-11.3173)]
      +2.2*(-3.0832)]/10^9
21 \text{ Hgas} = \text{Sniai}*(283-263) + \text{Snibi}*(283^2-263^2)/2 +
      Snici*(283^3-263^3)/3 + Snidi*(283^4-263^4)/4
      k.J
22 \text{ Hnh3} = 1533.8 //kJ
23 SniCmpi = (Hgas-Hnh3)/20 // kJ/(K 97.8 \text{ kmol gas})
      NH3 free gas
24 \text{ Go} = 97.8/.99995 //\text{kmol}
```

```
25 \text{ NH3a} = (2.2 - .005) *17 // kg
26 F1 = NH3a/.04 // flowrate of 4\% NH3 solution
27 Water = F1-NH3a //kg
28 \text{ dT1} = \text{Hgas/(Water*4.1868)} // \text{K}
29 Twater = 307 - dT1 //K
30 Wvp = 2.116 / kPa
31 P = 5101.325 //kPa
32 moist = Go*Wvp/(P-Wvp) // kg
33 W = Water + moist // total demineralised water
34 dTactual = Hgas/(W*4.1868) //K
35 // from table 5.59
36 \text{ dHf1} = -80.093 //\text{kJmol NH3} \text{ of } 4\% \text{ NH3 sol}
37 \text{ dHf2} = -46.11 //kJ/molNH3
38 H = dHf1-dHf2 // heat of 4\% NH3 sol
39 Hevl = -(H*NH3a*1000)/17 // total heat evolved
40 // in absorber gas is further heated from 283\mathrm{K} to
      291.4K
41 Hsol = Hevl-(2854.1*(291.4-283.15)) // kJ
42 // c 0f 4\% NH3 sol = c of water = 4.1868 kJ/kg K
43 \text{ dT2} = \text{Hsol}/(\text{F1}*4.1868)
44 \text{ To} = 291.4 + dT2
45 printf("(a) \n \n Temp of feed water to absorber = "
      NH3 sol leaving the absorber = "+string(To)+"K.")
```

Scilab code Exa 6.21 Direct contact counter current rotary drier

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
```

```
9 // Example 6.21
10 // Page 396
11 printf("Example 6.21, Page 396 n n");
12
13 // solution
14
15 // basis : product rate of 100 kg/h
16 H1 = .036 // kg moist/ kg dry solid
17 \text{ X}1 = .25/.75 // \text{kg /kg dry solid}
18 X2 = .02/.98 // kg/kg dry solid
19 // moist balance
20 // \text{ms}*(X1-X2) = \text{ma}*(H2-H1)
21 \text{ To} = 273.15 / \text{K}
22 \text{ is1} = 1.43*(30-0)+X1*4.1868*30
23 \text{ is2} = 1.43*80+.0204*4.1868*80
24 \text{ Tdb} = 393.15 / \text{K}
25 \text{ Tdp1} = 308.15 / \text{K}
26 \text{ iwb1} = 2565.4 //kJ/kg
27 \text{ Ch1} = 1.006 + 1.84 * .036
28 \text{ ia1} = 1.006*(Tdp1-273.15)+H1*iwb1+Ch1*(Tdb-Tdp1)
29 \text{ H2} = .056
30 \text{ Tdp2} = 315.55
31 \text{ iwb2} = 2578.7
32 \text{ ia2} = 1.006*(Tdp2-273.15)+H2*iwb2+(1.006+1.84*H2)
      *(323.15-Tdp2)
33 \text{ ma} = .085/(.056-.036)
34 iaa = 1.006*(Tdp1-273.15)+H1*iwb1
35 fi = 4.25*(218.68-iaa) //kW
36 \text{ lambda} = 2133.0
37 steam = fi/lambda // kg/h
38 printf("(a) \n \n Flowrate of incoming air on dry
      basis = "+string(ma)+" kg/s n \ln \ln \ln \ln \ln
      Humidity of air leaving the drier = "+string(H2)+
      " kg/kg dry air. \n \n \n(c) \n \n Steam
      consumption in the heater = "+string(steam)+" kg/
      h.")
```

Scilab code Exa 6.22 Hot air dryer of textile mill

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.22
10 // Page 398
11 printf("Example 6.22, Page 398 n n);
12
13 // solution
14 // \text{ basis cloth speed} = 1.15 \text{ m/s}
15 prod = 1.15*1.2*3600*.095
16 moisti = .90 // kg/kg bone dry cloth
17 \text{ moisto} = .06
18 \text{ evp} = 471.96*(\text{moisti-moisto})
19 // using fig 6.15 and 6.16
20 \text{ H1} = .01805
21 \text{ H2} = .0832
22 	 dH = H2 - H1
23 qm1 = evp/dH // kg dry air/h
24 Vh = .8837 / m^3 / kg dry air
25 \text{ qv} = \text{qm1*Vh}
26 \text{ DP1} = 296.5 \text{ //K}
27 \text{ DP2} = 322.5 / \text{K}
28 lambdaV2 = 2384.1 //kJ/kg
29 To = 273.15 / K
30 \text{ fil} = \text{prod}*1.256*(368-303)+\text{prod}*.06*(368-303)*4.1868
       // kJ/h
31 fi2 = evp*(322.5-303.15)+evp*lambdaV2 //kJ/h
```

```
32 \text{ ia1} = 1.006*(303.15-273.15)+2556.4*.01805 //kJ/kg
      dry air
33 \text{ ia2} = 1.006*(322.8-273.15)
      +2591.5*.0832+(1.006+1.84*.0832)*(393-328.8)
34 \text{ fi2} = \text{ia2-ia1}
35 hlost = fi2-fi1 // kJ/h
36 // using Appendix IV
37 h = 720.94 //kJ/kg
38 lambdav = 2046.5 // kJ/kg
39 steami = (h+lambdav)*885 // kJ/h
40 fi4 = h*885 / kJ/h
41 \text{ qm2} = 885/\text{evp}
42 printf("(a) \setminus n \setminus n \text{ Bone dry production of the dryer} =
       "+string(prod)+" kg/h. n n n b n
      evaporation taking place in the dryer = "+string(
      evp)+" kg/h. n n n(c) n m
      circulation rate = "+string(qv)+" m<sup>3</sup>/h.")
```

Scilab code Exa 6.23 Quadruple effect forward feed evaporator

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.23
10 // Page 401
11 printf("Example 6.23, Page 401 \n \n");
12
13 // solution
14
15 // basis : weak liquor flowrate = 1060 kg/h
```

```
16 \text{ s1} = 1060*.04 //\text{kg/h} solids in weak liquor
17 liqr = s1/.25 // kg/h conc liquor leaving 4th
      effect
18 evp = 1060-liqr // kg/h
19 lambdas = 2046.3 / kJ/kg
20 Wf = 1060 // \text{ kg/h}
21 \text{ C1f} = 4.04
22 \text{ T1} = 422.6
23 Tf = 303
24 \ lambdav1 = 2114.4
25 // enthalpy balance of 1st effect
26 / Ws*lambdas = Wf*C1f*(T1-Tf) + (Wf-W1)*2114.4
27 //putting values we get
28 / Ws = 1345.57 - 1.033*W1
29 // 2nd effect
30 //W1 = 531.38 + .510 *W2
31 // 3rd effect
32 / W1 - 1.990*W2 = -1.027*W3
33 // 4th effect
34 / W2 - 1.983*W3 = -176.84
35 //solving above eqs
36 \text{ W1} = 862 // \text{kg/h}
37 \text{ W2} = 648.2 // \text{kg/h}
38 \text{ W3} = 416.7 // \text{kg/h}
39 \text{ Ws} = 455.2 // \text{kg/h}
40 eco = evp/Ws // kg evaporation/kg steam
41 spcon = 1/eco // kg steam/kg evaporation
42 printf ("Specific heat consumption of the system is"
      +string(spcon)+" kg steam/kg evaporation.")
```

Scilab code Exa 6.24 Triple effect evaporation system

```
1 clear;
2 clc;
3
```

```
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.24
10 // Page 403
11 printf("Example 6.24, Page 403 \setminus n \setminus n");
12
13 // solution
14
15 Fspd1 = 4300 // kg/h
16 Bcrtn = Fspd1*600*10^-6 // kg/h
17 Fspd2 = Bcrtn/.00645 // kg/h
18 \text{ evp1} = \text{Fspd1} - \text{Fspd2}
19 \text{ Fspd3} = \text{Bcrtn/.057}
20 \text{ evp2} = \text{Fspd2} - \text{Fspd3}
21 C3 = Bcrtn/.4
22 \text{ evp3} = \text{Fspd3-C3}
23 fi1 = Fspd1*2.56*(468.15-373.15)+3900*450 // kJ/h
24 fi2 = Fspd2*2.56*(463.15-468.15)+354.737*450 // kJ/h
25 fi3 = Fspd3*2.56*(453.15-463.15)+38.813*450 // kJ/h
26 \text{ fi} = \text{fil+fi2+fi3}
27 mt = fi/(2.95*(503.15-478.15)) // kg/h
28 \text{ qt} = \text{mt}/.71 // l/h
29 mccw1 = 1755000/(8*4.1868) // kg/h
30 \quad mccw2 = mccw1*.9
31 \text{ dT2} = 159632/(\text{mccw2}*4.1868)
32 \text{ mccw3} = \text{mccw1} - \text{mccw2}
33 \text{ dT3} = 17466/(\text{mccw3}*4.1868)
34 \text{ dT} = (1755000+159632+17466)/(\text{mccw}1*4.1868)
35 Fw = 1932098/(8*4.1868) // kg/h
36 printf ("By mass balance, required cooling water flow
        in external cooler = "+string(Fw)+" kg/h.\n\nBy
       enthalpy balance, overall rise in CCW temperature
       = "+string(dT)+" K.")
```

Scilab code Exa 6.25 Four compartment washing thickner

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 6
6 // Stoichiometry and Unit Operations
7
8
9 // Example 6.25
10 // Page 405
11 printf("Example 6.25, Page 405 n n");
12
13 // solution
14
15 //stream M2
16 \ Vcaco3M2 = .349/2.711
17 \text{ VliqrM2} = .651/1.167
18 VslryM2 = Vcaco3M2+VligrM2
19 \text{ spgM2} = 1/\text{VslryM2}
20 \text{ FsM2} = 2.845*3600*\text{spgM2}
21 \text{ sM2} = \text{FsM2} * .349 // \text{kg/h}
22 \text{ liqrM2} = \text{FsM2} * .651
23 \text{ Na2OM2} = \text{liqrM2} * .1342/1.167
24 //stream O2
25 Fs02 = 14.193*3600*1.037 // kg/h
26 \text{ sO2} = \text{FsO2} * .0003
27 \text{ liqr02} = Fs02-s02
28 \text{ Na} = 2002 = 1 \text{iqr} = 0.02 \times 0.0272 \times 0.037
29 //stream M1
30 \text{ VM1} = .194/2.711 + .806/1.037 // 1
31 \text{ spgM1} = 1/VM1
32 \text{ FsM1} = 5206.9/.194
```

```
33 \text{ ligrM1} = \text{FsM1} - 5206.9
34 \text{ Na2OM1} = \text{ligrM1} * .0252/1.034
35 // stream O1
36 \text{ FsO1} = \text{FsO2+FsM1-FsM2}
37 \text{ sO1} = \text{FsO1} *.0002
38 \ \text{liqr01} = \text{Fs01} - \text{s01}
39 Na2001 = liqr01*.0096/1.014
40 // stream W
41 \text{ VW} = .037/2.711 + .963
42 \text{ spgW} = 1/VW
43 \text{ FsW} = 14.977*3600*spgW
44 \quad sW = FsW*.037
45 liqrW = FsW-sW
46 \text{ Na2OW} = \text{ligrW} * .0024
47 // stream Mo
48 \text{ VMo} = .402/2.711 + .598/1.022
49 \text{ spgMo} = 1/VMo
50 \text{ FsMo} = 3.627*3600*spgMo}
51 \text{ sMo} = \text{FsMo} *.402
52 ligrMo = FsMo - sMo
53 \text{ Na20Mo} = \text{ligrMo} * .0162/1.022
54 printf(" Material balance thickener \n \n ITEM
                              STREAM, kg/h n
                                  M2
                                                    O2
                                                           W
                      M1
                                         01
                      Mo\n Slurry
                                                    "+string(
      FsM2)+" "+string(FsO2)+" "+string(FsM1)
+" "+string(FsO1)+" "+string(FsW)+"
            "+string(FsMo)+"\n Suspended solids "+
      string(sM2)+"
                             "+string(s02)+"
                                                      "+string(
                     "+string(s01)+" "+string(sW)+"
            "+string(sMo)+"\n Liquor
                               "+string(liqr02)+"
      string(liqrM2)+"
                                "+string(liqr01)+"
      string(liqrM1)+"
      +string(liqrW)+" "+string(liqrMo)+" \n Na2O
                                                "+string(
                        "+string(Na20M2)+"
                                                    "+string(
      Na2002)+"
                        "+string(Na20M1)+"
                                                  "+string(
      Na2001)+"
                        "+string(Na2OW)+"
```

Na20Mo)+"")

Chapter 7

Combustion

Scilab code Exa 7.1 GCV and NCV calculations

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
8
9 // Example 7.1
10 // Page 434
11 printf("Example 7.1, Page 434 n n");
12
13 // solution
14
15 // basis 100 kg as received coal
16 \ 02 = 18.04 \ // kg
17 \text{ nH2} = 2.79 - (02/8) // \text{kg}
18 printf("(a) \n Net H2 in coal = "+string(nH2)+"
      kg. \langle n \rangle \langle n \rangle \langle n \rangle \langle n \rangle 
19 cbW = 1.128*18 // kg
20 printf("Combined water in the coal = "+string(cbW)+"
```

```
21 // Dulong's formula
22 \text{ GCV1} = 33950*(50.22/100) + 144200*nH2/100 +
      9400*.37/100 // kJ/kg
23 printf("GCV by Dulongs formula = "+string(GCV1)+" kJ
      /kg. n n n (d) n n ")
24 \text{ tH2} = 1.395 // \text{kmol}
25 \text{ wp} = tH2*18 + 7
26 Hv = 2442.5*wp/100 // kJ/kg fuel
27 \text{ GCV2} = 23392*(1-.21-.07) // as of received coal
28 \text{ NCV} = \text{GCV2} - \text{Hv}
29 printf ("NCV of the coal = "+string(NCV)+" kJ/kg. \n
     n \ n \ (e) \ n \ "
30 // Calderwood eq
31 // Total C = 5.88 + .00512(B-40.5S) +
      .0053[80-100*(VM/FC)]^1.55
32 C = 5.88 + .00512*(7240.8-40.5*.37)
     +.0053*[80-56.52]^1.55
33 printf("Total Carbon by Calderwood eq = "+string(C)+
     ".")
```

Scilab code Exa 7.2 NCV of crude oil

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
8
9 // Example 7.2
10 // Page 436
11 printf("Example 7.2, Page 436 \n \n");
12
```

Scilab code Exa 7.3 Gaseous propane

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
8
9 // Example 7.3
10 // Page 444
11 printf("Example 7.3, Page 444 n n");
12
13 // solution
14
15 // basis 1 mol of gaseous propane
16 \text{ H2O} = 4*18.0153 //g
17 \text{ NHV} = 2219.17 - (H20 * 2442.5 / 1000)
18 printf("NHV = "+string(NHV)+" kJ/mol.")
```

Scilab code Exa 7.4 GCV NCV for natural gas

```
1 clear;
2 clc;
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
9 // Example 7.4
10 // Page 444
11 printf("Example 7.4, Page 444 n n");
12
13 // solution
14
15 // basis 1 mol of natural gas
16 // using table 7.7
17 \text{ H20} = [2*.894+3*.05+.019+5*(.004+.006)]*18
18 \text{ Hv} = \text{H20} * 2442.5 / 1000
19 \text{ NCV1} = 945.16 - \text{Hv}
20 \text{ GCV} = 945.16*1000/18.132
21 \text{ NCV} = \text{NCV1}*1000/18.132
22 printf(" GCV = "+string(GCV) + " kJ/kg. \ \ NCV = "+
       string (NCV) + ^{\circ} kJ/kg.^{\circ})
```

Scilab code Exa 7.5 Coal burnt in excess air

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
8
9 // Example 7.5
```

```
10 // Page 451
11 printf("Example 7.5, Page 451 n n");
12
13 // solution
14
15 // basis 100 kg fuel
16 \text{ O2req} = 4.331*32 // kg
17 \text{ rO2req} = 02\text{req}/100
18 \text{ N2in} = (79/21)*4.331
                            // kmol
19 AIRreq = 02req+N2in*28 //kg
20 rAIRreq = AIRreq/100
21 R = AIRreq/100
22 AIRspld = R*2 // kg/kg coal
23 O2spld = 4.331*2 // kmol
24 \text{ N2spld} = \text{N2in}*2
25 \text{ N2coal} = 2.05/28
                        // kmol
26 \text{ tN2} = \text{N2spld} + \text{N2coal}
27 \text{ moist} = 1.395 + (7/18) // \text{kmol}
28 printf("(a) \n \n Theoratical O2 requirement per
      unit mass of coal = "+string(r02req)+" kg. \n
      \n \n \n \n Theoretical dry air requirement = "+
      string(rAIRreq)+" kg/kg coal.")
```

Scilab code Exa 7.6 Residue fuel oil sample

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
8
9 // Example 7.6
10 // Page 452
```

```
11 printf ("Example 7.6, Page 452 n \n");
12
13 // solution
14
15 // basis 100 kg of RFO
16 O2req = 9.786 / kmol
17 N2req = (79/21)*02req //kmol
18 AIRreq = 02req+N2req //kmol
19 rAIRreq = AIRreq*29/100
20 AIRspld = AIRreq*1.25
21 rAIRspld = AIRspld/100
22 // using table 7.11 and 7.12
23 \times SO2 = .07/(55.925+5.695) // kmol SO2/kmol wet gas
24 \text{ vSO2} = \text{xSO2}*10^6 // ppm
25 \text{ mSO2} = 4.48*10^6/(1696.14+102.51)
26 // at 523.15 K and 100.7 kPa
27 V = [(55.925+5.695)*8.314*523.15]/100.7 // m<sup>3</sup>
28 \text{ cSO2} = (4.48*10^6)/V // \text{mg/m}^3
29 //from fig 7.3
30 \text{ dp} = 424.4 \text{ //K}
31 printf("(a) \n Theoretical air required = "+
     string(rAIRreq)+" kg/kg fuel. n n n(b) n n
     Actual dry air supplied = "+string(rAIRspld)+" kg
     /kg fuel. \n \n \n \c) \n \n Concentration of SO2
     = "+string(mSO2)+" mg/kg. n n n (d) n n
     Concentration of SO2 = "+string(vSO2)+" ppm vol/
     gases are discharged at 523.15K and 100.7kPa = "+
     string(cSO2)+" mg/m^3. n n n f
     Point of flue gas = "+string(dp)+" K.")
```

Scilab code Exa 7.7 Orsat analysis of flue gases

```
1 clear;
2 clc;
```

```
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
8
9 // Example 7.7
10 // Page 454
11 printf("Example 7.7, Page 454 n \n");
12
13 // solution
14
15 // basis 100 kmol of dry flue gas
16 \ \text{O2acntd} = 11.4 + 4.2 \ // \ \text{kmol}
17 O2avlbl = (21/79)*84.4 // kmol
18 O2excs = 4.2 / \text{kmol}
19 O2unactd = O2avlbl-O2acntd
20 H2brnt = O2unactd*2
21 \ \text{O2req} = 11.4 + \text{O2unactd}
22 \text{ pexcsAIR} = 02 \text{excs} * 100 / 02 \text{req}
23 mH2brnt = H2brnt*2 // kg
24 \text{ mCbrnt} = 11.4*12
25 r = mCbrnt/mH2brnt
26 printf("(a) \n Percent excess air = "+string(
      pexcsAIR)+". n n n b n In fuel C:H = "+
      string(r)+".")
```

Scilab code Exa 7.8 Sugar factory boiler

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
```

```
7
8
9 // Example 7.8
10 // Page 459
11 printf ("Example 7.8, Page 459 n n);
12
13 // solution
14
15 // basis 100 kg of bagasse fired in the boiler
16 //(a)
17 \text{ O2req} = 2.02 // \text{kmol}
18 N2in = (79/21)*02req // kmol
19 AIRreq = (02req+N2in)*29 // kg
20 \text{ rAIR} = AIRreq/100
21 printf("(a) \setminus n \setminus n \text{ Theoretical air required} = "+
      string(rAIR)+" kg dry air/kg fuel. \n \n \n \b
      n \setminus n")
22 // (b)
23 tflugas = 1.95/.1565 //kmol
24 \text{ xcsO2N2} = \text{tflugas} - 1.95
25 \times (xcs02N2-7.6)/4.76 // kmol
26 \text{ pxcsAIR} = x*100/02req
27 printf("Percent excess air = "+string(pxcsAIR)+". \n
       n (c) n n "
28 //(c)
29 pW = 100*.2677 // kPa partial p of water vap
30 // from fig 6.13
31 \text{ dp} = 339.85 / \text{K}
32 printf ("Dew Point of flue gas = "+string(dp)+"K. \
      n \ n \ (d) \ n \ "
33 // (d)
34 // from appendix IV
35 hfw = 292.97 //kJ/kg enthalpy of feed water at
      343.15 K
36 Hss = 3180.15 // kJ/kg enthalpy of super heated
      steam at 2.15 bar and 643.15K
37 Hgain = Hss - hfw
38 H6 = Hgain*2.6*100 // kJ heat gained by water
```

```
39 H1 = 100*1030000  // kJ
40 GCV = H6*100/H1
41 printf("Thermal efficiency of the boiler = "+string(GCV)+".")
```

Scilab code Exa 7.9 Stoker fired water tube boiler

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
9 // Example 7.9
10 // Page 465
11 printf("Example 7.9, Page 465 n \n");
12
13 // solution
14
15 // using mean heat capacity data Table 7.21
16 // basis 100 kmol of dry flue gas
17 \text{ H7} = 1.0875*100*30.31*(423.15-298.15)
18 \text{ H71} = 3633.654*(423.15-298.15)
19 fi7 = H71*3900*.7671/162.2 // kJ/h
20 fi1 = 3.9*1000*26170 // kJ/h
21 // performing heat balance
22 Hsteamgen = 23546.07
23 eff = Hsteamgen*100/fi1 // overall efficiency rate
24 printf("Overall efficiency rate = "+string(eff)+"
      percent.")
```

Scilab code Exa 7.10 Atomization of fuel

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
8
9 // Example 7.10
10 // Page 468
11 printf("Example 7.10, Page 468 n \n");
12
13 // solution
14
15 // basis 100 kg of fuel oil
16 \text{ O2req} = 9.364 // \text{kmol}
17 \text{ N2in} = (79/21)*02req
18 \text{ tN2} = \text{N2in} + .036
19 AIRreq = 02req*32 + tN2*28
20 \text{ rAIR} = AIRreq/100
                        // kg/kg
21 \text{ wp} = 4.5 // \text{kmol}
22 Hloss = 2442.8*wp*18/100 // kJ/kg fuel
23 \text{ NCV} = 43540 - \text{Hloss}
\n (b) \n Theoretical air required = "+string"
      (rAIR)+" kg/kg fuel. \n \n \n \c) \n \n \n \
                       // kJ
25 \text{ H1} = 100*41561.33
26 // from table 5.1
27 \text{ H71} = 1349.726*(1500-298.15)+252.924*10^-3 *
      ((1500^2 - 298.15^2)/2)
      +257.436*10^-6*((1500^3-298.15^3)/3)
      -137.532*10^-9*((1500^4-298.15^4)/4) // upto
      1500 K
28 H711 = H1-H71 // above 1500K
29 // F(T) = \{1500 \text{ to } T\} \text{ integr} [1477.301+375.2710*10^{-3}]
      T-91.2760*10^{-}-6T^{2}+8.146*10^{-}-9T^{3}dT-2147118
```

```
(i)
30 // solving it for T = 2000
31 \text{ AFT} = 2612.71 // \text{ K}
32 printf ("When fluid is burnt with theoretical air AFT
       = "+string(AFT)+" K. n n n (d) n n "
33 // with 30\% excess air
34 \quad 02spld = 9.364*1.3
35 \text{ xcsO2} = \text{O2spld-O2req}
36 \text{ N2in1} = (79/21)*02spld
37 \text{ tN21} = \text{N2in1} + .036
38 // now, using table 7.26, table 7.27 and eq(i) we
      get
39 \text{ AFT1} = 2178.66 // K
40 // from fig 7.3
41 \text{ dp} = 429 // \text{ K}
42 // similarly for incomplete combustion we find
43 AFT2 = 2561.42 / K
44 printf("When 30 percent excess air is supplied AFT =
       "+string(AFT1)+" K. \n \n \n \d \n \n Dew Point
       = "+string(dp)+" K. n n (e) n row For
      incomplete combustion AFT = "+string(AFT2)+" K.")
```

Scilab code Exa 7.11 Water tube boiler

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
8
9 // Example 7.11
10 // Page 473
11 printf("Example 7.11, Page 473 \n \n");
```

```
12
13 // solution
14
15 // basis 100 kg of fuel
16 // material balance of carbon
17 \text{ CO2} = 7.092 + .047 //\text{kmol} in flue gases
18 N2 = 11.94*7.139/7.01
19 \quad 02 = 11.94*7.139/7.01
20 \text{ flue} = C02 + N2 + 02
21 // material balance of O2
22 \quad 02air = 21*N2/79
23 airin = N2+02air
24 t02in = 02air+.078 // O2 in burner
25 \quad 02xcs = t02in - 9.864
26 // material balance of water vapour
27 moistfrmd = 5.45 // \text{ kmol} from combustion of H2
28 H = .0331 // kmol/kmol of dry air humidity at
       100.7 kPa
29 moistair = H*104.482 //kmol
30 tmoist = moistfrmd+moistair
31 \text{ pxcsair} = 02xcs*100/9.786
32 // now using table 7.32
33 H7 = 3391.203*(563.15-298.15) //kJ
34 Ff = 400 // \text{kg/h} fuel firing rate
35 tH = 2791.7-179.99 // kJ/kg total heat supplied
      in boiler
36 fi5 = tH*4365 // kJ/h
37 fi8 = 5.45*18*Ff*2403.5/100 // kJ/h
38 \text{ GCVf} = 42260
                  //kJ/kg
39 \text{ fil} = \text{Ff}*\text{GCVf}
40 \text{ Fdryair} = 104.482*29*Ff/100
41 Cha = 1.006+1.84*.0205 // kJ/kg dry air K
42 \text{ fi3} = \text{Fdryair}*\text{Cha}*(308.15-298.15)
43 fi2 = Ff*1.758*(353.15-298.15)
44 BOILEReff1 = fi5*100/fi1
45 NCVf = GCVf - (18.0153/2.016)*.109*2442.8 // kJ/kg
46 BOILEReff2 = fi5*100/(Ff*NCVf)
47 r = 4365/Ff // steam: fuel
```

```
48 BOILERcapacity = fi5/2256.9
49 printf(" After performing material and thermal
    balance operations we get \n \n Overall thermal
    efficiency of the boiler based on GCV of the fuel
    = "+string(BOILEReff1)+" percent. \n \n Overall
    efficiency of the boiler based on NCV of the fuel
    = "+string(BOILEReff2)+" percent. \n \n Steam to
    fuel ratio = "+string(r)+" at 16 bar. \n \n
    Equivalent boiler capacity = "+string(
    BOILERcapacity)+" kg/h.")
```

Scilab code Exa 7.12 Gassification by coal

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
9 // Example 7.12
10 // Page 478
11 printf("Example 7.12, Page 478 n \n");
12
13 // solution
14
15 // basis 100 kmol of dry producer gas
16 \ C = 33*12 // kg
17 \ 02 = 18.5*32 \ //kg
18 \text{ H2} = 20*2 // \text{ kg}
19 O2air = 21*51/79 / kmol
20 COALgassified = 396/.672 // kg
21 O2coal = COALgassified*.061/32 // kmol
22 \text{ tO2} = 02\text{coal} + 02\text{air}
```

```
23 O2steam = 18.5 - t02 // kmol
24 H2steam = 2*02steam // kmol
25 H2fuel = 20-H2steam
26 dryproducergas = 100*22.41/\text{COALgassified} // Nm<sup>3</sup>/kg
      coal
27 \text{ Pw} = 2.642 \text{ // kPa}
28 \text{ Ha} = Pw/(100.7-Pw)
                      // kmol/kmol dry gas
29 water = Ha*100
30 moistproducergas = (100+water)*22.41/COALgassified
     // Nm<sup>3</sup>/kg coal
31 dryair = (51*28+02air*32)/COALgassified
                                           // kg/kg
32 tsteamsupplied = H2steam+water-(COALgassified
     *.026/18)
                // kmol
33 steam = tsteamsupplied*18/COALgassified
34 printf(" (a) n \in Moistproducer gas obtained = "+
     (b) \n \n Air supplied = "+string(dryair)+" kg/
     kg coal gassified. \n \n \n (c) \n \n Steam
     supplied = "+string(steam)+" kg/kg coal.")
```

Scilab code Exa 7.13 Open Hearth steel furnace

```
1 clear;
2 clc;
3
4 // Stoichiometry
5 // Chapter 7
6 // Combustion
7
8
9 // Example 7.13
10 // Page 479
11 printf("Example 7.13, Page 479 \n \n");
12
```

```
13 // solution
14
15 // solving by alternate method on page 483
16 // basis 100 kmol of dry producer gas
17 // using tables 7.38 and 7.39
18 fi7 = 6469.67*(833.15-298.15)*(27650/2672) // kJ/h
19 // heat output basis 1 kg of steam
20 // referring Appendix IV
21 \text{ H4} = 675.47 - 272.03 // kJ/kg
22 \text{ Ts} = 463 // \text{ K}
23 h = 806.69 // kJ/kg
24 lambdav = 1977.4 // kJ/kg
25 Hss = 2784.1 // kJ/kg at Ts
26 i = 3045.6 // kJ/kg
27 \text{ H6} = i-\text{Hss}
28 fi4 = H4*7100 // kJ/h
                             // kJ/h
29 \text{ fi5} = (\text{Hss}-675.47)*7100
30 fi6 = H6*7100 // kJ/h
31 recovery = fi4+fi5+fi6
32 BOILERcapacity = recovery *3600/2256.9 // kg/h
33 fi8 = 6125.47*(478.15-298.15)*(27650/2672) // kJ/h
34 hloss = fi7-fi4-fi5-fi6-fi8 /// kJ/h
35 printf (" Heat Balance of Waste Heat Boiler \n \n \n
                                      kJ/h \n Heat Output
       \n Steam rising \n Economiser
                          "+string(fi4)+" \n Steam
                               "+string(fi5)+" \n Super
      generator
                               "+string(fi6)+" n n
      heater
                                     "+string(fi8)+" \n
      Heat loss in flue gases
                                      "+string(hloss)+"")
      Unaccounted heat loss
```