Scilab Textbook Companion for Advanced Engineering Chemistry by M. Senapati[1]

Created by
Nitya Lakkaraju
BTech
Electronics Engineering
VBIT
College Teacher
None
Cross-Checked by
Aviral

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Book Description

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

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

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

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

Contents

List of Scilab Codes

Chapter 1

Structure and Bonding

Scilab code Exa 1.1 Prob 1

```
//Chapter 1: Structure and Bonding
//Problem: 1
clc;

//Declaration of Constant
c = 3 * 10 ** 10                        // Velocity of light,in cm/sec

//Declaration of Variable
w = 3500 * 10 ** -8     // Wavelength of radiation,in cm

// Solution
mprintf("v = c / w\n")  //v is Velocity, c is Speed of light ,w is the wavelength

v = c / w

mprintf(" The frequency of radiation is %.2e Hz",v)
```

Scilab code Exa 1.2 Prob 2

```
//Chapter 1: Structure and Bonding
//Problem: 2
clc;

//Declaration of Constant
c = 3 * 10 ** 8                    // speed of light ,in
    m/sec

//Declaration of Variable
f = 5 * 10 ** 16                   // frequency ,in
    cycles/sec

// Solution
v = f / c
mprintf("The wave number is %.2e cycles/m",v)
```

Scilab code Exa 1.3 Prob 3

```
//Chapter 1: Structure and Bonding
//Problem: 3
clc;

//Declaration of Constant
c = 3 * 10 ** 8                    // Speed of light ,in
    m/sec

//Declaration of Variable
T = 2.4 * 10 ** -10                // Time period ,in
    sec

```

```
// Solution
f = 1 / T                          // Frequency, per sec
lamda = c / f                      // Wavelength, in m
v = 1 / lamda                      // Wavenumber, per meter

mprintf("Frequency: %.2e /sec\n', f)
mprintf(" Wavelength: %.2e m\n", lamda)
mprintf(" Wave number: %.2e /m", v)
```

Scilab code Exa 1.4 Prob 4

```
//Chapter 1: Structure and Bonding
//Problem: 4
clc;

//Declaration of Constants
c = 3 * 10 ** 8                    // Speed of light, in m/sec
m = 9.1 * 10 ** -31                // Mass of electron, in kg
h = 6.626 * 10 ** -34              // Plank's constant, in J.sec

//Declaration of Variable
ke = 4.55 * 10 ** -25              // Kinetic Energy, in J

// Solution
v = sqrt(ke * 2 / m)

lamda = h / (m * v)

mprintf("The de Broglie wavelength is : %.2e m', lamda)
```

Scilab code Exa 1.5 Prob 5

```
//Chapter 1: Structure and Bonding
//Problem: 5
clc;

//Declaration of Constant
h = 6.626 * 10 ** -34             // Plank's constant,
    in J.sec

//Declaration of Variables
m = 10 * 10 ** -3                 // Mass of the ball,
    in kg
v = 10 ** 5                       // Velocity of ball,
    in cm / sec

// Solution
lamda = (h * 10 ** 7) / (m * v)
mprintf("The Wavelength of iron ball is %.2e cm",
    lamda)
```

Scilab code Exa 1.6 Prob 6

```
//Chapter 1: Structure and Bonding
//Problem: 6
clc;

//Declaration of Constant
h = 6.626 * 10 ** -34             // Plank's constant,
    in J.sec

// Variable
```

```
lamda = 2 * 10 ** -10                // wavelength, in m

// Solution
p = h / lamda

mprintf("The momentum of the particle is :%.2e kg m/
   s",p)
```

Scilab code Exa 1.7 Prob 7

```
//Chapter 1: Structure and Bonding
//Problem: 7
clc;

//Declaration of Constants
m = 9.1 * 10 ** -31                  // Mass of electron,
    kg
h = 6.626 * 10 ** -34                // Plank's constant,
    J.sec
pi = 3.141                           // Pi

// Variable
delta_x = 1 * 10 ** -10              // Uncertainty in
   Velocity, m

// Solution
delta_v = h / (4 * pi * m * delta_x)

mprintf( "Uncertainty in position of electron >= :%
   .1e m/s",delta_v)
```

Scilab code Exa 1.8 Prob 8

```
//Chapter 1: Structure and Bonding
//Problem: 8
clc;

//Declaration of Constants
h = 6.626 * 10 ** -34               // Plank's constant, J.sec
pi = 3.141                          // Pi

// Variables
m = 10 ** -11                       // Mass of particle, g
v = 10 ** -4                        // Velocity of particle, cm/sec
delta_v = 0.1 / 100                 // Uncertainty in velocity

// Solution
delta_v = v / 1000
delta_x = (h * 10 ** 7) / (4 * pi * delta_v * m)

printf("Uncertainty in position >=%.3e cm",delta_x)
```

Scilab code Exa 1.9 Prob 9

```
//Chapter 1: Structure and Bonding
//Problem: 9
clc;

//Declaration of Constants
c = 3 * 10 ** 8                     // Speed of light, m/sec
h = 6.626 * 10 ** -34               // Plank's constant, J.sec

```

```
// Variable
lamda = 650 * 10 ** -12          // Wavelength of radiation , m

// Solution
E = h * c / lamda

mprintf("Energy per photon :%.3e J",E)
```

Scilab code Exa 1.10 Prob 10

```
//Chapter 1: Structure and Bonding
//Problem: 10
clc;

//Declaration of Constant
h = 6.625 * 10 ** -34           // Plank's constant , J.sec

// Variables
v = 6.5 * 10 ** 7               // Velocity of particle , m/s
lamda = 5 * 10 ** -11           // Wavelength , m

// Solution
P = h / lamda

mprintf("The momentum of the particle :%.2e kg m/s", P)
```

Scilab code Exa 1.11 Prob 11

```
//Chapter 1: Structure and Bonding
```

```
//Problem: 11
clc;

//Declaration of Constants
c = 3 * 10 ** 8                     // Speed of light, m/sec
m = 9.1 * 10 ** -31                 // Mass of electron, kg
h = 6.626 * 10 ** -34               // Plank's constant, J.sec

// Variables
lamda = 200 * 10 ** -7              // Wavelength, cm
wf = 6.95 * 10 ** -12               // Work function, erg

// Solution
E = (h * c) * 10 ** 9 / lamda

mprintf("Energy of photon :%.3e erg\n",E)

ke = E - wf

v = sqrt((2 * ke) / (m * 10 ** 3)) * 10 ** -2

mprintf(" The maximum velocity of electron :%.3e m/sec",v)
```

Scilab code Exa 1.12 Prob 12

```
//Chapter 1: Structure and Bonding
//Problem: 12
clc;

//Declaration of Constant
```

```
h = 6.626 * 10 ** -34              // Plank's constant, J.sec

// Variables
m = 150                            // Weight of ball, gm
v = 50                             // Velocity, m/sec

lamda = h / (m * v * 10 ** -8)
mprintf("Wavelength of ball :%.3e m\n",lamda)
mprintf(" Its wavelength is so short that it does not fall in visible range, so we cannot observe it.")
```

Scilab code Exa 1.13 Prob 13

```
//Chapter 1: Structure and Bonding
//Problem: 13
clc;

//Declaration of Constant
h = 6.626 * 10 ** -34              // Plank's constant, J.sec
pi = 3.141                         // Pi

// Variables
m = 0.1                            // Mass of base ball, kg
delta_x = 10 ** -10                // Uncertainty in position, m

// Solution
delta_v = h / (4 * pi * m * delta_x)

mprintf("Uncertainty in velocity >= %.2e m/s",
```

```
delta_v)
```

Scilab code Exa 1.14 Prob 14

```
//Chapter 1: Structure and Bonding
//Problem: 14
clc;

//Declaration of Constant
t_v = 1.3 * 10 ** 15                // Threshold freq.
    Pt, /sec
h = 6.626 * 10 ** -34               // Planck's constant
    , J.sec


// Solution
mprintf("The threshold frequency is the lowest
    frequency that photons may possess to produce the
     photoelectric effect.\n")
E = h * t_v
mprintf(" The energy corresponding to this frequency
     is the minimum energy = %.2e erg",E)
```

Scilab code Exa 1.15 Prob 15

```
//Chapter 1: Structure and Bonding
//Problem: 15
clc;

//Declaration of Constants
m = 9.1 * 10 ** -31                 // Mass of electron,
     kg
```

```
h = 6.626 * 10 ** -34                 // Plank's constant, J.sec
e = 1.602 * 10 ** -19                 // Charge of electron, C

// Variable
v = 1.87 * 10 ** 9                    // Velocity of electron, m/sec

// Solution
V = m * v ** 2 / (2 * e)
lamda = h / (m * v)

mprintf("The voltage is %.2e Volts\n",V)
mprintf(" The de Broglie wavelength is %.2e m",lamda)
```

Scilab code Exa 1.16 Prob 16

```
//Chapter 1: Structure and Bonding
//Problem: 16
clc;

//Declaration of Constants
m = 9.1 * 10 ** -31                   // Mass of electron, kg
h = 6.626 * 10 ** -34                 // Plank's constant, J.sec

// Variable
lamda = 4.8 * 10 ** -9                // Wavelength of electron, m

// Solution
ke = ((h / lamda) ** 2) / (2 * m)
```

```

mprintf("The Kinetic Energy of moving electron is %.2e J",ke)
```

Scilab code Exa 1.17 Prob 17

```
//Chapter 1: Structure and Bonding
//Problem: 17
clc;

//Declaration of Constants
m = 9.1 * 10 ** -31                    // Mass of electron, kg
h = 6.626 * 10 ** -34                  // Plank's constant, J.sec
c = 3 * 10 ** 8                        // Speed of light, m/sec

// Variables
v = 6.46 * 10 ** 5                     // Velocity of electron, m/sec
lamda = 200 * 10 ** -9                 // Wavelength of light, m

// Solution
E = (h * c) / lamda
ke = m * v ** 2
w = E - ke

mprintf("The Workfunction of the metal surface is %.3e J",w)
```

Scilab code Exa 1.18 Prob 18

```
//Chapter 1: Structure and Bonding
//Problem: 18
clc;

//Declaration of Constants
e = 1.602 * 10 ** -19                    // Charge of proton ,
    C
m_p = 1.66 * 10 ** -27                   // Mass of proton ,
    kg
m_e = 9.1 * 10 ** -31                    // Mass of electron ,
    kg
h = 6.626 * 10 ** -34                    // Plank's constant ,
    J.sec

// Variable
V = 35                                   // Acceleration
    potential , volt

// Solution
lamda_p = h / sqrt(2 * e * V * m_p)
lamda_e = h / sqrt(2 * e * V * m_e)

mprintf("The wavelength of electron when accelerated
    with same potential is %.3e m",lamda_e)
```

Scilab code Exa 1.19 Prob 19

```
//Chapter 1: Structure and Bonding
//Problem: 19
clc;

B_O1 = (10 - 6) / 2                       // Bond Order for
    O2
B_O2 = (10 - 7) / 2                       // Bond Order for
    O2-
```

```
r=B_O1 > B_O2

if r==%t then disp("Bond length of O2− > O2 as Bond
   order of O2 > Bond order of O2−")
end

mprintf(" Both are paramagnetic , because they
   contain unpaired electrons.")
```

Scilab code Exa 1.20 Prob 20

```
//Chapter 1: Structure and Bonding
//Problem: 20
clc;

B_O = (9 - 4) / 2.0          // Bond order of N2+

printf( "MO configuration of N2+ is\n")
printf("    (1s2)   *(1s2)   (2s2)   *(2s2) [   (2px2) =
      (2py2)]    (2pz1)\n")
printf("\n The Bond order of N2+, 1/2[Nb − Na] =%.1f
   ", B_O)
```

Scilab code Exa 1.21 Prob 21

```
//Chapter 1: Structure and Bonding
//Problem: 21
clc;

// Solution
v_n = 2 * 5              // number of valence e− in
   nitrogen
```

```
v_co = 4 + 6                 // number of valence e- in CO

mprintf("The Number of valence electrons in N2 is %d\n", v_n)
mprintf(" The Number of valence electrons in CO is %d", v_co)
```

Chapter 2

Spectroscopy and Photochemistry

Scilab code Exa 2.1 Prob 1

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem: 1
clc;

//Declaration of Constants
m_br79 = 78.9183                // Mass of 79Br,in amu
m_br81 = 80.9163                // Mass of 91Br,in amu
Na = 6.022 * 10 ** 23           // Mole constant,per mol
pi = 3.141                      // Pi
c = 3 * 10 ** 10                // Speed of light,in cm/s

//Declaration of Variable
wave_no = 323.2                 // Wave no. of fund. vibration of 79Br - 81Br, /cm

// Solution
mu = (m_br79 * m_br81) / ((m_br79 + m_br81) * Na)

```

```
k = 4 * (pi * c * wave_no) ** 2 * mu * 10 ** -3

mprintf("The force constant of the bond is %.2e N/m\n",k)
```

Scilab code Exa 2.2 Prob 2

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem: 2
clc;

//Declaration of Constants
Na = 6.022 * 10 ** 23              // Mole constant, per mol
pi = 3.141                         // Pi
c = 3 * 10 ** 10                   // Speed of light, in cm/s
h = 6.626 * 10 ** -34              // Plank's constant, in J.sec

//Declaration of Variables
b_l = 112.81 * 10 ** -12           // Equillibrium bond length, in m
m1 = 12                            // Mass of Carbon, in g per mol
m2 = 16                            // Mass of Oxygen, in g per mol

// Solution
mu = m1 * m2 / ((m1 + m2) * Na)  //in g
mu = mu * 10 ** -3                     //in kg

B = h / (8 * pi ** 2 * mu * b_l ** 2 * c)
v2_3 = B * 6

```

```
mprintf("The reduced mass of CO is %.3e kg\n",mu)
mprintf(" The frequency of 3->2 transition is %.2f /cm",v2_3)
```

Scilab code Exa 2.3 Prob 3

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem: 3
clc;

//Declaration of Constants
Na = 6.022 * 10 ** 23        // Mole constant,permol

//Declaration of Variables
d_NaCl = 2.36 * 10 ** -10            // Intermolecular dist. NaCl,in m
m_Cl = 35 * 10 ** -3                 // Atomic mass, in kg /mol
m_Na = 23 * 10 ** -3                 // Atomic mass, in kg /mol

// Solution
mu = m_Na * m_Cl / ((m_Na + m_Cl) * 10 ** -3 * Na) * 10 ** -3

I = mu * d_NaCl ** 2

mprintf("The reduced mass of NaCl is %.3e kg\n",mu)
mprintf(" The moment of inertia of NaCl is %.3e kg m square",I)
```

Scilab code Exa 2.4 Prob 4

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem: 4
clc;

//Declaration of Constant
e = 4000        // Extinction coeff.,in dm cube per mol per cm

// Variable
x = 3           // Solution thickness,in cm

// Solution
A = log10(1 / 0.3)     // Absorbance
C = A / (e * x)

mprintf("The concentration of the solution is %.2e mol per dm cube",C)
```

Scilab code Exa 2.5 Prob 5

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem: 5
clc;

//Declaration of Constants
pi = 3.141                    // Pi
c = 3 * 10 ** 10              // Speed of light,in cm/s

//Declaration of Variables
v_bar = 2140                  // Fundamental vibrating freq, per cm
m_C = 19.9 * 10 ** -27        // Atomic mass of C,in kg
m_O = 26.6 * 10 ** -27        // Atomic mass of O,in
```

```
    kg

// Solution
mu = m_O * m_C / (m_C + m_O)
k = 4 * (pi * c * v_bar) ** 2 * mu

mprintf("The force constant of the molecule is %.3e
    N/m",k)
```

Scilab code Exa 2.7 Prob 7

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem: 7
clc;

//Declaration of Constants
pi = 3.141                    // pi
c = 3 * 10 ** 10              // speed of light, cm /s
h = 6.626 * 10 ** -34         // Plank's constant, J.
    sec
Na = 6.022 * 10 ** 23         // Mole constant, /mol

//Declaration of Variables
d = 20.7                      // Interspacing, /cm
m1 = 1                        // Mass of H, g / mol
m2 = 35.5                     // Masso f Cl, g / mol

// Solution
B = 0.1035 * 10 ** 2          // /m
I = h / (8 * pi ** 2 * B * c)
mu = m1 * m2 / ((m1 + m2) * Na)
mu = mu * 10 ** -3
r = sqrt(I / mu)

mprintf("The intermolecular distance of HCl is %.3e
```

```
    m",r)
// The answer provided in the textbook is wrong
```

Scilab code Exa 2.8 Prob 8

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem: 8
clc;

//Declaration of Constant
e = 8000        // Molar absorbtion coeff,in dm cube
    per mol per cm

//Declaration of Variable
l = 2.5         // Thickness of solution,in cm

// Solution
C = log10(1 / 0.3) / (e * l)

mprintf("The concentration of Solution from Lambert-
    Beer Law is %.2e mol per dm cube",C)
```

Scilab code Exa 2.10 Prob 10

```
//Chapter 2: Spectroscopy and Photochemistry
//Problem:10
clc;

mprintf("Because CO2 is a linear molecule.\n")
v_deg = 3 * 3 - 5
mprintf(" The vibrational degree of freedom is %d",
    v_deg)
```

Chapter 3

Thermodynamic and Chemical Equilibrium

Scilab code Exa 3.1 Prob 1

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 1
clc;

//Declaration of Variables
q = 120        // Heat from surrounding, cal
W = 70         // Work done, cal

// Solution
delta_E = q - W

mprintf("Change in Internal Energy :%d cals", delta_E)
```

Scilab code Exa 3.2 Prob 2

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 2
clc;

//Solution
mprintf("CH4 (g) + 2O2 (g) -> CO2 (g) + 2H20 (l)\n")

delta_n = 1 - (1 + 2)
solution = - 2 * 2 * 298                 // cals

mprintf(" Delta H - Delta E is: %d cals", solution)
```

Scilab code Exa 3.3 Prob 3

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 3
clc;

//Declaration of Variables
delta_g = -16.0         // Kelvin cal
delta_h = -10.0         // Kelvin cal
T = 300                 // Kelvin

// Solution
delta_s = (delta_h - delta_g) * 10 ** 3 / T     //
   cal/deg
new_t = 330                          // Kelvin
new_delta_g = (delta_h * 10 ** 3) - new_t * delta_s

mprintf("The free energy at 330K is: %.2e K cal",
   new_delta_g)
```

Scilab code Exa 3.4 Prob 4

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 4
clc;

//Declaration of Variables
delta_s = -20.7         // cal per deg per mol
delta_h = -67.37        // K cal
T = 25                  // deg C

// Solution
T = T + 273                 // K
delta_g = delta_h - (T * delta_s * 10 ** -3)

mprintf("The change in free energy at 25deg C is: %
   .4f K cal per mol", delta_g)
```

Scilab code Exa 3.5 Prob 5

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 5
clc;

//Declaration of Variables
wt = 1                  // g
delta_h = 149           // joules

// Solution
delta_h_f = delta_h * (10 * 12 + 8 * 1)
delta_h_f_c=delta_h_f * 10 ** -3

mprintf("Enthalpy of fusion of naphthalene:%.3f kJ/
   mol", delta_h_f_c)
```

Scilab code Exa 3.6 Prob 6

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 6
clc;

//Declaration of Variables
d_h_acetylene = 230        // kJ per mol
d_h_benzene = 85           // kJ per mol
T = 298                    // K

// Solution
d_h = d_h_benzene - 3 * d_h_acetylene

mprintf("The enthalpy change for the reaction is: %d
    kJ/mole", d_h)
```

Scilab code Exa 3.7 Prob 7

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 7
clc;

//Declaration of Constant
d_h_vap = 2.0723          // kJ per g
Tb = 373                          // K

// Solution
d_h_vap = d_h_vap * 18              // kJ per mol
d_s = d_h_vap / Tb
d_g = d_h_vap - Tb * d_s
d_s = d_s * 1000

mprintf("The Entropy change is: %.1f J / mol / K\n",
   d_s)
```

```
mprintf(" The Free Energy change is:%d kJ/mol", d_g)
```

Scilab code Exa 3.8 Prob 8

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 8
clc;

//Declaration of Constant
R = 1.987                  // cal per K per mol

//Declaration of Variables
m = 5
Vo = 4                     //in litres , Initial Volume
Vf = 40                    //in litres , Final Volume
T = 27                     //in deg C

// Solution
mprintf("dS = nRln(V2 / V1)\n")

dS = m * R * 2.303 * log10(Vf / Vo)

mprintf(" The change in entropy is: %.2f cal /
   degree",dS)
```

Scilab code Exa 3.9 Prob 9

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 9
clc;

//Declaration of Variables
wt = 10              //in g
```

```
heat_a = 4.5        //in K

// Solution
m = 10 / 100.0      // mol
d_h = heat_a / m
mprintf("The heat of the reaction is:%d K cal / mol"
   , d_h)
```

Scilab code Exa 3.10 Prob 10

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 10
clc;

//Declaration of Constant
R = 8.314                    //in J / K

//Declaration of Variables
V_O2 = 2.8                   //in litres
V_H2 = 19.6                  //in litres

// Solution
na = V_O2 / 22.4             //in mol
nb = V_H2 / 22.4             //in mol
Xa = na / (na + nb)
Xb = nb / (na + nb)
d_s = (- R) * (na * log(Xa) + nb * log(Xb))

mprintf("The increase in entropy on mixing is : %.3f
    J /K",d_s)
```

Scilab code Exa 3.12 Prob 12

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 12
clc;

//Declaration of Variables
d_g_25 = - 85.77         // kJ, Free Energy at 25 C
d_g_35 = - 83.68         // kJ, Free Energy at 35 C
Ti = 273 + 25                // K
Tf = 273 + 35                // K

// Solution
mprintf("Equating the entropy change at both the temperatures.\n")
mprintf(" (d_h + d_g_25) / Ti = (d_h + d_g_35) / Tf\n")
d_h = - 148
mprintf(" The change in enthalpy for the process at 30C is %d kJ", d_h)
```

Scilab code Exa 3.13 Prob 13

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 13
clc;

//Declaration of Constants
l_v = 101              //in cal /g, Latent headt of vap.
mwt = 78              // molecular weight of benzene

//Declaration of Variable
m = 2
Tb = 80.2            // C, boiling point of benzene

// Solution
```

```
Tb = Tb + 273       // K
d_h = l_v * mwt
d_s = d_h / Tb
d_g = d_h - Tb * d_s

mprintf("d_s = %.2f cal / K\n",d_s)
mprintf(" d_g = d_a = %d", d_g)
```

Scilab code Exa 3.14 Prob 14

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 14
clc;

//Declaration of Variables
V1 = 6              //in dm cube
V2 = 2              //in dm cube
T1 = 27             //in C
m = 5

// Solution
mprintf("T1*V1 ^ (gamma - 1) = T2 * V2 ^ (gamma - 1)\n")

T1 =T1 + 273        // K
T2 = T1 * (V1 / V2) ** (8.314 / 20.91)

mprintf(" The Final Temperature is %.1f K\n",T2)

q = 0               //For Adiabatic process
d_E = - m * 20.91 * (T2 - T1)
d_E = d_E / 1000

mprintf(" q =%d \n", q)
mprintf(" Change is Energy is %.2f kJ / mol\n",d_E)
```

```

W = - d_E

mprintf(" W = %.2f kJ /mol",d_E)
```

Scilab code Exa 3.15 Prob 15

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 15
clc;

//Declaration of Constant
R = 8.314           //in J / K mol

//Declaration of Variables
m = 1
V1 = 5              // dm cube
V2 = 10             // dm cube
T = 300             // K

// Solution
mprintf("For isothermal and reversible process,\n")

d_E = 0
d_H = 0
d_A = - 2.303 * m * R * T * log10(V2 / V1)
d_G = - 2.303 * m * R * T * log10(V2 / V1)
q = - d_G
W = - d_G

mprintf(" d_E = d_H = %d \n", d_H)
mprintf(" d_G = d_A =%.3f J / mol\n",d_G)
mprintf(" For isothermal and reversible expansion\n"
   )
mprintf(" q = W = -d_G = %.3f J / mol",W)
```

Scilab code Exa 3.16 Prob 16

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 16
clc;

//Declaration of Constant
R = 8.314          //in J per K mol

//Declaration of Variables
n = 5              // moles
T = 27             // C
V1 = 50.0          // L, Initial Volume
V2 = 1000          // L, Final Volume

//Solution
T = T + 273
d_G = 2.303 * n * R * T * log10(V1 / V2)
d_G = d_G / 1000
mprintf("The free energy change is :%.3f kJ",d_G)
```

Scilab code Exa 3.17 Prob 17

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 17
clc;

//Declaration of Variables
d_H_n = - 51.46         // kJ/mol, neutralization
d_H_i = - 57.1          // kJ/mol, ionization

```

```
//Solution
d_H = - d_H_i + d_H_n

mprintf("The head of ionization for NH4OH is %.2f kJ
    / mol", d_H)
```

Scilab code Exa 3.20 Prob 20

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 20
clc;

// Solution
Eq_HI = 1.56 / 2
Eq_H2 = 0.22 / 2
Eq_I2 = 0.22 / 2
Kc = Eq_H2 * Eq_I2 / (Eq_HI ** 2)
mprintf("The equilibrium constant for the
   dissociation reaction %.4f",Kc)
```

Scilab code Exa 3.21 Prob 21

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 21
clc;

//Declaration of Variables
Kc = 0.5          // mole square litre square
T = 400           // K
R = 0.082         // litre atm per degree  per mole

// Solution
Kp = Kc * (R * T) ** (-2)
```

```
mprintf("The given equilibrium is\n")
mprintf(" N2(g) + 3H2(g) <--> 2NH3(g)\n")
mprintf(" Kp is %.3e",Kp)
```

Scilab code Exa 3.22 Prob 22

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 22
clc;

//Declaration of Variables
solubility = 7.5 * 10 ** - 5        // mol per L

// Solution
Ksp = 4 * (solubility ** 3)
mprintf("Solubility product of the salt is %.3e mol
   cube L cube",Ksp)
```

Scilab code Exa 3.23 Prob 23

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 23
clc;

//Declaration of Variables
Ti = 25            // C
S = 0.00179        // g / L

// Solution
S =S / 170         // mol / L
Ksp = S ** 2
```

```
mprintf("Solubility product at 25 C is %.4e mol square L square",Ksp)
```

Scilab code Exa 3.24 Prob 24

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 24
clc;

//Declaration of Variables
Ksp = 8 * 10 ** - 5                    // Solubility product PbBr2
diss = 80 / 100                        // % dissociation

// Solution
S = (Ksp / 4) ** (1 / 3.0)             // Solubility is 100%
S_80 = S * (80 / 100.0)
S_per_g = S_80 * 367 - 1.621
mprintf("Solubility in gm per litre is %.3f gm / l",S_per_g)
```

Scilab code Exa 3.27 Prob 27

```
//Chapter 3: Thermodynamic and Chemical Equilibrium
//Problem: 27
clc;

//Declaration of Variables
n_salt = 0.02        // mole
n_base = 0.2         // mole
pKb = 4.7

```

```
// Solution
pOH = pKb + log10(n_salt / n_base)
pH = 14 - pOH
mprintf("pH of a buffer solution is %.1f", pH)
```

Chapter 5

Chemical Kinetics and Catalysis

Scilab code Exa 5.1 Prob 1

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 1
clc;

//Declaration of Variables
K = 3.5 * 10 ** - 2               // Rate constant

// Solution
mprintf("First order reaction = 0.693 / K\n")
t = 0.693 / K
mprintf(" Time taken for half the initial
   concentration to react:%.1f minutes", t)
```

Scilab code Exa 5.2 Prob 2

```
//Chapter 5: Chemical Kinetics and Catalysis
```

```
//Problem: 2
clc;

//Declaration of Variables
t = 40        //in minutes

// Solution
mprintf("Rate constant = 0.693 / t\n")
K = 0.693 / t
mprintf(" Rate constant = %.4f / min",K)
```

Scilab code Exa 5.3 Prob 3

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 3
clc;

//Declaration of Variables
t0 = 37.0                    //in cm cube of KMnO4
t5 = 29.8                    //in cm cube of KMnO4
t15 = 19.6                   //in cm cube of KMnO4
t25 = 12.3                   //in cm cube of KMnO4
t45 = 5.00                   //in cm cube of KMnO4

// Solution
K5 = 2.303 / 5 * log10(t0 / t5)
K15 = 2.303 / 15 * log10(t0 / t15)
K25 = 2.303 / 25 * log10(t0 / t25)
K45 = 2.303 / 45 * log10(t0 / t45)

mprintf("At t = 5 min, K = %.3e /min\n",K5)
mprintf(" At t = 15 min, K = %.3e /min\n",K15)
mprintf(" At t = 25 min, K = %.3e /min\n",K25)
mprintf(" At t = 45 min, K = %.3e /min\n",K45)
mprintf(" As the different values of K are nearly
```

```
   same, the reaction is of first-order\n")
K = (K45 + K25 + K5 + K15) / 4
mprintf(" The average value of K = %.3e /min",K)
```

Scilab code Exa 5.4 Prob 4

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 4
clc;

//Declaration of Variables
t = 60                       //in min
x = "0.5a"
K = 5.2 * 10 ** - 3          //in per mol L per min

// Solution
a = 1 / (t * K)
mprintf("Initial concentration = %.3f mol / L",a)
```

Scilab code Exa 5.5 Prob 5

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 5
clc;

// Solution
t = ((2.303 * log10(100 / (100 - 99.9))) / (2.303 *
   log10(100 / (100 - 50))))
mprintf("99.9 percent / 50 percent =%.1f",t)
```

Scilab code Exa 5.6 Prob 6

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 6
clc;

//Declaration of Constants
R = 1.987                    //in cal per K per mol

//Declaration of Variables
T1 = 273.0                   //in K
T2 = 303.0                   //in K
K1 = 2.45 * 10 ** -5
K2 = 162 * 10 ** -5

// Solution
Ea = log10(K2 / K1) * R * 2.303 / ((T2 - T1) / (T1 *
    T2))
mprintf("The activation energy of the reaction is %d
    cal / mol",Ea)
```

Scilab code Exa 5.7 Prob 7

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 7
clc;

//Declaration of Variables
t05 = 30                     //in minutes
a = 0.1                      //in M

// Solution
mprintf("For second order reaction,\n t0.5 = 1 / Ka\
   n")
K = 1 / (a * t05)
```

```
mprintf(" The rate constant is %.3f mol per lit per
    min",K)
```

Scilab code Exa 5.8 Prob 8

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 8
clc;

//Declaration of Variables
T = 500         //in C
Pi = 350        //in torr
r1 = 1.07       //in torr / s
r2 = 0.76       //in torr / s

// Solution
mprintf("1.07 = k(0.95a)^n\n")
mprintf(" 0.76 = k(0.80a)^n\n")
n = log(r1 / r2) / log(0.95 / 0.80)
n=ceil(n)
mprintf(" Hence, order of reaction is %d",n)
```

Scilab code Exa 5.10 Prob 10

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 10
clc;

//Declaration of Constant
R = 1.987                    //in cal per K per mol

//Declaration of Variables
K2_K1 = 4    // factor increase
```

```
T1 = 27       //in C
T2 = 47       //in C

// Solution
T1 = T1 + 273.0
T2 = T2 + 273.0
Ea = log10(4) * 2.303 * R * (T1 * T2 / (T2 - T1))
mprintf("The activation energy for the reaction is %
   .2e cal /mol",Ea)
```

Scilab code Exa 5.11 Prob 11

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 11
clc;

//Declaration of Variables
a = 1            //in mole
x = 3 / 4.0      // reaction completed

// Solution
K = (2.303 / 6) * log10(1 / (1 - x))
mprintf("The rate constant is :%.3f / min",K)
```

Scilab code Exa 5.12 Prob 12

```
//Chapter 5: Chemical Kinetics and Catalysis
//Problem: 12
clc;

// Solution
mprintf("Let the initial concentration be 100, when
   x = 25,t = 30 minutes\n")
```

```
a = 100
x = 25.0
t = 30
K = 2.303 / t * log10(a / (a - x))
t05 = 0.683 / K
t = 2.303 / K * log10(a / x)
mprintf(" K = %.2e / min\n",K)
mprintf(" T0.5 = %.2f min\n",t05)
mprintf(" t = %.1f min",t)
```

Chapter 6

Electrochemistry

Scilab code Exa 6.2 Prob 2

```
//Chapter 6: Electrochemistry
//Problem: 2
clc;

//Declaration of Variables
T = 25          // C
Cu = 0.1        // M
Zn = 0.001      // M
Eo = 1.1

// Solution
E = Eo + 0.0296 * log10(Cu / Zn)
mprintf("The emf of Daniell cell is %.4f V",E)
```

Scilab code Exa 6.3 Prob 3

```
//Chapter 6: Electrochemistry
//Problem: 3
```

```
clc;

//Declaration of Constant
R = 8.314        //in J per K
F = 96500        //in C per mol

//Declaration of Variables
Cu = 0.15       //in M
Eo = 0.34       //in V
T = 298         //in K
n = 2           //in moles

// Solution
E = Eo + (2.303 * R * T) / (n * F) * log10(Cu)
mprintf("The single electrode potential for copper
   metal is %.4f V",E)
```

Scilab code Exa 6.4 Prob 4

```
//Chapter 6: Electrochemistry
//Problem: 4
clc;

//Declaration of Variable
Eo_Cu = 0.3370       // Cu+2 -> Cu
Eo_Zn = - 0.7630     // Zn -> Zn +2

// Solution
Eo_cell = Eo_Cu - Eo_Zn

mprintf("Daniel cell is, Zn | Zn +2 || Cu+2 | Cu\n")
mprintf(" Eo (cell) is %.1f V", Eo_cell)
```

Scilab code Exa 6.5 Prob 5

```
//Chapter 6: Electrochemistry
//Problem: 5
clc;

//Declaration of Variable
Eo_Cu = 0.3370          // Cu+2 -> Cu
Eo_Cd = - 0.4003        // Cd -> Cd +2

// Solution
Eo_cell = Eo_Cu - Eo_Cd

mprintf("Cell is, Cd | Cd +2 || Cu+2 | Cu\n")
mprintf(" Eo (cell) is %.4f V", Eo_cell)
```

Scilab code Exa 6.6 Prob 6

```
//Chapter 6: Electrochemistry
//Problem: 6
clc;

//Declaration of Constant
F = 96500           // C / mol

//Declaration of Variables
n = 2
T = 25              // C
Eo_Ag = 0.80        // Ag+ / Ag
Eo_Ni = - 0.24      // Ni+2 / Ni

// Solution
Eo_Cell = Eo_Ag - Eo_Ni
delta_Go = - n * F * Eo_Cell

```

```
mprintf("Standard free energy change %d J / mol",
    delta_Go)
```

Scilab code Exa 6.8 Prob 8

```
//Chapter 6: Electrochemistry
//Problem: 8
clc;

//Declaration of Constant
F = 96500      //in C per mol

//Declaration of Variables
E1o = - 2.48   //in V
E2o = 1.61     //in V

// Solution
delta_G1 = - 3 * F * (- 2.48)
delta_G2 = - 1 * F * 1.61

mprintf("delta_G3 = delta_G1 + delta_G2\n")
mprintf(" delta_G3 = - 4 * F * E3o\n")

E3o = (delta_G1 + delta_G2) / (- 4 * F)

mprintf(" The reduction potential for the half-cell
    Pt/Ce, Ce+4 is %.4f V",E3o)
```

Scilab code Exa 6.10 Prob 10

```
//Chapter 6: Electrochemistry
//Problem: 10
clc;
```

```
//Declaration of Variables
T = 25          // C
Cu = 0.1        // M
Zn = 0.001      // M
Eo = 1.1        // V

// Solution
mprintf("Zn(s) | Zn+2 (0.001M) || Cu+2(0.1M) | Cu(s)
    \n")

Ecell = Eo + 0.0592 / 2 * log10(Cu / Zn)

mprintf(" The emf of a Daniel cell is %.4f V",Ecell)
```

Scilab code Exa 6.11 Prob 11

```
//Chapter 6: Electrochemistry
//Problem: 11
clc;

//Declaration of Variables
pH = 7          // O2
Eo = 1.229      // V
pO2 = 0.20      // bar

// Solution
mprintf("Nernst equation at 25C is,\n")
mprintf(" E = Eo - (0.0592 / 2) * log(1 / ([H+]^2 *
    [pO2]^ (1/2)))\n")

E = Eo - (0.0592 / 2) * log10(1.0 / (((10 ** (- 7))
    ** 2) * (pO2 ** (1 / 2.0))))

mprintf(" The reduction potential for the reduction
```

```
    is %.3f V",E)

// The answer provided in the textbook is wrong
```

Scilab code Exa 6.12 Prob 12

```
//Chapter 6: Electrochemistry
//Problem: 12
clc;

//Declaration of Variables
E_KCl = 0.2415        // V
E_cell = 0.445        // V


// Solution
mprintf("Emf of the cell is\n")
mprintf(" At 25C,\n")
mprintf(" E = Er - El = Eref - ((RT)/ F) * ln H+\n")

pH = (E_cell - E_KCl) / 0.059
Eo_cell = - 0.8277     // V

mprintf(" Thus, equilibrium constant for the
    reaction\n")
mprintf(" 2H2O --> H3O+  + OH- may be calculated as\
    n")

K = 10 ** (Eo_cell / 0.0591)

mprintf(" K = %.e",K)
```

Scilab code Exa 6.13 Prob 13

```
//Chapter 6: Electrochemistry
//Problem: 13
clc;

//Declaration of Variables
EoSn = 0.15          // V
EoCr = - 0.74        // V

// Solution
mprintf("3Sn+4  +  2Cr  -->  3Sn+2 + 2Cr+3\n")

Eo_cell = EoSn - EoCr
n = 6
K = 10 ** (n * Eo_cell / 0.0591)

mprintf(" The equillibrium constant for th reaction
    is %.2e ",K)
```

Scilab code Exa 6.14 Prob 14

```
//Chapter 6: Electrochemistry
//Problem: 14
clc;

//Declaration of Variables
T = 25             // C
Eo = - 0.8277      // V

// Solution
mprintf("The reversible reaction,\n")
mprintf(" 2H2O  <--> H3O+ + OH-\n")
mprintf(" May be divided into two parts.\n")
mprintf(" 2H2O + e- --> 1/2 H2 + OH-    (cathode) Eo
     = -0.8277 V\n")
mprintf(" H2O  + 1/2 H2 --> H3O+ + e-    (anode) Eo =
```

0")

Scilab code Exa 6.15 Prob 15

```
//Chapter 6: Electrochemistry
//Problem: 15
clc;

//Declaration of Variables
E = 0.4           // V

// Solution

mprintf( "The cell is Pt(H2) | H+, pH2 = 1 atm\n")
mprintf(" The cell reaction is\n")
mprintf(" 1/2 H2 --> H+ + e-\n")

pH = E / 0.0591

mprintf(" pH = %.3f ",pH)
```

Chapter 7

Solid State

Scilab code Exa 7.2 Prob 2

```
//Chapter 7: Solid State
//Problem: 2
clc;

//Declaration of Variable
a = 450      //in pm

// Solution
d = a / sqrt(2 ** 2 + 2 ** 2 + 0)
mprintf("Interplanar spacing : %d",d)
```

Scilab code Exa 7.4 Prob 4

```
//Chapter 7: Solid State
//Problem: 4
clc;

//Declaration of Variables
```

```
r_Na = 0.98 * 10 ** - 10      //in m
r_Cl = 1.81 * 10 ** - 10      //in m

// Solution
rr = r_Na / r_Cl
mprintf("When the radius ration is :%.2f, the coordination number is 6.",rr)
```

Scilab code Exa 7.5 Prob 5

```
//Chapter 7: Solid State
//Problem: 5
clc;

//Declaration of Variables
r_Li = 68        //in pm
r_F = 136.       //in pm

// Solution
rr = r_Li / r_F
mprintf("Radius ratio = %.1f\n", rr)
mprintf(" The structure of LiF is SCC and Co-ordination Number of Li+ is 6")
```

Scilab code Exa 7.6 Prob 6

```
//Chapter 7: Solid State
//Problem: 6
clc;

//Declaration of Variables
l = 2 * 10 ** - 10   //in m
t = 30               //in degrees
```

```
// Solution
mprintf("For first-order reflection\n")
d = l / (2 * sin(t))
dist = 2 * d
mprintf(" Hence, distance between planes is : %.0e m",abs(dist))
```

Scilab code Exa 7.7 Prob 7

```
//Chapter 7: Solid State
//Problem: 7
clc;

//Declaration of Variables
r = 174.6          // pm

// Solution
a = r * sqrt(8)
mprintf("For 200 plane: h = 2, k = 0, l = 0\n")
d200 = a / sqrt(2 ** 2)
mprintf(" d200 = %.1f pm\n",d200)
mprintf(" For 200 plane: h = 2, k = 2, l = 0\n")
d220 = a / sqrt(2 ** 2 + 2 ** 2)
mprintf(" d220 = %.1f pm", d220)
```

Scilab code Exa 7.8 Prob 8

```
//Chapter 7: Solid State
//Problem: 8
clc;

//Declaration of Constant
```

```
N = 6.023 * 10 ** 23

//Declaration of Variables
wt = 55.6
p = 0.29                    // nm
n = 2

// Solution
mprintf( "For BCC pattern,\n Number of Atoms per
   unit cell = 2\n")
d = n * (wt * 10 ** -3) / (N * (p * 10 ** - 9) ** 3)
mprintf(" Density of the metal is %.2e kg per m
   cube\n",d)
mprintf(" Number of nearest neighbours for BCC = 8")
```

Scilab code Exa 7.10 Prob 10

```
//Chapter 7: Solid State
//Problem: 10
clc;

//Declaration of Constant
N = 6.023 * 10 ** 23

// Variables
D = 0.53                    //in g per cm cube
MM = 6.94                   //in g per mol
n = 2

// Solution
mprintf("For BCC pattern,\n")
mprintf(" Number of Atoms per unit cell = 2\n")
V = D * N / (n * MM)
V = 1 / V
mprintf(" Volume of a unit cell of lithium metal is
```

```
%.2e cc",V)
```

Scilab code Exa 7.11 Prob 11

```
//Chapter 7: Solid State
//Problem: 11
clc;

mprintf("AB remain in BCC structure if the edge
   length is a then body diagonal ,is root(3)a\n")
mprintf(" root(3)a = 2(r+ + r-)\n")
A = (sqrt(3) * 0.4123 - 2 * 0.81) / 2
mprintf(" A+ = %.2f nm",A)
```

Chapter 12

Polymers and Polymerization

Scilab code Exa 12.1 Prob 1

```
//Chapter 12: Polymers and Polymerization
//Problem: 1
clc;

//Declaration of Variable
Mwt = 21150                 // in g per mol

// Solution
m = 2 * 12 + 3 * 1.008 + 1 * 35.45       // g per mer
n = Mwt / m
mprintf("The degree of polymerization is %d",n)
```

Scilab code Exa 12.2 Prob 2

```
//Chapter 12: Polymers and Polymerization
//Problem: 2
clc;

```

```
//Declaration of Variables
n = 10000                    // degree of polymerisation

// Solution
m = 8 * 12 + 8 * 1.008    // g / mer
M = n * m
mprintf("Molecular weight of polystyrene chain = %.1f g/mol", M)
```

Scilab code Exa 12.3 Prob 3

```
//Chapter 12: Polymers and Polymerization
//Problem: 3
clc;

//Declaration of Variables
d1 = 920                           // density,in kg per m cube
d2 = 961.97                        // density,in kg per m cube
dp = 44                            // density %

// Solution
mprintf("dp = [d2 * (p - d1)] * [100/p * (d2 - d1)]\n")
p = 937.98
mprintf(" Density of sample is %.2f kg per m cube", p)
```

Scilab code Exa 12.4 Prob 4

```
//Chapter 12: Polymers and Polymerization
//Problem: 4
```

```
clc;

//Declaration of Constant
Na = 6.022 * 10 ** 23         // Avogadros number

// Variables
wt_ethylene = 28              // g
deg = 500

// Solution
n = Na / deg

mprintf("28 g of ethylene contains %.3e molecules\n"
   ,Na)
mprintf(" No. of polyethylene formed %.3e molecules"
   ,n)
```

Chapter 13

Fuel and Combustions

Scilab code Exa 13.1 Prob 1

```
//Chapter 13: Fuel and Combustions
//Problem: 1
clc;

//Declaration of Variables
C = 84          // %
S = 1.5         // %
N = 0.6         // %
H = 5.5         // %
O = 8.4         // %

// Solution
GCV = (8080 * C + 34500 * (H - O / 8) + 2240 * S) / 100
LCV = (GCV - 9 * H / 100 * 587)
mprintf("Gross Calorific Value :%d kcal / kg\n",GCV)
mprintf(" Net Calorific Value : %.2f kcal / kg",LCV)
```

Scilab code Exa 13.2 Prob 2

```
//Chapter 13: Fuel and Combustions
//Problem: 2
clc;

//Declaration of Variables
C = 90                    // %
O = 3.0                   // %
S = 0.5                   // %
N = 0.5                   // %
ash = 2.5                 // %
LCV = 8490.5              // kcal / kg

// Solution
mprintf("HCV = LCV + 9 * H / 100 * 587\n")
mprintf(" HCV = 1/100 * (8080 * C + 34500 * (H - O /
    8) + 2240 * N)\n")
H = (8490.5 - 7754.8) / (345 - 52.8)
H = 4.575
mprintf(" The percentage of H is %.3f percent\n", H)
HCV = LCV + 52.8 * H
mprintf(" Higher calorific value of coal %.1f kcal /
    kg",HCV)
```

Scilab code Exa 13.3 Prob 3

```
//Chapter 13: Fuel and Combustions
//Problem: 3
clc;

//Declaration of Variables
x = 0.72      // g
W = 250       // g
w = 150       // g
t1 = 27.3     // C
t2 = 29.1     // C
```

```

// Solution
HCV = ((W + w) * (t2 - t1)) / x
HCV = HCV * 4185.0 / 10 ** 6
mprintf("HCV of fuel is : %.3f KJ / Kg",HCV)
```

Scilab code Exa 13.4 Prob 4

```
//Chapter 13: Fuel and Combustions
//Problem: 4
clc;

//Declaration of Variables
x = 0.84            // g
W = 1060            // g
w = 135             // g
d_t = 2.5       // C

// Solution
HCV = ((W + w) * d_t) / x
mprintf("HCV of fuel is : %.2f kcal / kg",HCV)
```

Scilab code Exa 13.5 Prob 5

```
//Chapter 13: Fuel and Combustions
//Problem: 5
clc;

//Declaration of Variables
V = 0.1         // metre cube
W = 25          // kg
t1 = 20         // C
t2 = 33         // C
```

```
m = 0.025      // kg

// Solution
HCV = W * (t2 - t1) / V
LCV = HCV - (m / V) * 580
mprintf("HCV is %d kcal / metre cube\n", HCV)
mprintf(" LCV is %d kcal / metre cube", LCV)
```

Scilab code Exa 13.6 Prob 6

```
//Chapter 13: Fuel and Combustions
//Problem: 6
clc;

//Declaration of Variables
w1 = 2.5           // g
w2 = 2.415         // g
r = 1.528          // g
ma = 0.245         // Mass of ash, g

// Solution
m = w1 - w2        // Mass of moisture in coal
mv = w2 - r        // Mass of volatile matter

moip = m * 100 / w1
vp = mv * 100 / w1
ap = ma * 100 / w1
cp = 100 - (moip + vp + ap)

mprintf("Percentage of moisture:%.1f percentage\n",
   moip)
mprintf(" Percentage of volatile matter:%.2f
   percentage\n", vp)
mprintf(" Percentage of ash:%.1f percentage\n", ap)
mprintf(" Percentage of fixed carbon:%.2f percentage
```

", cp)
```

**Scilab code Exa 13.7** Prob 7

```
//Chapter 13: Fuel and Combustions
//Problem: 7
clc;

// Solution
wt_O = 2 * 32 / 12.0
wt_a = wt_O * 100 / 23.2
vol_a = wt_a / 28.94 * 22.4

mprintf("Volume of air needed for the complete
    combustion of 2kg coke is %.3f litres at NTP",
    vol_a)
```

Scilab code Exa 13.8 Prob 8

```
//Chapter 13: Fuel and Combustions
//Problem: 8
clc;

//Declaration of Variables
C = 86       // %
H = 4        // %
N = 1.3      // %
S = 3        // %
O = 4        // %
Ash = 1.7    // %
wt = 500     // g

// Solution
```
```

```
wt_C = C / 100.0
wt_S = S / 100.0
wt_H = H / 100.0
wt_O = O / 100.0

mprintf("Nitrogen and ash are incombustible, so they do not require oxygen\n")

wt_O_C = 32 / 12.0 * wt_C
wt_O_S = 32 / 32.0 * wt_S
wt_O_H = 32 / 4.0 * wt_H

totw = wt_O_H + wt_O_S + wt_O_C
wt_O_n = totw - wt_O
wt_a = (100.0 / 23.0 * wt_O_n) * 500 / 1000.0

mprintf(" Minimum Wt. of air required by 500g of fuel %.2f kg",wt_a)
```

Scilab code Exa 13.9 Prob 9

```
//Chapter 13: Fuel and Combustions
//Problem: 9
clc;

//Declaration of Variables
wt_C = 3          // kg

// Solution
wt_a = wt_C * 32 * 100 / 12.0 / 23.0
vol_a = wt_a * 1000 * 22.4 / 28.94

mprintf("H2(g)  +  1/2 O2(g)  --> H20(l)\n")
mprintf(" 1             0.5            1\t\t(By Vol.)\n")
```

```
mprintf(" CO(g)   +   1/2  O2(g)   --> CO2(g)\n")
mprintf(" 1                0.5         1\t\t(By Vol.)\n")
mprintf(" CH4(g) +   2    O2(g)   --> CO2(g) + 2H2O(l)\n")
mprintf(" 1                2           1\t\t(By Vol.)\n")

mprintf(" Weight of air for the combustion of 3kg carbon %.3f kg\n",wt_a)
mprintf(" Vol. of air required for combustion of 3kg carbon %.3e L (or) %.2f metre cube",vol_a,vol_a / 1000)
```

Scilab code Exa 13.10 Prob 10

```
//Chapter 13: Fuel and Combustions
//Problem: 10
clc;

//Declaration of Variables
H = 0.30        // metre cube
CO = 0.10       // metre cube
CH4 = 0.04      // metre cube
N2 = 0.56       // metre cube

// Solution
vol_o = H * 0.5 + CO * 0.5 + CH4 * 2
vol_a = vol_o * 100 / 21

mprintf("Volumer of air required for complete combustion of 1 metre cube of producer gas: %.3f metre cube",vol_a)
```

Scilab code Exa 13.11 Prob 11

```
//Chapter 13: Fuel and Combustions
//Problem: 11
clc;

//Declaration of Variables
H = 15.4            //in %
C = 84.6            //in %
wt_fuel = 1         //in kg
wt_C = 0.846        //in kg
wt_H = 0.154        //in kg

// Solution
mprintf("The combustion reactions are,\n")
mprintf(" C + O2 --> CO2\n")
mprintf(" 12  32  \t(by Weight)\n")
mprintf(" 2H2 + O2 --> H20\n")
mprintf(" 4     32\t(by Weight)\n")

wt_O = 32 / 12.0 * wt_C
wt_O_H = 32 / 4.0 * wt_H
totwt = wt_O + wt_O_H
totwc=22.4 / 32 * totwt * 1000

mprintf(" Because 32 gm of O2 occupies a volume of
   22.4 liters at NTP\n")
mprintf(" 3.488 * 1000 gm of O2 will occupy %.1f l",
   totwc)
```

Scilab code Exa 13.12 Prob 12

```
//Chapter 13: Fuel and Combustions
//Problem: 12
clc;

//Declaration of Variables
C = 750         // g
H = 52          // g
O = 121         // g
N = 32          // g
ash = 45        // g

// Solution
min_wt_a = (C * 32 / 12. + H * 16 / 2. - O) * 100 /
   23.
HCV = 1 / 1000. * (8080 * C + 34500 * (H - O / 8.) +
    2240 * O)
LCV = HCV - 0.09 * H * 587 / 10.0

mprintf("HCV is %d kcal/kg\n",HCV)
mprintf(" LCV is %d kcal/kg",LCV)
```

Scilab code Exa 13.13 Prob 13

```
//Chapter 13: Fuel and Combustions
//Problem: 13
clc;

//Declaration of Variables
C = 81          // %
H = 8           // %
N = 2           // %
O = 5           // %

// Solution
mprintf("In 1kg coal,\n")
```

```
wt_C = C * 10
wt_H = H * 10
wt_N = N * 10
wt_O = O * 10
wt_ash = 100 - (wt_O + wt_N + wt_H + wt_C)

wt_a = ((wt_C * 32 / 12. + wt_H * 16 / 2. - wt_O) *
    100 / 23.) / 1000.

mprintf(" Weight of air required for complete
    combustion of 10kg coal = %.2f kg\n",wt_a * 10)

HCV = 1 / 100. * (8080 * C + 34500 * (H - O / 8.))
LCV = HCV - 0.09 * H * 587

mprintf(" HCV is %d kcal/kg\n",HCV)
mprintf(" LCV is %d kcal/kg\n",LCV)
```

Scilab code Exa 13.14 Prob 14

```
//Chapter 13: Fuel and Combustions
//Problem: 14
clc;

//Declaration of Variables
C = 80        // %
H = 7         // %
N = 2.1       // %
O = 3         // %
S = 3.5       // %
Ash = 4.4     // %

// Solution
HCV = 1 / 100. * (8080 * C + 34500 * (H - O / 8.) +
```

```
   2240 * S)
LCV = HCV - 0.09 * H * 587

mprintf("HCV is %d kcal/kg\n",HCV)
mprintf(" LCV is %d kcal/kg",LCV)
```

Chapter 14

Water Treatment

Scilab code Exa 14.1 Prob 1

```
//Chapter 14: Water Treatment
//Problem: 1
clc;

//Declaration of Variables
wt_CaSO4 = 160 //in mg/L

//Solution
hardness = 100 * wt_CaSO4 / 136.
mprintf("The hardness is:%.2f mg/L of CaCO3 eqv.",
    hardness)
```

Scilab code Exa 14.2 Prob 2

```
//Chapter 14: Water Treatment
//Problem: 2
clc;

```

```
//Declaration of Variables
wt1 = 9.3 //in mg/L
wt2 = 17.4 //in mg/L
wt3 = 8.7 //in mg/L
wt4 = 12.6 //in mg/L

//Solution
temp_h = wt1 * 100 / 146 + wt2 * 100 / 162 //where temp_h is temporary hardness
perm_h = wt3 * 100 / 95 + wt4 * 100 / 136 //where perm_h is permanent hardness
total_h = temp_h + perm_h //where total_h is total hardness

mprintf("Temporary hardness: %.2f mg/L\n",temp_h)
mprintf(" Total hardness: %.2f mg/L",total_h)
```

Scilab code Exa 14.3 Prob 3

```
//Chapter 14: Water Treatment
//Problem: 3
clc;

//Initialisation of Variables
wt1 = 32.4    //in mg/L
wt2 = 29.2    //in mg/L
wt3 = 13.5    //in mg/L

//Solution
temp_h = wt1 * 100 / 162. + wt2 * 100 / 146. //where temp_h is temporary hardness
perm_h = wt3 * 100 / 136. //where perm_h is permanent hardness

mprintf("Temporary hardness: %.2f mg/L\n",temp_h)
```

```
mprintf(" Total hardness: %.2f mg/L",perm_h)
```

Scilab code Exa 14.4 Prob 4

```
//Chapter 14: Water Treatment
//Problem: 4
clc;

//Initialisation of Variables
i1 = 180     //in mg/L for CaCl2
i2 = 210     //in mg/L for Ca(NO3)2
i3 = 123     //in mg/L for MgSO4
i4 = 90      //in mg/L for Mg(HCO3)2

//Solution
i1_req = i1 * 100 / 111.
i2_req = i2 * 100 / 164.
i3_req = i3 * 100 / 120.
i4_req = i4 * 100 / 146.

lime_req = 74 / 100. * (2 * i4_req + i3_req) * 100 / 70. * 10000 //where lime_req is the required value
alime_req=lime_req / (10 ** 6) //where alime_req is the approximated value
soda_req = 106 / 100. * (i1_req + i3_req + i2_req) * 100 / 80. * 10000 //where soda_req is the required value
asoda_req=soda_req / (10 ** 6) //where asoda_req is the approximated value

mprintf("Lime Required : %.1e mg ~ %.1f Kg\n", lime_req,alime_req)
mprintf(" Soda Required : %.1e mg ~ %.1f Kg", soda_req,asoda_req)
```

Scilab code Exa 14.5 Prob 5

```
//Chapter 14: Water Treatment
//Problem: 5
clc;

//Initialisation of Variables
wt1 = 32.4     //in mg/L for Ca(HCO3)2
wt2 = 29.29    //in mg/L for Mg(HCO3)2
wt3 = 13.5     //in mg/L for CaSO4

//Solution
wt1_eq = wt1 * 100 / 162.
wt2_eq = wt2 * 100 / 146.
wt3_eq = wt3 * 100 / 136.

temp_h = wt1_eq + wt2_eq //where temp_h is temporary hardness
perm_h = wt3_eq //where perm_h is permanent hardness

mprintf("Temporary hardness {caused by Ca(HCO3)2 & Mg(HCO3)2} is:%d ppm\n",temp_h)
mprintf(" Permanent hardness {caused by CaSO4} is:%.1f ppm",perm_h)
```

Scilab code Exa 14.6 Prob 6

```
//Chapter 14: Water Treatment
//Problem: 6
clc;

```

```
//Initialisation of Variables
v1 = 150    //in litres for NaCl

//Solution
a_hardwater = 22500 * v1 /(3 * 0.6 * 58.5)

mprintf("The amount of hard water that can be
   softened using this softner is:%.1f litres",
   a_hardwater)
```

Scilab code Exa 14.7 Prob 7

```
//Chapter 14: Water Treatment
//Problem: 7
clc;

//Initialisation of Variables
v1 = 30       //in litres for NaCl
w = 1500      //in mg/L for NaCl

//Solution
hardness = 45 * 50 / 58.5 * 1000 / 1000
mprintf("Hardness of water is :%.2f ppm",hardness)
```

Scilab code Exa 14.8 Prob 8

```
//Chapter 14: Water Treatment
//Problem: 8
clc;

//Initialisation of Variables
//EDTA=Ethylenediaminetetraacetic acid
v1_water = 50     //in ml for water
```

```
w1_CaCO3 = 1.5    //in mg for pure CaCO3
v1_EDTA = 44      //in ml for EDTA
v2_EDTA = 40      //in ml for EDTA
v2_water = 20     //in ml for water

//Solution
EDTA_1 = v1_water * w1_CaCO3 / v1_EDTA
hardw_40 = v2_water * 1.704
total_h1 = hardw_40 * 1000 / 40
total_h2 = total_h1 * 0.07

mprintf("Total hardness is :%.2f  Cl",total_h2)
```

Scilab code Exa 14.9 Prob 9

```
//Chapter 14: Water Treatment
//Problem: 9
clc;

//Given Constants For Specific Elements
Fe = 56
S = 32
O = 16

//Solution
hardness = Fe + S + O * 4
hardn= (hardness * 215 )/100

mprintf("215 ppm of hardness is : %.1f ppm of FeSO4"
   ,hardn)
```

Scilab code Exa 14.10 Prob 10

```
//Chapter 14: Water Treatment
//Problem: 10
clc;

//Initialisation of Variables
v1 = 50.    //in ml for hardwater
v2 = 15     //in ml for EDTA
m = 0.01    //in M for EDTA

//Solution
M = v2 * m / v1
N = M * 2
S = N * 50 * 1000

mprintf("Molarity of hardness is :%.3f M\n", M)
mprintf(" Normality of hardness is :%.3f N\n", N)
mprintf(" Strength of hardness is :%d ppm", S)
```

Scilab code Exa 14.11 Prob 11

```
//Chapter 14: Water Treatment
//Problem: 11
clc;

//Initialisation of Variables
C = 16.5     //in ppm for CO3-2

//Solution
Molarity = C * 10 ** - 6 / 60.

mprintf("Molarity of CO3-2 is : %.1e mol/L",Molarity
    )
```

Chapter 15

Environmental Pollution and Control

Scilab code Exa 15.1 Prob 1

```
//Chapter 15: Environmental Pollution and Control
//Problem: 1
clc;

MM = 294// Molar mass, K2Cr2O7

//Declaration of Variables
v_eff = 25    // cm cube,
v = 8.3       // cm cube, K2Cr2O7
M = 0.001     // M, K2Cr2O7

// Solution
w = v * 8 * 6 * M / 1000.

mprintf("8.3 cm cube of 0.006 N K2Cr2O7 =%.2e g of
    O2\n",w)
mprintf(" 25 ml of the effluent requires %.2e g of
    O2\n",w)

```

```
cod = w * 10 ** 6 / 25.
mprintf(" 1l of the effluent requires %.2fg of O2\n"
   ,cod)
mprintf(" COD of the effluent sample is %.2f ppm or
   mg/L",cod)
```

Scilab code Exa 15.2 Prob 2

```
//Chapter 15: Environmental Pollution and Control
//Problem: 2
clc;

//Declaration of Variables
v0 = 30      // cm cube, effluent
v1 = 9.8     // cm cube, K2Cr2O7
M = 0.001    // M, K2Cr2O7

// Solution
Oeff = 6 * 8 * v1 * M
mprintf("30 cm cube of effluent contains =:%.4f mg
   of O2\n",Oeff)

cod = Oeff * 1000 / 30.

mprintf(" 1l of the effluent requires %.2f mg of O2\
   n",cod)
mprintf(" COD of the effluent sample=%.2f ppm",cod)
```

Scilab code Exa 15.3 Prob 3

```
//Chapter 15: Environmental Pollution and Control
//Problem: 2
clc;
```

```
//Declaration of Variables
v0 = 25        // ml, sewage
d0 = 410    // ppm, dissolved oxygen
d1 = 120    // ppm, dissolved oxygen
v1 = 50        // ml, sewage

// Solution
mprintf("BOD = (DOb - DOi) * Dilution Factor\n")
mprintf(" BOD = (DOb - DOi) * (ml of sample after
   dilution) / (ml of sample before dilution)\n")

BOD = (d0 - d1) * (v1 / v0)
mprintf(" BOD = %d ppm",BOD)
```