# Scilab Textbook Companion for Engineering & Chemical Thermodynamics by M. D. Koretsky[1]

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# Book Description

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

**Exa** Example (Solved example)

**Eqn** Equation (Particular equation of the above book)

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

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

# Contents

# List of Scilab Codes

# Chapter 1

# Measured thermodynamic Properties and Other Basic Concepts

**Scilab code Exa 1.1** Example 1 1

```
//Engineering and Chemical Thermodynamics
//Example 1.1
//Page no :22

clear ; clc
// Given the quality of the system is ,x=0.2

// V_l = Specific volume of pure liquid
// V_v = Specific volume of pure vapour
// V = Molar volume of liquid-vapour mixture
disp(" Example: 1.1    Page no : 22") ;
disp("              V = V_l + x*(V_v - V_l)");
disp("              0.2 = (V - V_l) / (V_v - V_l)");
disp("              0.8 = (V_v - V) / (V_v - V_l)");

disp("          The tie line is devided into two
   parts according to the fraction of each phase to
```

```
    get the state of the mixture . ");

// The line segment representing the liquid is four
    times greater than      that of vapour

disp("           As no numerical values are given for
    specific volumes , we can not  get numerical
    answer .");
```

**Scilab code Exa 1.2** Example 1 2

```
//Engineering and Chemical Thermodynamics
//Example 1.2
//Page no :25

clear ; clc
P = 1.4 ; // [MPa]
T = 333 ; //[K]

//Given values are
T1 = 320 ; //[K]
T2 = 360 ; //[K]
P_low = 1 ; //[MPa]
P_high = 1.5 ; //[MPa]
V_cap_T1_P1 = 0.2678 ;
V_cap_T2_P1 = 0.2873 ;
V_cap_T1_P1_5 = 0.1765 ;
V_cap_T2_P1_5 = 0.1899 ;

//At P = 1 MPa
V_cap_T333_P1 = V_cap_T1_P1 + (V_cap_T2_P1 -
    V_cap_T1_P1)*((T - T1)/(T2- T1)); //[m^3/kg]

//Similarly at P=1.5 MPa
V_cap_T333_P1_5 = V_cap_T1_P1_5 + (V_cap_T2_P1_5 -
```

```
    V_cap_T1_P1_5)*((T - T1)/(T2 - T1)); //[m^3/kg]

//At T=333*C
V_cap_P1_5 = V_cap_T333_P1_5 ;
V_cap_P1 = V_cap_T333_P1 ;
V_cap_P1_4 = V_cap_P1 + (V_cap_P1_5 - V_cap_P1)*((P
    - P_low)/(P_high - P_low)) ; //[m^3/kg]
disp(" Example: 1.2    Page no : 25") ;
printf('\n         Required specific volume = %g m^3/
    kg',V_cap_P1_4);
```

**Scilab code Exa 1.3** Example 1 3

```
//Engineering and Chemical Thermodynamics
//Example 1.3
//Page no :27

clear ; clc

disp("              The problem contains only theory
    and different substitutions.There is no numerical
     part involved. Users can go through the book to
    obtain the required expression.")
```

**Scilab code Exa 1.4** Example 1 4

```
//Engineering and Chemical Thermodynamics
//Example 1.3
//Page no :27

clear ; clc
//From Ideal gas law we have v=(R*T)/P

```

```
//Given data
P = 1.4 ; //[MPa]
P_low = 1 ;//[MPa]
P_high = 1.5;//[MPa]

//At T=333*C from interpolation we have
v_cap_P1_5 = 0.18086 ;//[m^3/kg]
v_cap_P1 = 0.27414 ;//[m^3/kg]

//Molar volume is inversely proportional to pressure
v_cap_P1_4 = v_cap_P1 +(v_cap_P1_5 - v_cap_P1)*((1/P
    - 1/P_low)/(1/P_high - 1/P_low));
x=(0.19951-0.19418)/0.19418*100 ;
disp(" Example: 1.4   Page no : 28") ;
printf('\n        Specific volume (m^3/kg) = %g',
   v_cap_P1_4);
printf('\n        Percentage difference = %g',x);
```

# Chapter 2

# The First law of Thermodynamics

**Scilab code Exa 2.1** Example 2 1

```
//Engineering and Chemical Thermodynamics
//Example 2.1
//Page no :33

clear ; clc
z1 = 10 ; //[m]
z2 = 0 ; //[m],Taking ground as state 2,reference
v1 = 0 ;

//From conservation of total energy we get
// (1/2*m*v2^2-1 / 2*m*v1^2)+(m*g*z2 - m*g*z1) = 0
//   1/2*m*v2^2 - m*g*z1 = 0
v2 = sqrt(2 * 9.8 * z1) ; //[m/s]
disp(" Example: 2.1   Page no : 33") ;
printf('\n      Final velocity = %g (m/s) ',v2);
```

**Scilab code Exa 2.2** Example 2 2

```
//Engineering and Chemical Thermodynamics
//Example 2.2
//Page no :36

clear ; clc

//Given data
V2 = 14 ; // [m/s]
u_cap_l1 = 104.86 ; //[kJ/kg],at 25*C internal energy of saturated water
u_cap_l_t25 = 104.86 ; //[kJ/kg], From steam table
u_cap_l_t30 = 125.77 ; //[kJ/kg], From steam table
T1 = 25 ; //[*C]
T2 = 30 ; //[*C]

//For unit mass change in kinetic energy
Delta_e_cap_k = 1/2 * V2^2 * 10^-3 ; //[kJ/kg]

Delta_u_cap = Delta_e_cap_k ;

//For final state of water:
u_cap_l2 = Delta_u_cap + u_cap_l1 ;

//From table

x = (u_cap_l2 - u_cap_l_t25) / (u_cap_l_t30 - u_cap_l_t25) ;
T_unknown = T1 + x*(T2 - T1) ;
disp(" Example: 2.2    Page no : 36") ;
printf('\n          Final temperature of water = %g *C',T_unknown);
```

---

**Scilab code Exa 2.3** Example 2 3

```
//Engineering and Chemical Thermodynamics
//Example 2.3
//Page no :38

clear ; clc

//External pressure is constant
P_ex = 1*10^5 ; //[Pa]}

//To calculte work done
function y = f(x),y = 1,endfunction
I = intg(10,15.2,f) ;
W = -P_ex * I * 10^-3 ; //[J]
disp(" Example: 2.1    Page no : 33") ;
printf('\n          Work done = %g J',W);
```

**Scilab code Exa 2.4** Example 2 4

```
//Engineering and Chemical Thermodynamics
//Example 2.4
//Page no :55

clear ; clc
//From steam table specific enthalpy at state1 and
    state2 are
h_cap_1 = 3373.6 ; //[kJ/kg]
h_cap_2 = 2675.5 ; //[kJ/kg]

m_dot1 = 10; //[kg/s],As we are dealing with steady
    state
m_dot2 = 10; //[kg/s]

//Neglecting heat dissipation compared to shaft work
     we have
// m_dot1*h_cap_1 - m_dot2*h_cap_2 + Ws_dot = 0
```

```
Ws_dot = m_dot1 * (h_cap_2 - h_cap_1) ; //[kW]
disp(" Example: 2.4    Page no : 55") ;
printf('\n        Power generated = %g kW',Ws_dot);
```

**Scilab code Exa 2.5** Example 2 5

```
//Engineering and Chemical Thermodynamics
//Example 2.5
//Page no :55

clear ; clc

//Solution(a)
//Unsteady state analysis
h_cap_in = 3241 ; //[kJ/kg] , From steam table
P_final = 10 ; //[MPa]

//From Eqn. Eq2.5A , Eq2.5B , Eq2.5C we get
u_cap_2 = h_cap_in ;
//At codition of P = 10MPa , u_cap_2 = 3241 kJ/kg
   the final temperature of the system is
T2 = 600 ; // From steam table .No calculation is
   involved .
disp(" Example: 2.5    Page no : 55") ;
printf('\n       (a)\n              The final
   temperature of the system = %g *C\n',T2);

//Closed system analysis
//From equation E2.5E , E2.5F , E2.6G we get
u_cap_2 = h_cap_in ;
// So temperature is T2 = 600*C (From table).

//Solution(b)
disp("      (b)    The temperature of the fluid
   increases in the system due to the receipent of
```

```
    flow work .")
```

**Scilab code Exa 2.6** Example 2 6

```
//Engineering and Chemical Thermodynamics
//Example 2.6
//Page no :62

clear ; clc
//Q=n*Delta_h
//Given data
n =2 ; //[mol]
A = 3.470 ;
B = 1.450*10^-3 ;
D = 0.121*10^5 ;
T1 = 473 ; //[K]
T2 = 773 ; //[K]

function y = f(T),y = 8.314*(A + B*T + D*T^-2),
    endfunction
Delta_h = intg(T1,T2,f);

Q = n * Delta_h ;
disp(" Example: 2.6    Page no : 62") ;
printf('\n       (a)Heat required = %g J',Q);

//Solution (b)

//From steam table
h_cap_1 = 2827.9 ; //[kJ/kg]
h_cap_2 = 3478.4 ; //[kJ/kg]
m = 2*0.018 ; //[kg]

Delta_h_cap = (h_cap_2 - h_cap_1) * 10^3 ; //[J/kg]
Q = m * Delta_h_cap;
```

```
printf('\n\n         (b)Heat required = %g J',Q);
```

**Scilab code Exa 2.7** Example 2 7

```
//Engineering and Chemical Thermodynamics
//Example 2.7
//Page no :63

clear ; clc
//Given data
T1 = 298;
T2_start = 300;
A = 3.355;
B = 0.575*10^-3;
D = -0.016*10^5;

function y = f(T),y = 8.314*[A*T + B/2*T^2 - D/T]
endfunction;
disp(" Example: 2.7    Page no : 63") ;
for T2_start = 300:100:1000;
    del_h = f(T2_start) - f(T1);
    Cp = del_h /(T2_start - 298);
    mprintf('\n        At temperature(K) %g,       Molar
        heat capacity (J/molK) %g',T2_start,Cp);
end
```

**Scilab code Exa 2.8** Example 2 8

```
//Engineering and Chemical Thermodynamics
//Example 2.8
//Page no :64

clear ; clc
```

```
// Given data
n_dot_air = 10 ; //[mol/min]
C_bar_P_900 = 30.71 ; //[J/molK]
C_bar_P_600 = 29.97 ; //[J/molK]
T1 = 600 ; //[K]
T2 = 900 ; //[K]
T_ref = 298 ; //[K]

// Q_dot = n_dot_air * (h_900 - h_600)...........Eqn E2.8A
Q_dot = n_dot_air * (C_bar_P_900 * (T2 - T_ref) - C_bar_P_600 * (T1 - T_ref));
disp(" Example: 2.8    Page no : 33") ;
printf('\n        Heat rate required = %g J/min',
   Q_dot);
```

**Scilab code Exa 2.9** Example 2 9

```
//Engineering and Chemical Thermodynamics
//Example 2.9
//Page no :65

clear ; clc
//solution(a)

// Given data:
P1 = 100000 ; // [N/m^2]
T1 = 298 ; //[K]
V1 = 0.1 * 0.1 ; // [m^3]
T2 = 373 ; // [N]
P_ext = 100000 ; //[N/m^2]
k = 50000 ; //[N/m]
A = 0.1 ; //[m^2]

// Applying ideal gas law we getan quadritic eqn of
```

```
    the form :
// a * V2^2 + b * V2 + c = 0 where
a = k / (T2 * A^2) ;
b = (P_ext / T2) - k * V1 / (A^2 * T2) ;
c = -P1 * V1 / T1 ;
V2 = (-b + sqrt ( b^2 - (4*a*c))) / (2 * a) ;
W = -P_ext * (V2 - V1) - ( k * (V2 - V1)^2)/(2 * A
    **2);//From eqn E2.9C
disp(" Example: 2.9    Page no : 65") ;
printf('\n       (a) Work required = %g J \n\n',W);


//Solution(b):

//Given data:
A = 3.355 ;
B = 0.575 * 10^-3 ;
D = -0.016 * 10^5 ;
P1 = 10^5 ; //[N/m^2]
V1 = 0.01 ; //[m^3]
R = 8.314 ;
T1 = 298 ;

n = (P1 * V1) / (R * T1) ;
function y=f(T),y=R*((A - 1) * T + B/2 * T^2 -D/T)
endfunction
del_u = f(373) - f(298) ;
del_U = n * del_u ;
Q = del_U - W;
printf('\n       (b).Heat transfered  = %.4f  J',Q);
```

**Scilab code Exa 2.10** Example 2 10

```
//Engineering and Chemical Thermodynamics
//Example 2.10
```

```
//Page no :68

clear ; clc
//Given data:
n_dot = 10 ; //[mol/s]
T1 = 298.2 ; //[K]
T2 = 342 ; //[K]
T3 = 373.2 ; //[K]
Cp_298_342 = 216.3 ; //[J/molK]
A = 3.025 ;
B = 53.722 * 10^-3 ;
C = -16.791 * 10^-6 ;
del_h_vap = 28.88 ; //[kJ/mol]

del_h_1 = Cp_298_342 * (T2 - T1) * 10^-3 ; //[kJ/mol]
del_h_2 = del_h_vap ;
function y=f(T),y=8.314*(A*T + (B/2)*(T^2) + (C/3)*(T^3))* 10^-3 ;
endfunction
del_h_3 = f(T3) - f(T2) ;

Q = n_dot * (del_h_1 + del_h_2 + del_h_3) ;
disp(" Example: 2.10    Page no : 68") ;
printf('\n        Rate of heat supplied = %d kJ/s',Q);
```

**Scilab code Exa 2.11** Example 2 11

```
//Engineering and Chemical Thermodynamics
//Example 2.11
//Page no :69

clear ; clc ;
//Given data:
```

```
m_1_v = 4.3 ; //[kg]
m_1_l = 50 ; //[kg]
u_cap_1_v = 2437.9 ; //[kJ/kg],From steam table
u_cap_1_l = 191.8 ; //[kJ/kg],From steam table
v_cap_1_v = 14.67 ; //[m^3],From steam table
v_cap_1_l = 0.001 ; //[m^3],From steam table

V2 = m_1_l * v_cap_1_l + m_1_v * v_cap_1_v ;
m_2_v = m_1_l + m_1_v ;
v_cap_2_v = V2 / m_2_v ; //[m^3/kg]

// From table this specific volume matches at
P2= 0.15 ; //[MPa]
//At this condition
u_cap_2_v = 2519.6 ; //(kJ/kg)
Q = ((m_2_v * u_cap_2_v) -(m_1_l * u_cap_1_l + m_1_v
    * u_cap_1_v))*1000;
disp(" Example: 2.11    Page no : 69") ;
printf('\n      Minimum amount of heat required = %e
    J',Q);
```

**Scilab code Exa 2.12** Example 2 12

```
//Engineering and Chemical Thermodynamics
//Example 2.12
//Page no :73

clear ; clc ;
// From table we have
del_h0_f_CO2 = -393.51 ; // [kJ/mol]
del_h0_f_H2 = 0 ; // [kJ/mol]
del_h0_f_H2O = -241.82 ; // [kJ/mol]
del_h0_f_CH3OH = -200.66 ; // [kJ/mol]

del_h0 = del_h0_f_CO2 + 3 * del_h0_f_H2 -
```

```
    del_h0_f_H2O - del_h0_f_CH3OH ;
disp(" Example: 2.12   Page no : 73") ;
printf('\n        Enthalpy of reaction = %g kJ/mol',
    del_h0);
```

**Scilab code Exa 2.13** Example 2 13

```
//Engineering and Chemical Thermodynamics
//Example 2.13
//Page no :73

clear ; clc ;
//Given data :
del_h0_f_CO2 = -393.51 ; //[kJ/mol], From Appendix A
    .3
del_h0_f_CO = -110.53 ; //[kJ/mol], From Appendix A
    .3
del_h0_f_H2O = -241.82 ; //[kJ/mol], From Appendix A
    .3
del_h0_f_C3H8 = -103.85 ; //[kJ/mol], From Appendix
    A.3
del_h0_f_O2 = 0 ; //[kJ/mol], From Appendix A.3
A_CO2 = 5.457 ; // From table E2.13
B_CO2 = 1.05 * 10^-3 ;
D_CO2 = -1.16 * 10^5 ;
A_CO = 3.379 ;
B_CO = 5.57 * 10^-4;
D_CO = -3.1 * 10^3 ;
A_H2O = 3.470 ;
B_H2O = 1.45 * 10^-3;
D_H2O = 1.21 * 10^4 ;
A_N2 = 3.280 ;
B_N2 = 5.93 * 10^-4;
D_N2 = 4.00 * 10^3 ;

```

```
//Let
n_C3H8 = 10 ; //[mol]
n_N2 = (0.79/0.21) * (9.7/2) * n_C3H8 ; //[mol]
n_CO2 = 2.7 * n_C3H8 ; //[mol]
n_CO = 0.3 * n_C3H8 ; //[mol]
n_H2O = 4 * n_C3H8 ; //[mol]
n_O2 = (9.7 / 2)* n_C3H8 ; //[mol]
T_reff = 298 ; //[K]
del_H_rxn_298 = n_CO2 * del_h0_f_CO2 + n_CO * del_h0_f_CO + n_H2O * del_h0_f_H2O - n_C3H8 * del_h0_f_C3H8 - n_O2 * del_h0_f_O2 ; //[kJ]

//The co-efficients of T2 in the equation of degree 3 are
a = 8.314*(n_CO2 * (B_CO2/2) + n_CO * (B_CO/2) + n_H2O * (B_H2O/2) + n_N2 * (B_N2/2));
b = 8.314*(n_CO2 * A_CO2 + n_CO * A_CO + n_H2O * A_H2O + n_N2 * A_N2) ;
d =8.314*(- n_CO2 * D_CO2 - n_CO * D_CO - n_H2O * D_H2O -n_N2 * D_N2) ;
c = (del_H_rxn_298 *1000) + 8.314 * (n_CO2 * (- T_reff * A_CO2 - B_CO2/2 * T_reff^2 + D_CO2/T_reff) + n_CO * (- T_reff * A_CO - B_CO/2 * T_reff^2 + D_CO/T_reff) + n_H2O * (- T_reff * A_H2O - B_H2O/2 * T_reff^2 + D_H2O/T_reff) + n_N2 * (-T_reff * A_N2 - B_N2/2 * T_reff^2 + D_N2/T_reff));

T2=poly(0,'T2');
P = d + c*T2 + b*T2^2 + a*T2^3 ;
M = roots(P);

disp(" Example: 2.13    Page no : 73") ;
disp("  The roots of the equation containig T2 as variable are (K)-")
disp(M);
disp("  But T2 must be more than 298K . So we have to choose the most suitable solution .")
```

```
// The answer in the textbook does not statisfy the
   equation while it  is counter-checked .
```

**Scilab code Exa 2.14** Example 2 14

```
//Engineering and Chemical Thermodynamics
//Example 2.14
//Page no :75

clear ; clc ;
disp("  Example 2.14    Page no : 75")
disp("              The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.")
```

**Scilab code Exa 2.15** Example 2 15

```
//Engineering and Chemical Thermodynamics
//Example 2.15
//Page no :80

clear ; clc ;

//Given data
V1 = 350 ; //[m/s]
A = 3.355 ;
B = 0.575*10^-3 ;
D = -0.016*10^5 ;
Tin = 283 ; //[K]
MW = 29 * 10^-3 ; //[kg/mol]

ek = 1/2 * MW * V1**2 ;
```

```
//The co-efficients of T2 in the equation of degree 3 are
a = B/2 ;
b = A ;
c = -(Tin * A + Tin^2*B/2 - (D/Tin) + ek/8.314) ;
d=-D ;

T2=poly(0,'T2');
P = d + c*T2 + b*T2^2 + a*T2^3 ;
M = roots(P);
disp(" Example: 2.15    Page no : 80") ;
disp( " The solutions are ")
disp(M);
disp("                But the outlet temp should be more than 283K(inlet temperature) .So we have to choose the most suitable solution .")
```

**Scilab code Exa 2.16** Example 2 16

```
//Engineering and Chemical Thermodynamics
//Example 2.16
//Page no :81

clear ; clc ;
//Given data:
V_dot_2 = 0.001 ; //[m^3/kg]
v_cap_2 = 0.001 ; //[m^3/kg], Specific volume of water
z2 = 250 ; //[m] ; Taking ground as the reference level
e_cap_2 = 9.8 * z2 ; //[kg*m^2/s^2]

m_dot_2 = V_dot_2 / v_cap_2 ; //[kg/s]
//Neglecting the kinetic energy ,frictional losses ftrom energy balance  equation we have
```

```
W_dot_s = m_dot_2 * e_cap_2 * 10^-3 ;
disp(" Example: 2.16    Page no : 81") ;
printf('\n       Minimum power required is = %g kW',
    W_dot_s);
```

**Scilab code Exa 2.17** Example 2 17

```
//Engineering and Chemical Thermodynamics
//Example 2.17
//Page no :82

clear ; clc ;
//Given data
n_dot = 10 ; //[mol/min]
del_h_vap_CO2 = 10400 ; //[J/mol]
A_CO2 = 5.457 ; //From appendix A.3
B_CO2 = 1.045 * 10^-3 ;
D_CO2 = -1.157 * 10^5 ;
A_air = 3.355 ;
B_air = 0.575 * 10^-3 ;
D_air = -0.016 * 10^5 ;
T1 = 273 ; //[K]
T2 = 283 ; //[K]
T3 = 323 ; //[K]
T4 = 293 ; //{k}

function y=f1(T),y=8.314 * (A_CO2 * T + (B_CO2/2) *
    T^2 - D_CO2/T)
endfunction

sen_heat_CO2 = f1(T2) - f1(T1) ;
Q_dot = n_dot * (del_h_vap_CO2 + sen_heat_CO2) ; //[
    J/min]

function y=f2(T),y=8.314 * (A_air * T + B_air/2*T^2
```

```
   - D_air /T)
endfunction
sen_heat_air = f2(T4) - f2(T3);
n_dot_air = - Q_dot / sen_heat_air ;
disp(" Example: 2.17    Page no : 82") ;
printf('\n        Air required = %g mol/min',
   n_dot_air);
```

**Scilab code Exa 2.18** Example 2 18

```
//Engineering and Chemical Thermodynamics
//Example 2.18
//Page no :84

clear ; clc ;
m_dot_1 = 10 ; //[kg/s]
h_cap_1 = 3238.2 ;//[kJ/kg], Super heated steam at
   500*C & 200bar
h_cap_2 = 93.3 ;//[kL/kg], subcooled liquid at 20*C
   & 100bar
h_cap_3 = 2724.7 ;//{kJ/kg}, Super heated vapour at
   100bar

m_dot_2 = m_dot_1 * (h_cap_1 - h_cap_3) / (h_cap_3 -
    h_cap_2);
disp(" Example: 2.18    Page no : 84") ;
printf('\n       Flow of liquid stream = %.2f kg/s',
   m_dot_2);
```

**Scilab code Exa 2.19** Example 2 19

```
//Engineering and Chemical Thermodynamics
//Example 2.19
```

```
//Page no :85

clear ; clc ;
//From steam table
h_cap_st_1 = 2923.4 ; // [kJ/kg]
h_cap_200 = 2875.3 ; // {kJ/kg} , At 100kPa
h_cap_250 = 2974.3 ; // {kJ/kg} , At 100 kPa
del_T = 250-200 ;

T1 = 200 ; //[K]
h_cap_st_2 = h_cap_st_1 ;//Assumimg bulk kinetic
    energy of the stream and heat transfered is
    negligible
T2 = T1 + del_T * (h_cap_st_2 - h_cap_200) / (
    h_cap_250 - h_cap_200) ;
disp(" Example: 2.19   Page no : 85") ;
printf('\n      The exit temperature is = %d *C',T2)
    ;
```

**Scilab code Exa 2.20** Example 2 20

```
//Engineering and Chemical Thermodynamics
//Example 2.20
//Page no :89

clear ; clc ;
//solution (a)
//Given data
Cv = 3/2 * 8.314 ;
Cp = 5/2 * 8.314 ;
n = 1;
R = 8.314 ;
T1 = 1000 ; //[K]
P1 = 10 ; //[bar]
T2 = 1000 ; //[K]
```

```
P2 = 0.1 ; //[bar]
T3 = 300 ; //[K]
T4 = 300 ; //[K]

k = Cp / Cv ;
P3 = P2 * (T3 / T2)^(k/(k-1)); //[bar]
P4 = P1 * (T4 / T1)^(k/(k-1)) ; //[bar]

// (1)
  del_U_12 = 0 ; // As process 1-2 is isothermal
  W_12 = n * R * T1 * log(P2 / P1);
  Q_h_12 = W_12 ;
  disp(" Example: 2.20   Page no : 89") ;
printf('(a)\n    (1)\n            del_U = %d J',
   del_U_12) ;
printf('\n            Work  = %d J',W_12) ;
printf('\n            Heat = %d J',Q_h_12) ;

//(2)
   Q_23 = 0 ; // As adiabatic process
   del_U_23 = n * Cv *(T3 - T2) ;
   W_23 = del_U_23 ;
printf('\n     (2)\n            del_U  = %g J',
   del_U_23) ;
printf('\n            Work (J) = %d J',W_23) ;
printf('\n            Heat (J) = %d J',Q_23) ;

//(3)
   del_U_34 = 0 ; // As isothermal process
   W_34 = n * R * T3 * log(P4 / P3) ; // Eqn E2.20.A
   Q_c_34 = del_U_34 - W_34 ;
printf('\n     (3)\n            del_U = %g J',
   del_U_34) ;
printf('\n            Work = %d J',W_34) ;
printf('\n            Heat = %d J',Q_c_34) ;

//(4)
    Q_41 = 0 ; // As adiabatic process
```

```
    del_U_41 = n * Cv * (T1 - T4) ;
    W_41 = del_U_41 ;
printf('\n    (4)\n            del_U = %g J', del_U_41) ;
printf('\n            Work = %d J',W_41) ;
printf('\n            Heat = %d J',Q_41) ;

//Solution (b)
//Users can refer figure E2.20

//Solution (c)
  W_total = W_12 + W_23 + W_34 + W_41 ;
  Q_absor = Q_h_12 ;
  effi = W_total / Q_absor ;
printf('\n\n(c)   efficiency = %g',effi)

//Solution (d)
x = 1 - T3 / T1 ;
printf('\n\n(d)   1 - Tc/Th = %g',x);
disp("    i.e  Efficiency = 1 - Tc/Th");

//Solution (e)
disp("(e) The process can be made more efficient by raising Th or by  lowering Tc .");
disp("Table E2.20B") ;
disp("       T(K)        P(bar)    v(m^3/mol)") ;
P = [P1 , P2 , P3 , P4 ] ;
T = [T1 , T2 , T3 , T4 ] ;
for i = 1:4
    v(i) = R * T(i) * 10^-5/ P(i) ;
    printf("\n       %d     %.4f     %f \n",T(i) ,P(i) ,v(i)) ;
end
```

# Chapter 3

# Entropy and the Second law of Thermodynamics

**Scilab code Exa 3.2** Example 3 2

```
//Engineering and Chemical Thermodynamics
//Example 3.2
//Page no : 119

//Solution(a)
clear ; clc ;
//Given
del_U = 0 ; // As no work or heat transfered across
   its boundaries during the process
T_1 = 500 ; // [K]
V1 = 1.6682 / 2 * 10^-3; // [m^3]
V2 = 2 * V1 ;
del_S_sur = 0 ; // As no heat transfered across its
   boundaries during the process
disp(" Example 3.2   Page no : 119")
disp("(a)");
disp("  For an ideal gas u = u(T only)") ;
printf('\n   Final temperature = %g K \n\n',T_1);

```

```
//Solution(b)
q_rev = 8.314 * T_1 * log(V2/V1) ;
del_S_sys = q_rev / T_1 ;
del_S_univ = del_S_sys + del_S_sur ;
printf('(b)\n\n  Entropy change for universe = %.2f
    J/(molK)',del_S_univ);
```

**Scilab code Exa 3.3** Example 3 3

```
//Engineering and Chemical Thermodynamics
//Example 3.3
//Page no:121

clear  ; clc ;
// Given
T_1_1 = 273 ;// {K}
T_1_2 = 373 ; //[K]
Cp = 24.5 ; // [J/molK]
del_S_sur = 0 ; //Since the system is isolated
T2 = (T_1_1 + T_1_2)/2 ;
del_S = Cp / 2 * log(T2^2 / (T_1_1 * T_1_2)) ;

disp(" Example 3.3   Page no : 121") ;
printf("\n      Entropy change for the system = %.2f
    J/(mol K)", del_S);
```

**Scilab code Exa 3.4** Example 3 4

```
//Engineering and Chemical Thermodynamics
// Example 3.4
//Page no : 122

clear ; clc ;
```

```
//Given
del_h_vap = 38.56 * 10^3 ; //[J/mol] , From Table
Tb = 78.2 + 273 ; //[K] ,From table

del_S = - del_h_vap / Tb * 10^-3 ;
disp(" Example 3.4   Page no : 122") ;
printf("\n     Change in entropy = %.4f kJ/mol K",
    del_S);
```

**Scilab code Exa 3.5** Example 3 5

```
//Engineering and Chemical Thermodynamics
//Example 3.5
//Page no:124

clear ; clc ;
//Given
P_1 = 300 * 10^3 ; //[N/m^2]
T_1 = 700 ; // [*C]
V_bar_1 = 20 ; //[m/s]
P_2 = 200 * 10^3 ; // [N/m^2]
h_cap_1 = 3927.1 * 10^3 ; // [J/kg] , From table
S_cap_1 = 8.8319 ; // [kJ/kgK] , From table

S_cap_2 = S_cap_1 ; // Reverssible adiabatic process
T2 = 623 ; // [*C] ,From table by interpolation
h_cap_2 = 3754.7 * 10^3 ; // [J/kgK] ,From table by
    interpolation
V_bar_2 = sqrt(2 * (h_cap_1 - h_cap_2) + V_bar_1^2)
    ;
disp(" Example: 3.5   Page no : 124") ;
printf('\n   The final temperature is %g C and the
    exit velocity is %g m/s',T2,V_bar_2);
```

**Scilab code Exa 3.6** Example 3 6

```
//Engineering and Chemical Thermodynamics
//Example 3.6
//Page no:125

clear ; clc ;
//Given
m_dot_1 = 10 ; // [kg/s]
m_dot_2 = 1.95 ; // [kg/s]
P_1 = 200 * 10^5 ; //[N/m^2]
T_1 = 500 ; //[*C]
P_2 = 100 * 10^5 ; // [N/m^2]
T_2 = 20 ; //[*C]
P_3 = 100 * 10^5 ; //[N/m^2]
S_cap_1 = 6.14 * 10^3 ; //[J/kgK] , From table
S_cap_2 = 0.2945 * 10^3 ; //[J/kgK] , From table
S_cap_3 = 5.614 * 10^3 ; //[J/kgK] , From table

m_dot = m_dot_1 + m_dot_2 ;
dS_dt_univ = (m_dot * S_cap_3 -(m_dot_1 * S_cap_1 +
    m_dot_2 * S_cap_2)) * 10^-3;
disp(" Example: 3.6    Page no : 125") ;
printf('\n      Entropy generated = %.2f kW/K ',
    dS_dt_univ);
```

**Scilab code Exa 3.7** Example 3 7

```
//Engineering and Chemical Thermodynamics
//Example3.7
//Page no:128

```

```
//Solution:(a)
clear ; clc ;
//Given
V_1 = 0.5 ; //[m^3]
P_1 = 150 ; //[kPa]
T_1 = 20 + 273 ; //[K]
P_2 = 400 ; // [kPa]
Cp = 2.5 * 8.314 ;
Q = V_1 * (P_1 - P_2);
disp(" Example: 3.7    Page no : 128") ;
printf("\n    (a)\n      Heat transferd = %g kJ\n\n",Q
    );

//Solution:(b)
del_S_sys = (P_1 * V_1) / T_1 * -log(P_2 / P_1) ;
printf('    (b)\n       Entropy change of system = %.2
    f kJ/K \n',del_S_sys);
Q_surr = - Q ;
del_S_surr = Q_surr / T_1 ;
printf('       Entropy change of surrounding = %.2f
    kJ/K \n',del_S_surr) ;
del_S_univ = del_S_sys + del_S_surr ;
printf('       Entropy change of universe =%.2f kJ/K
    \n',del_S_univ) ;

//Solution:(c)
disp("  (c)");
disp("       Since entropy of the universe increases
     , the process is irreverssible .")
```

---

**Scilab code Exa 3.8** Example 3 8

```
//Engineering and Chemical Thermodynamics
//Example 3.8
//Page no :129
```

```
clear ; clc ;
//Given
A = 3.355 ; // from table
B = 0.575 * 10^-3 ; // from table
D = -0.016 * 10^5 ; // from table
R = 8.314 ;
P1 = 1 ; //[bar]
P2 = 0.5 ; //[bar]
function y=f(T),y = R * (A * log(T) + B * T + D / (2
    * T^2)) ;
endfunction ;
S1 = f(373) - f(298) ;
S2 = R * log(P1 / P2) ;
del_S = S1 - S2 ;

disp(" Example: 3.8    Page no : 129") ;
printf('\n      Entropy change = %.2f J/(mol K )',
   del_S);
```

---

**Scilab code Exa 3.9** Example 3 9

```
//Engineering and Chemical Thermodynamics
//Example 3.9
//Page no:129

clear ; clc ;
//Given
P = 1 ; //[bar]
p_O2 = 0.5 ; //[bar]
p_N2 = 0.5 ; // [bar]
n_O2 = 1 ; //[mol]
n_N2 = 1 ; //[mol]
R = 8.314 ; // J/mol K
del_S_1_O2 = -n_O2 * R * log(p_O2 / P) ;
```

```
del_S_1_N2 = -n_N2 * R * log(p_N2 / P) ;
del_S_2 = 0 ; // As both O2 and N2 behave idealy
del_S = del_S_2 + del_S_1_O2 + del_S_1_N2 ;
disp(" Example: 3.9    Page no : 129") ;
printf("\n     Entropy of mixing = %.2f J/K",del_S);
```

**Scilab code Exa 3.10** Example 3 10

```
//Engineering and Chemical Thermodynamics
//Example 3.10:
//Page no:131

clear ; clc ;
disp(" Example: 3.10    Page no : 131") ;
disp("            The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.") ;
```

**Scilab code Exa 3.11** Example 3 11

```
//Engineering and Chemical Thermodynamics
//Example 3.11
//Page no:131

clear ; clc ;
P_1 = 10 ; //[bar]
T_1 = 298 ; // [K]
P_2 = 1 ; //[bar]
T_2 = 298 ; // [K]
P_3 = 1 ; //[bar]
R = 8.314 ; // [J/mol K]
n = 4 ; //[mol]
```

```
X = 0.01 ;

//Step 1 :
del_S_sys = - R * log(P_2 / P_1);
del_S_surr = - R * (1 - P_2 / P_1) ;
del_s_univ_1 = del_S_sys + del_S_surr ;
Del_S_univ_1 = n * del_s_univ_1 ;

//Step 2 :
Del_S_univ_2 = 0 ;
n_3 = n * P_3 / P_1 ;

//Step 3 :
n_out = n - n_3 ;
del_S_sys_3 = - n_out * R * log(X) ;
Del_S_univ_3 = del_S_sys_3 ; // Assuming the
    composition of air in the room does not
    noticeably change by the dilute addition of argon
Del_S_univ = Del_S_univ_1 + Del_S_univ_2 +
    Del_S_univ_3 ;

disp(" Example: 3.11    Page no : 131") ;
printf("\n        Total entropy change of universe =
    %.2f J/K \n\n",Del_S_univ) ;
disp("        No matter how slow the leak , the
    driving force for the expansion is finite . So
    the process canot be reverssible .")
```

**Scilab code Exa 3.12** Example 3 12

```
//Engineering and Chemical Thermodynamics
// Example 3.12
//Page no:136

clear ; clc ;
```

```
//Given
n_dot = 250 ; // [mol/s]
P_1 = 125 * 10^5 ; // [N/m^2]
V_cap_1 = 5 * 10^-4 ; // [m^3/mol]
P_2 = 8 * 10^5 ; // [N/m^2]

X = 3 * P_1^0.6667 * V_cap_1 * ( P_2^(1/3) - P_1^(1/3)) ;
W_dot_s = n_dot * X * 10^-6 ;

disp(" Example: 3.12   Page no : 136") ;
printf('\n     Power generated = %.1f MW',W_dot_s) ;
```

**Scilab code Exa 3.13** Example 3 13

```
//Engineering and Chemical Thermodynamics
// Example 3.13
//Page no:137

clear ; clc ;
//Given
Ws_real = -2.1 ; //[MW]
Ws_rev = -2.8 ; // [MW]
n_tur = Ws_real / Ws_rev ;
disp(" Example: 3.13   Page no : 137") ;
printf("\n     Isentropic efficiency of turbine = %.2f %%", n_tur * 100);
```

**Scilab code Exa 3.14** Example 3 14

```
//Engineering and Chemical Thermodynamics
//Example 3.14
//Page no:140
```

```
clear ; clc ;
//Given
P_1 = 10 * 10^6 ; // [N/m^2]
T_1 = 600 + 273 ; //[K]
T_H = T_1 ;
T_C = 100 + 273 ; //[K]
P_3 = 10 * 10^4 ; //[N/m^2]
P_4 = P_1 ;
h_cap_1 = 3625.3 ; // [kJ/kg],From steam table
S_cap_1 = 6.9028 ; //[kJ/kgK],From steam table
S_cap_2 = S_cap_1 ; //[kJ/kgK],From steam table
S_cap_v = 7.3593 ; //[kJ/kgK],From steam table
S_cap_l = 1.3025 ; //[kJ/kgK],From steam table
h_cap_l = 417.44 ;// [kJ/kg],From steam table
h_cap_v = 2675.5 ;// [kJ/kg],From steam table
V_cap_l = 10^-3 ; // [m^3/kg],From steam table

X = (S_cap_2 - S_cap_l) / (S_cap_v - S_cap_l);
h_cap_2 = (1 - X) * h_cap_l + X * h_cap_v ;
W_cap_s = h_cap_2 - h_cap_1 ;
h_cap_3 = h_cap_l ;

W_cap_c = V_cap_l * (P_4 - P_3) * 10^-3 ;
h_cap_4 = h_cap_3 + W_cap_c ;
W_net = W_cap_s + W_cap_c ; // [kJ/kg]

n_turb = ( -W_cap_s - W_cap_c) / (h_cap_1 - h_cap_4)
    ;
disp(" Example: 3.14   Page no : 140") ;
printf("\n    Efficiency of the Rankine cycle = %.3f
    %% \n\n",n_turb * 100 );

n_carnot = 1 - T_C / T_H ;
printf("    Efficiency of the Carnot cycle = %.3f %%
    \n\n",n_carnot * 100);

disp("   The Rankine efficiecy is lower than Carnot
```

```
efficiency .")
```

**Scilab code Exa 3.15** Example 3 15

```
//Engineering and Chemical Thermodynamics
//Example 3.15
//Page no:141

clear ; clc ;
//Given
n_turb = 0.85 ;
n_comp = 0.85 ;
W_cap_s_rev = -1120 ; //[kJ/kg]
h_cap_1 = 3625.3 ; //[kJ/kg]
h_cap_l = 417.44 ; //[kJ/kg]
W_cap_c_rev = 9.9 ; //[kJ/kg]

W_cap_s_act = n_turb * W_cap_s_rev ;
h_cap_2_act = W_cap_s_act + h_cap_1 ;
h_cap_3 = h_cap_l ;
W_cap_c_act = W_cap_c_rev / n_comp ;
h_cap_4_act = W_cap_c_act + h_cap_3 ;
W_cap_net = W_cap_s_act + W_cap_c_act ;
n_rank_act = (-W_cap_s_act - W_cap_c_act) / (h_cap_1
    - h_cap_4_act) ;

disp(" Example: 3.15    Page no : 141") ;
printf("\n          W_cap_net = %.1f kJ/kg",W_cap_net
   ) ;
printf("\n       Efficiency of Rankine cycle = %.3f
   %%",n_rank_act*100) ;
```

**Scilab code Exa 3.16** Example 3 16

```
//Engineering and Chemical Thermodynamics
// Example 3.16
//Page no:144

clear ; clc ;
//Given
P_1 = 120 * 10^3 ; //[N]
P_2 = 900 * 10^3 ; //[N]
h_4 = 25.486 ; //[kJ/mol], From table
h_1 = h_4 ;
h_2 = 39.295 ; //[kJ/mol], From table
S_2 = 177.89 ;  //[kJ/molK], From table
S_3 = S_2 ;  //[kJ/mol]
h_3 = 43.578 ; //[kJ/mol] , Enthalpy corresponding
   to S3 value which    equales to S2
Q_dot_c_des = 10 ; //[kW]

q_c = h_2 - h_1 ;
Q_dot_c = h_2 - h_1 ;
W_dot_c = h_3 - h_2 ;

COP = Q_dot_c / W_dot_c ;
n_dot = Q_dot_c_des / q_c ;
disp(" Example: 3.16   Page no : 144") ;
printf("\n     COP of the refrigerator is = %.2f \n\
   n     Mass flow rate needed = %.3f mol/s",COP,
   n_dot)
```

**Scilab code Exa 3.17** Example 3 17

```
//Engineering and Chemical Thermodynamics
// Example 3.17
//Page no :151

clear ; clc ;
```

```
disp("  Example: 3.17   Page no : 151") ;
disp("          The problem contains only theory
    and different substitutions.There is no numerical
     part involved .")

// Del_S_magnetization > 0 ;
// Del_S_magnetization + Del_S_temperature = 0 ;
   therefore
// Del_S_temperature < 0 ;
// i.e.   T2 < T1 ;
```

# Chapter 4

# Equation of states and intermolecular forces

**Scilab code Exa 4.1** Example 4 1

```
//Engineering and Chemical Thermodynamics
//Example 4.1
//Page no :175

clear ; clc ;
//Let
H2O = 1 ;
NH3 = 2 ;
CH4 = 3 ;
CH3Cl = 4 ;
CCl4 = 5 ;

M_11 = 1.85 ; alp_12 = 14.80 ;  I_13 = 12.62 ;
M_12 = 1.47 ; alp_22 = 22.20 ;  I_23 = 10.07 ;
M_31 = 0.00 ;    alp_32 = 26.00 ;    I_33 = 12.61 ;
M_41 = 1.87 ; alp_42 = 45.30 ;  I_43 = 11.26 ;
M_51 = 0.00 ;    alp_52 = 105.0 ;   I_53 = 11.47 ;

k =1.38 * 10^-16 ; //[ J/K]
```

```
T = 298 ; //[K]
A =[M_11 , alp_12 , I_13;
M_12 , alp_22 , I_23 ;
M_31 , alp_32 , I_33 ;
M_41 , alp_42 , I_43 ;
M_51 , alp_52 , I_53 ;] ;
disp(" Example: 4.1 Page no : 175") ;
disp(" Molecule M alp*10^25 I C*10^60 Cd_d Cind Cdis") ;
for i=1:5
    A(i,5) = ceil( 2/3 * A(i,1)^4 / (k * T) * 10^-12) ;
    A(i,6) = ceil(2 * A(i,2) * A(i,1)^2 * 10^-1) ;
    A(i,7) = ceil(3/4 * A(i,2)^2 * A(i,3) * 1.6 * 10^-2) ;
    A(i,4) = ceil(A(i,5) + A(i,6) + A(i,7)) ; //....E4.1D
end ;

printf(" H2O %.2f %.1f %.2f %d %d %d %d ",A(1,1),A(1,2),A(1,3),A(1,4),A(1,5),A(1,6),A(1,7)) ;
printf("\n NH3 %.2f %.1f %.2f %d %d %d %d ",A(2,1),A(2,2),A(2,3),A(2,4),A(2,5),A(2,6),A(2,7)) ;
printf("\n CH4 %.2f %.1f %.2f %d %d %d %d ",A(3,1),A(3,2),A(3,3),A(1,4),A(3,5),A(3,6),A(3,7)) ;
printf("\n CH3Cl %.2f %.1f %.2f %d %d %d %d ",A(4,1),A(4,2),A(4,3),A(4,4),A(4,5),A(4,6),A(4,7)) ;
printf("\n CCl4 %.2f %.1f %.2f %d %d %d %d \n",A(5,1),A(5,2),A(5,3),A(5,4),A(5,5),A(5,6),A
```

```
    (5,7)) ;

disp("        Even though it is non polar , CCl4
    exhibit the largest intermolecular forces . It is
     due to the large polarizability accociated with
    the four Cl atom in CCl4 .") ;
```

**Scilab code Exa 4.2** Example 4 2

```
//Engineering and Chemical Thermodynamics
//Example 4.2
//Page no :176

clear ; clc ;
//Given //
C6_Ar_HCl_tab = 76 * 10^-60 ;//From table E4.2
C6_Ar_Ar_tab = 52 * 10^-60 ;//From table E4.2
C6_HCl_HCl_tab = 134 * 10^-60 ;//From table E4.2

C6_Ar_HCl_gmean = sqrt(C6_Ar_Ar_tab * C6_HCl_HCl_tab
    ) ; //[erg/cm^6]
x = (C6_Ar_HCl_gmean - C6_Ar_HCl_tab) /
    C6_Ar_HCl_tab * 100 ;

disp(" Example: 4.2    Page no : 176") ;
printf("\n    The geometric mean is different from
    that in table E4.2 by %d %%",x)
```

**Scilab code Exa 4.3** Example 4 3

```
//Engineering and Chemical Thermodynamics
//Example 4.3
//Page no :177
```

```

clear ; clc ;
//The problem contains only theory . There is no
   numerical part involved. Users can go through the
    book to obtain the required expression.

disp(" Example: 4.3    Page no : 177") ;
disp("      (C6)SiCl4 > (C6)CCl4 > (C6)CF4")
```

**Scilab code Exa 4.4** Example 4 4

```
//Engineering and Chemical Thermodynamics
//Example 4.4
//Page no :185

clear ; clc ;
//Given
Psat_wat_25 = 3.169 * 10^3 ;// From steam table
Psat_wat_50 = 1.235 * 10^4 ;// From steam table
Psat_wat_100 = 1.014 * 10^5 ;// From steam table
A =11.9673 ;
B = 3626.55 ;
C = -34.29 ;
T1 = 25 ; //[*C]
T2 = 50 ; //[*C]
T3 = 100 ; //[*C]

M = [T1 , Psat_wat_25 ; T2 , Psat_wat_50 ; T3 ,
   Psat_wat_100];
for i=1:3
    M(i,3) = exp(A - B / (M(i,1) + 273 + C)) * 10^5
        ;
end
disp(" Example: 4.4    Page no : 185") ;
disp("  T(*C)    Water(Pa)    Methanol(Pa)") ;
```

```
disp(M);

//Solution(1) :
printf("\n(1)\n     Water can form two hydrogen
   bonds . While CH4Oh can form only one . Thus at a
    given temperature , water has stronger
   attractive forces in the liquid and a lower
   vapour pressure .\n\n")

//Solution(2):
printf("(2)\n      Since the Maxwell-Boltzmann
   distribution depends exponentially on temperature
    , Psat also increses exponentially with
   temperature .")
```

**Scilab code Exa 4.5** Example 4 5

```
//Engineering and Chemical Thermodynamics
//Example 4.5
//Page no :189

clear ; clc ;
//The problem contains only theory . There is no
   numerical part involved. Users can go through the
    book to obtain the required expression.

disp(" Example: 4.5    Page no : 189") ;
disp(" (a)  a_SiCl3H > a_SiCl4 > a_CCl4 > a_CF4 ");
disp(" (b)  b_SiCl4 > b_CCl4 > b_SiCl3H > b_CF4 ");
```

**Scilab code Exa 4.6** Example 4 6

```
//Engineering and Chemical Thermodynamics
```

```
//Example 4.6
//Page no :190

clear ; clc ;
//Given
Pc_B = 49.1 ; // [bar] , From table
Pc_T = 42.0 ; // [bar] , From table
Pc_C = 40.4 ; // [bar] , From table
Tc_B = 562 ; // [K] , From table
Tc_T = 594 ; // [K] , From table
Tc_C = 553 ; // [K] , From table
R = 8.314 ;

A = [Pc_B , Tc_B ; Pc_T , Tc_T ; Pc_C , Tc_C];
for i=1:3
    A(i,3) = 27/64 * (R * A(i,2))^2 /( A(i,1) *
        10^5) ;
    A(i,4) = R * A(i,2) / (8 * A(i,1) * 10^5) ;
end
disp(" Example: 4.6    Page no : 190") ;
disp("    P_c      T_c          a                        b "
   ) ;
disp(A) ;
disp("                              The attractive
   interactions of all three compounds are dominated
    by dispersion interactions ( parameter a) ,
   while size affects parameter b .")
```

**Scilab code Exa 4.7** Example 4 7

```
//Engineering and Chemical Thermodynamics
//Example 4.7
//Page no :191

clear ; clc ;
```

```
disp(" Example: 4.7 Page no : 191") ;
disp(" The problem contains only theory and different substitutions.There is no numerical part involved. Users can go through the book to obtain the required expression.")
```

**Scilab code Exa 4.8** Example 4 8

```
//Engineering and Chemical Thermodynamics
//Example 4.8
//Page no :197

clear ; clc ;
//Given
B = 0.0486 * 10^-3 ;
T1 = 20 + 273 ; //[K]
T2 = 500 + 273 ; //[K]
v1 = 7.11 ; // [cm^3/mol]

v2 = v1 * exp( B * (T2 - T1)) ;
disp(" Example: 4.8 Page no : 197") ;
printf("\n Molar volume of solid state 2 = %.2f cm^3/mol", v2);
```

**Scilab code Exa 4.9** Example 4 9

```
//Engineering and Chemical Thermodynamics
//Example 4.9
//Page no :199

clear ; clc ;
//Given
```

```
P_c = 37.9 * 10^5 ;//[N/m^2] , From compressibility chart
T_c = 425.2 ;// [K , From compressibility chart
P = 50 * 10^5 ; //N/m^2]
T = 333.2 ;//[K]
R = 8.314 ;
z_0 = 0.2148 ; // Using interpolation from table C.1 and C.2
z_1 = -0.0855 ; // Using interpolation from table C.1 and C.2
w = 0.199 ;
m = 10 ;
MW = 0.05812 ;

// Using Redlich Kwong equation
a = (0.42748 * R^2 * T_c^2.5) / P_c ;
b = 0.08664 * R * T_c / P_c ;
A = P * T^(1/2) ;
B = -R * T^(3/2) ;
C = (a - P * T^(1/2) * b^2 - R * T^(3/2)*b) ;
D = - a * b;

mycoeff = [ D , C , B , A] ;
p = poly(mycoeff , "v" , "coeff" );
M = roots(p);

disp(" Example: 4.9   Page no : 199") ;
for i = 1:3
    sign(M(i,1)) ;
        if ans == 1 then
          V = m / MW *(M(i,1)) ;
          printf("\n       Using Redlich Kwong equation the volume is = %.3f m^3\n\n",V)
        end
end

// Using compressibility chart
```

```
z = z_0 + w * z_1 ;
v = z * R * T / P ;
V = m / MW * v ;
        printf("        Using compressibility chart
            the volume is = %.3f m^3\n\n",V)
```

**Scilab code Exa 4.10** Example 4 10

```
//Engineering and Chemical Thermodynamics
//Example 4.10
//Page no :202

//Solution(a)
clear ; clc ;
T = 100 + 273 ; //[K]
P = 70 * 10^5 ; //[N/m^2]
P_c = 42.2 * 10 ^ 5 ;
T_c = 370 ; //[K]
w = 0.153 ;// Interpolating from table C.1 and C.2
z_0 = 0.2822 ;// Interpolating from table C.1 and C
   .2
z_1 = - 0.0670 ;// Interpolating from table C.1 and
   C.2
m = 20 * 10^3 ;//[g]
MW = 44 ; //[g/mol]
R = 8.314 ;

P_r = P / P_c ;
T_r = T / T_c ;
z = z_0 + w * z_1 ;
V = m / MW *z * R * T / P ;
disp(" Example: 4.10    Page no : 202") ;
printf("\n    (1)\n          Volume = %.4f m^3 \n\n"
   , V )

```

```
//Solution(b)
T = 295 ;//[K]
n = 50 ; // [mol]
a = 0.42748 * R^2 * T_c^2.5 / P_c ;
b = 0.08664 * R * T_c / P_c ;
v = 0.1 ;
P = R * T / (v - b) - a / (T^0.5 * v * (v + b)) ;
x = P * n * 10^-6 ;
printf("\n     (2)\n               Pressure = %d MPa \n\n", x )

//Solution (c)
y1 = 0.4 ;
y2 = 1 - y1 ;
n = 50 ;
P_c = 48.7 * 10^5 ;//[N/m^2]
T_c = 305.5 ; //[K]
a1 = a ;
b1 = b ;
a2 = 0.42748 * R^2 * T_c^2.5 / P_c ;
b2 = 0.08664 * R * T_c / P_c ;

a_mix = y1^2 * a1 + 2 * y1 * y2 * sqrt(a1 * a2) + y2^2 * a2 ;
b_mix = y1 * b1 + y2 * b2 ;
P = R * T / (v - b_mix) - a_mix /(T^0.5 * v * (v + b_mix));
x = P * n * 10^-6 ;

printf("\n     (3)\n               Pressure = %.2f MPa \n\n", x )
```

# Chapter 5

# The thermodynamic web

**Scilab code Exa 5.1** Example 5 1

```
//Engineering and Chemical Thermodynamics
//Example 5.1
//Page no :218

clear ; clc ;
disp(" Example: 5.1   Page no : 218") ;
disp("          The problem contains only theory
    and different substitutions.There is no numerical
     part involved. Users can go through the book to
    obtain the required expression.")
```

---

**Scilab code Exa 5.2** Example 5 2

```
//Engineering and Chemical Thermodynamics
//Example 5.2
//Page no :222

clear ; clc ;
```

```
//Given
T_c = 370 ; //[K]
P_c = 41.58 * 10^5 ;//[N/m^2]
R = 8.314 ;
V1 = 0.001 ;//[m^3]
V2 = 0.04 ; //[m^3]
q = 600 ; //[J]

a = 27/64 * (R ^2)*(T_c)^2 / P_c ;
//Using E5.2D , E5.2E in E5.2C
del_U = -0.96 * (1 / V2 - 1 / V1) ;
W = del_U - q ;

disp(" Example: 5.2    Page no : 222") ;
printf("\n      Work done for the expansion = %g J/
    mol",W) ;
```

**Scilab code Exa 5.3** Example 5 3

```
//Engineering and Chemical Thermodynamics
//Example 5.3
//Page no :223

clear ; clc
disp("  Example: 5.3    Page no : 223") ;
disp("             The problem contains only theory
    and different substitutions.There is no numerical
     part involved. Users can go through the book to
    obtain the required expression.") ;
```

**Scilab code Exa 5.4** Example 5 4

```
//Engineering and Chemical Thermodynamics
```

```
//Example 5.4
//Page no :225

clear ; clc ;
//Given
P_1 = 9.43 * 10^5 ; //[N/m^2]
P_2 = 18.9 * 10^5 ; //[N/m^2]
T_1 = 80 + 273 ; //[K]
T_2 = 120 + 273 ; //[K]
A = 1.935 ;
B = 36.915 * 10^-3 ;
C = -11.402 * 10^-6 ;
T_c = 425.2 ; // [K]
P_c = 37.9 * 10^5 ;//[N/m^2]
R = 8.314 ;
del_h_1 = 1368 ; //[J/mol]
del_h_3 = -2542 ; //[J/mol]
Ws = 2100 ; //[J/mol]

a = 0.42748 * R^2 * T_c^2.5 / P_c ;
b = 0.08664 * R * T_c / P_c ;


  function y = f1 (v) , y  = R * T_1 / (v - b) - a / (sqrt(T_1) * v *(v + b)) - P_1;
  endfunction ;
za=  fsolve([0.001] , f1) ;

  function y = f2 (v) , y  = R * T_2 / (v - b) - a / (sqrt(T_2) * v *(v + b)) - P_2;
  endfunction ;
 zb=  fsolve([0.001] , f2) ;

   function y = f(T),
       y = R * ( A * T + B/2 * T^2 + C/3 * T^3) ;
   endfunction ;

del_h_2 = f(T_2) - f(T_1) ;
```

```
del_h_total = del_h_1 + del_h_2 + del_h_3 ;
q = del_h_total - Ws ;


disp(" Example: 5.4    Page no : 225") ;
printf("\n              v1 = %f m^3/mol\n              v2 =
    %f m^3/mol",za ,zb ) ;
printf("\n\n      The heat input = %g J/mol",ceil(q))
    ;
```

**Scilab code Exa 5.5** Example 5 5

```
//Engineering and Chemical Thermodynamics
//Example 5.5
//Page no :234

clear ; clc ;
//Given
T_c = 425.2 ; //[K] ,From Appendix A.1
P_c = 37.9 * 10^5 ; //[N/m^2] ,From Appendix A.1
w = 0.199 ;// From Appendix A.1
A = 1.935 ;
B = 36.915 * 10^-3 ;
C = -11.402 * 10^-6 ;
Ws = 2100 ; //[J/mol]
T1 = 353.15 ;//[K]
T2 = 393.15 ;//[K]
P1 =7.47 * 10^5 ;//[N/m^2]
P2 = 18.9 * 10^5 ; //[N/m^2]
R = 8.314 ;
enth_dep1_0 = -0.413 ;// Table C.3,C.4 in Appendix C
enth_dep1_1 = -0.622 ;// Table C.3,C.4 in Appendix C
enth_dep1 = enth_dep1_0 + w * enth_dep1_1 ;//....E5
    .5B
enth_dep2_0 = -0.771 ;// Table C.3,C.4 in Appendix C
```

```
enth_dep2_1 = -0.994 ;// Table C.3,C.4 in Appendix C
enth_dep2 = enth_dep2_0 + w * enth_dep2_1 ;//....E5
    .5C

T1_r = T1 / T_c ;
P1_r = P1 / P_c ;
T2_r = T2 / T_c ;
P2_r = P2 / P_c ;

function y=f(T) , y = R * (A * T + B/2 * T^2 + C/3 *
    T^3)
endfunction
del_h = f(T2) - f(T1) ;//.....E5.5D

Del_h = -enth_dep1 * R * T_c + del_h + enth_dep2 * R
    * T_c ;
q = Del_h - Ws ;

disp(" Example: 5.5    Page no : 235") ;
printf("\n      Heat input = %d J/mol",q)
```

**Scilab code Exa 5.6** Example 5 6

```
//Engineering and Chemical Thermodynamics
//Example 5.6
//Page no :237

clear ; clc ;
disp("  Example: 5.6    Page no : 237") ;
disp("            The problem contains only theory
    and different substitutions.There is no numerical
     part involved. Users can go through the book to
    obtain the required expression.")
```

**Scilab code Exa 5.7** Example 5 7

```
//Engineering and Chemical Thermodynamics
//Example 5.7
//Page no :239

clear ; clc ;
disp("  Example: 5.7   Page no :239") ;
disp("            The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.")
```

---

**Scilab code Exa 5.8** Example 5 8

```
//Engineering and Chemical Thermodynamics
//Example 5.8
//Page no :241

clear ; clc ;
//Given
T_c = 126.2 ; //[K]  , From appendix A.1
P_c = 33.8 * 10^5 ; //[N/m^2]  , From appendix A.1
w = 0.039 ;// From appendix A.1
enth_dep_1 = -2.81 ; // From table C.1 Appendix C
A = 3.28 ;// From Appendix A.2
B = 0.593 * 10^-3 ;// From Appendix A.2
del_h_dep_l = -5.1 ;
del_h_dep_v = -0.1 ;
T1 = 151 ; //[K]
P1 = 100 * 10^5 ; //[N/m^2]
P2 = 1 * 10^5 ; //[N/m^2]
```

```
T2_r = 0.61 ; // From figure 5.4
T1_r = T1 / T_c ;
P1_r = P1 / P_c ;
P2_r = P2 / P_c ;

T2 = T2_r * T_c ; //[K]
function y=f(T),y = A * T + B/2 * T^2
endfunction
x = 1 / T_c *(f(T2) - f(T1)) ;

y = enth_dep_1 - x ;

disp(" Example: 5.8    Page no : 241") ;
disp(y)
X = ( y - del_h_dep_l) / (del_h_dep_v - del_h_dep_l)
    ;
printf("\n    Quality = %.2f",X) ;
```

# Chapter 6

# Multi component Phase Equillibrium

**Scilab code Exa 6.1** Example 6 1

```
//Engineering and Chemical Thermodynamics
//Example 6.1:
//Page no :257

clear ; clc  ;
disp("  Example: 6.1   Page no : 257") ;
disp("            The problem contains only theory
  and different substitutions.There is no numerical
   part involved. Users can go through the book to
  obtain the required expression.")
```

**Scilab code Exa 6.2** Example 6 2

```
//Engineering and Chemical Thermodynamics
//Example 6.2
//Page no :261
```

```
clear ; clc ;
//Given
slop = -4222.1 ;
R = 8.314 ;
del_h_vap = -R * slop * 10^-3 ;

disp(" Example: 6.2    Page no : 261") ;
printf("\n      Enthalpy of vapourisation of Ga(CH3)3
    = %.1f kJ/mol",del_h_vap) ;
```

**Scilab code Exa 6.3** Example 6 3

```
//Engineering and Chemical Thermodynamics
//Example 6.3
//Page no :261

clear ; clc ;
//The problem contains only theory and different
   substitutions.There is no numerical part involved
   . Users can go through the book to obtain the
      required expression.


disp(" Example: 6.3    Page no : 261") ;
function y=f(x) , y = -4222.1 * x + 17.556
endfunction
xdata = linspace(0.0032,0.004,8) ;
ydata = f(xdata) ;
plot(xdata,ydata) ;
xtitle("Figure E6.2","1/T","ln P_sat (kPa)")
```

**Scilab code Exa 6.4** Example 6 4

```
//Engineering and Chemical Thermodynamics
//Example 6.4
//Page no :268

clear ; clc ;
disp("  Example: 6.4   Page no : 268") ;
disp("           The problem contains only theory and different substitutions.There is no numerical part involved. Users can go through the book to obtain the required expression.")
```

**Scilab code Exa 6.5** Example 6 5

```
//Engineering and Chemical Thermodynamics
//Example 6.5
//Page no :271

clear ; clc ;
disp("   Example 6.5   Page no:271")
disp("        There is no numerical part involved in this problem . Users can refer Figure 6.5.")
```

**Scilab code Exa 6.6** Example 6 6

```
//Engineering and Chemical Thermodynamics
//Example 6.6
//Page no :277

clear ; clc ;
//Given
MW1 = 119.5 ;
MW2 = 58 ;
```

```
A =
    [0,4.77,9.83,14.31,19.38,23.27,25.53,25.07,21.55,13.56,0]
    ;
B = [0,.1 , .2 , .3 ,.4 ,.5 ,.6 ,.7 ,.8 ,.9,1] ;

disp(" Example: 6.6   Page no : 277") ;
for i = 1:11

    x1 = (B(1,i) / MW1) / (B(1,i) / MW1 + (1 - B(1,i
       )) / MW2) ;
    x2 = 1 - x1 ;
    MW = x1 * MW1 + x2 * MW2 ;
    del_h_mix = - 1*(A(1,i)) * MW ;
    C(1,i) = del_h_mix ;
    D(1,i) = x1 ;

    printf("\n    For weight percent  %.3f
       del_h_mix = %.1f J/mol\n",x1,del_h_mix)
end

xdata = D ;
ydata = C ;
plot(xdata ,ydata) ;
xtitle("Figure E6.6B","x_CHCl3","Del_h_mix  (J/mol)"
   ) ;
```

**Scilab code Exa 6.7** Example 6 7

```
//Engineering and Chemical Thermodynamics
//Example 6.7
//Page no :279

clear ; clc ;
//Given
A =
```

```
[-32669,-31840,-28727,-26978,-24301,-20083,-13113]
  ;
B = [20 ,10 ,5 ,4 ,3 ,2 ,1] ;

disp(" Example: 6.7   Page no : 279") ;
for i = 1:7
    del_h_mix = A(1,i) / (1 + B(1,i)) ;
    C(1,i) = del_h_mix ;
    D(1,i) = 1 / (1 + B(1,i)) ;
    printf("\n      For mole fraction %.3f   the
       entropy of mixing is %d J/mol\n",D(1,i),C(1,i
       )) ;
end
```

**Scilab code Exa 6.8** Example 6 8

```
//Engineering and Chemical Thermodynamics
//Example 6.8
//Page no :280

clear ; clc ;
disp("  Example: 6.8   Page no : 280") ;
disp("           The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.")
```

**Scilab code Exa 6.9** Example 6 9

```
//Engineering and Chemical Thermodynamics
//Example 6.9
//Page no :282

```

```
clear ; clc ;
//Given
x1 = 0.1 ;
x2 = 1- x1 ;
B11 = -910 ;
B22 = -1330 ;
B12 = -2005 ;
T = 333 ; //[K]
P = 10 * 10^5 ;
R = 8.314 ;
v1 = R * T /P * 10^6 + B11 ;//....E6.9A

disp(" Example: 6.9    Page no : 282") ;
printf("\n      v1 = %g cm^3/mol\n",v1)
V_bar_1 = (R * T / P) * 10^6+ (x1^2 + 2 * x1 * x2) *
    B11 + 2 * x2^2 * B12  - x2^2 * B22 ;//.....E6.9B
printf("\n      V_bar_1 = %g cm^3/mol\n",V_bar_1) ;
del_v_mix = x1 * x2 * (2 * B12 - B11 - B22) ;//.....
   E6.9C
printf("\n      del_v = %g cm^3/mol",del_v_mix);
```

**Scilab code Exa 6.10** Example 6 10

```
//Engineering and Chemical Thermodynamics
//Example 6.10
//Page no :283

clear ;clc ;
//Given
h_H2SO4 = 1.596 ; //[kJ/mol]
h_H2O = 1.591 ; //[kJ/mol]
C1 = -74.40 ;
C2 = 0.561 ;
A = [0 ,0.1 , 0.2 ,0.3 ,0.4 ,0.5 ,0.6 ,0.7 ,0.8 ,0.9
    ,1] ;
```

```
B = [1 ,0.9 ,0.8 ,0.7 ,0.6 ,0.5 ,0.4 ,0.3 ,0.2 ,0.1
    ,0] ;

disp(" Example: 6.10    Page no : 283") ;
for i = 1:11
    H_bar_H2SO4 = h_H2SO4 + C1 * B(1,i)^2 - 2 * C2 *
        C1 * A(1,i) * B(1,i)^2 ;
    H_bar_H2O = h_H2O + C1 * A(1,i)^2 -C2 * C1 * A
        (1,i)^2 * (1 - 2 * B(1,i)) ;
    y_data_1(1,i) =  H_bar_H2SO4 ;
    y_data_2(1,i) =  H_bar_H2O ;
    x_data(1,i) = A(1,i) ;
end
plot(x_data,y_data_1) ;
plot(x_data,y_data_2) ;

m = y_data_1(1,6)  ;
s = y_data_2(1,6)  ;
xtitle("Figue E6.10","x_H2SO4"," Partial molar
    enthalpy");
printf("\n      For equimolar mixture del_H_H2SO4 = %
    .1f kJ/mol    del_H_H2O = %.1f kJ/mol",m,s);
```

**Scilab code Exa 6.11** Example 6 11

```
//Engineering and Chemical Thermodynamics
//Example 6.11
//Page no :283

clear ; clc ;
disp("  Example: 6.11    Page no : 283") ;
disp("              The problem contains only theory
    and different substitutions.There is no numerical
     part involved. Users can go through the book to
    obtain the required expression.")
```

**Scilab code Exa 6.12** Example 6 12

```
//Engineering and Chemical Thermodynamics
//Example 6.12
//Page no :287

clear ; clc ;
disp(" Example: 6.12   Page no : 287") ;
disp("            The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.")
```

**Scilab code Exa 6.13** Example 6 13

```
//Engineering and Chemical Thermodynamics
//Example 6.13
//Page no :287

clear ;clc ;
//Given
C1 = 1.596 ;
C2 = 1.591 ;
C3 = -74.40 ;
C4 = -0.561 ;
A = [ 0 ,0.1 ,0.2 ,0.3 ,0.4 ,0.5 ,0.6 ,0.7 ,0.8 ,0.9
    ,1] ;
m = (-C1 + C2 + C3 * ( C4 * 0.25)) * 1000 ;

disp(" Example: 6.13   Page no : 287") ;
for i = 1:11
```

```
    x_H2O = A(1,i) ;
    x_H2SO4 = 1- x_H2O ;
    h = C1 * x_H2SO4 + C2 * x_H2O + C3 * x_H2SO4 * x_H2O *(1 + C4 * x_H2SO4) ;
    C(1,i) = h * 10^3;
end
y1 = C(1,6) ;

function y = f613(x) ,
    y = -m * (x - 0.5 ) + y1 ;
endfunction

for i = 1:11
    F(1,i) = f613(A(1,i)) ;
end

plot(A,C);
plot(A,F)
xtitle("Figure E6.13","x_H2O","h (J/mol)");

printf("\n                    H_bar_H2SO4 = %d J/mol      H_bar_H2O = %d J/mol\n ",F(1,1),F(1,11)) ;
disp("      The partial molar property can be obtained by drawing tangent at mole fraction 0.5.")
```

---

**Scilab code Exa 6.14** Example 6 14

```
//Engineering and Chemical Thermodynamics
//Example 6.14:
//Page 291

clear ; clc ;
disp("  Example: 6.14    Page no : 291") ;
disp("           The problem contains only theory
```

and different substitutions.There is no numerical part involved. Users can go through the book to obtain the required expression.")

---

# Chapter 7

# Phase Equilibia 2 Fugacity

**Scilab code Exa 7.1** Example 7 1

```
//Engineering and Chemical Thermodynamics
//Example 7.1
//Page no :308

clear ; clc ;
//Given
h_cap_H2O = 2676.0 ; //[kJ/kg],From steam table
S_cap_H2O = 7.3548 ; //[kJ/kgK],From steam table
h_cap_0_H2O = 2687.5 ; //[kJ/kg],From Appendix B
S_cap_0_H2O = 8.4479 ; //[kJ/kgK],From Appendix B
P_0_H2O = 10 ;//[kPa]
T = 373.15 ;//[K]
R = 8.314 / 18 ;
P_sys = 101.35 ;//[kPa]

g_cap_H2O = h_cap_H2O - T * S_cap_H2O ;
g_cap_0_H2O = h_cap_0_H2O - T * S_cap_0_H2O ;

f_H2O = P_0_H2O * exp((g_cap_H2O - g_cap_0_H2O ) / (
    R * T)) ;

```

```
Sai_H2O = f_H2O / P_sys ;

disp(" Example: 7.1    Page no : 308") ;

printf("\n           The fugacity = %.2f kPa \n\n
           The fugacity coefficient = %.3f",f_H2O ,
   Sai_H2O);
```

**Scilab code Exa 7.2** Example 7 2

```
//Engineering and Chemical Thermodynamics
//Example 7.2
//Page no :309

clear ; clc ;
disp("  Example: 7.2    Page no : 309") ;
disp("               The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.")
```

**Scilab code Exa 7.3** Example 7 3

```
//Engineering and Chemical Thermodynamics
//Example 7.3
//Page no :311

clear ; clc ;
//Given
P = 50 ; //[bar]
T = 25 + 273.2 ;//[K]
P_c = 48.7 ; //[bar] , From Appendix A.1 Table C.7 &
    C.8
```

```
T_c = 303.5 ; //[K] , From Appendix A.1 Table C.7 & C.8
w = 0.099 ; // From Appendix A.1 Table C.7 & C.8
log_w_0 = -0.216 ;// By interpolation
log_w_1 = -0.060 ;// By interpolation

X = log_w_0 + w * log_w_1 ;
sai_eth = 10^(X) ;
f_eth = sai_eth * P ;

disp(" Example: 7.3    Page no : 311") ;
printf("\n       Fugacity = %g bar",f_eth);
```

**Scilab code Exa 7.4** Example 7 4

```
//Engineering and Chemical Thermodynamics
//Example 7.4
//Page no :316

clear ; clc ;
disp("  Example: 7.4    Page no : 316") ;
disp("            The problem contains only theory and different substitutions.There is no numerical part involved. Users can go through the book to obtain the required expression.") ;
```

**Scilab code Exa 7.5** Example 7 5

```
//Engineering and Chemical Thermodynamics
//Example 7.5
//Page no :319

clear ; clc ;
```

```
//Given
P = 50 ; // [bar]
T = 25 + 273.2 ; //[K]
y_eth = 0.2 ;
y_pro = 0.8 ;
T_c_eth = 305.5 ; //[K],From Appendix A.1
T_c_pro = 370 ; //[K],From Appendix A.1
P_c_eth = 48.7 ; //[bar],From Appendix A.1
P_c_pro = 42.4 ; // [bar],From Appendix A.1
w_eth = 0.099 ;//From Appendix A.1
w_pro = 0.153 ;//From Appendix A.1
log_w_0 = -0.579 ;// By double liner interpolation
log_w_1 = -0.406 ;// By double liner interpolation
T_pc = y_eth * T_c_eth + y_pro * T_c_pro ;
P_pc = y_eth * P_c_eth + y_pro * P_c_pro ;
w_mix = y_eth * w_eth + y_pro * w_pro ;

Pr = P / P_pc ;
Tr = T /T_pc ;
X = log_w_0 + w_mix * log_w_1 ;

sai = 10^(X) ;
f = sai * P ;

disp(" Example: 7.5   Page no : 319") ;
printf("\n     Fugacity co-efficient = %.2f\n\n
          Fugacity = %.1f bar",sai,f);
```

**Scilab code Exa 7.6** Example 7 6

```
//Engineering and Chemical Thermodynamics
//Example 7.6
//Page no :324

clear ; clc ;
```

```

// The problem does not contain any numerical part . The readers can refer the text book to get the answer .
disp(" Example: 7.6    Page no : 324") ;
disp("     Like interactions are stronger than unlike interaction .")
```

**Scilab code Exa 7.7** Example 7 7

```
//Engineering and Chemical Thermodynamics
//Example 7.7
//Page no :331

clear ; clc ;
disp("  Example: 7.7    Page no : 331") ;
disp("              The problem contains only theory and different substitutions.There is no numerical part involved. Users can go through the book to obtain the required expression.") ;
```

**Scilab code Exa 7.8** Example 7 8

```
//Engineering and Chemical Thermodynamics
//Example 7.8
//Page no :338

clear ; clc ;
disp("  Example: 7.8    Page no : 338") ;
disp("              The problem contains only theory and different substitutions.There is no numerical part involved. Users can go through the book to obtain the required expression.") ;
```

**Scilab code Exa 7.9** Example 7 9

```
//Engineering and Chemical Thermodynamics
//Example 7.9
//Page no :339

clear ; clc ;
disp("  Example: 7.9   Page no : 339") ;
disp("            The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.") ;
```

**Scilab code Exa 7.10** Example 7 10

```
//Engineering and Chemical Thermodynamics
//Example 7.10
//Page no :343

clear ; clc ;
//Given
gama_a_inf = 0.88 ;
gama_b_inf = 0.86 ;
R =  8.314 ;
T = 39.33 + 273 ;

A_1 = R * T * log(gama_a_inf) ;
A_2 = R * T * log(gama_b_inf) ;
A = (A_1 + A_2) / 2 ;
disp(" Example: 7.10   Page no : 343") ;
printf("\n      The average value of two-suffix
   Margules parameter A = %g J/mol",A);
```

**Scilab code Exa 7.11** Example 7 11

```
//Engineering and Chemical Thermodynamics
//Example 7.11
//Page no :343


clear ; clc ;
disp("  Example: 7.11    Page no : 343") ;
disp("              The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression.") ;
```

**Scilab code Exa 7.12** Example 7 12

```
//Engineering and Chemical Thermodynamics
//Example 7.12
//Page no :352

clear ; clc ;
//Given
A_T1 = 1401 ; //[J/mol]
T1 = 10 + 273 ;//[K]
T2 = 60 + 273 ; //[K]
C = 3250 ;
A_T2_prev = 1143 ;//[J/mol]

A_T2 = T2 * (C *(1/T2 - 1/T1) + A_T1 / T1);
disp(" Example: 7.12    Page no : 352") ;
printf("\n      Value of A at 60*C = %f J/mol\n\n",
   A_T2) ;
```

```
x = (A_T2_prev - A_T2) / A_T2_prev* 100 ;
printf("\n       The values differ by = %g %%",x)

// The results given in the text book are wrong .
```

# Chapter 8

# Phase Equilibria III Phase Diagrams

**Scilab code Exa 8.1** Example 8 1

```
//Engineering and Chemical Thermodynamics
//Example 8.1
//Page 369

clear ; clc ;
disp("  Example: 8.1    Page no : 369") ;
disp("             The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression .") ;
```

---

**Scilab code Exa 8.2** Example 8 2

```
//Engineering and Chemical Thermodynamics
//Example 8.2
//Page no :369
```

```
clear ; clc ;
//Given
A_C5H12 = 9.2131 ; //From table E8.2A
B_C5H12 = 2477.07 ; //From table E8.2A
C_C5H12 = -39.94 ; //From table E8.2A
A_C6H12 = 9.1325 ; //From table E8.2A
B_C6H12 = 2766.63 ; //From table E8.2A
C_C6H12 = -50.50 ; //From table E8.2A
A_C6H14 = 9.2164 ; //From table E8.2A
B_C6H14 = 2697.55 ; //From table E8.2A
C_C6H14 = -48.78 ; //From table E8.2A
A_C7H16 = 9.2535 ; //From table E8.2A
B_C7H16 = 2911.32 ; //From table E8.2A
C_C7H16 = -56.51 ; //From table E8.2A

x_C5H12 = 0.3 ;
x_C6H12 = 0.3 ;
x_C6H14 = 0.2 ;
x_C7H16 = 0.2 ;

function y82 = f82(T), y82 = -1 + (x_C5H12 * exp(
   A_C5H12 - B_C5H12 / (T + C_C5H12)) + x_C6H12 *
   exp(A_C6H12 - B_C6H12 / (T + C_C6H12)) + x_C6H14
   * exp(A_C6H14 - B_C6H14 / (T + C_C6H14)) +
   x_C5H12 * exp(A_C5H12 - B_C5H12 / (T + C_C5H12))
   + x_C7H16 * exp(A_C7H16 - B_C7H16 / (T + C_C7H16)
   ));
endfunction ;
y =fsolve([300],f82) ;
disp(" Example: 8.2    Page no : 369") ;
printf("\n     The temperature at which the liquid
   develops the first bubble of vapour = %d K",y);
```

**Scilab code Exa 8.3** Example 8 3

```
//Engineering and Chemical Thermodynamics
//Example 8.3
//Page no :370

clear ; clc ;
//Given
A_C5H12 = 9.2131 ; //From table E8.2A
B_C5H12 = 2477.07 ; //From table E8.2A
C_C5H12 = -39.94 ; //From table E8.2A
A_C6H12 = 9.1325 ; //From table E8.2A
B_C6H12 = 2766.63 ; //From table E8.2A
C_C6H12 = -50.50 ; //From table E8.2A
A_C6H14 = 9.2164 ; //From table E8.2A
B_C6H14 = 2697.55 ; //From table E8.2A
C_C6H14 = -48.78 ; //From table E8.2A
A_C7H16 = 9.2535 ; //From table E8.2A
B_C7H16 = 2911.32 ; //From table E8.2A
C_C7H16 = -56.51 ; //From table E8.2A

y_C5H12 = 0.3 ;
y_C6H12 = 0.3 ;
y_C6H14 = 0.2 ;
y_C7H16 = 0.2 ;
P = 1 ; //[bar]

function y83 = f83(T), y83 = -1 + P * ( y_C5H12 / exp(A_C5H12 - B_C5H12 / (T + C_C5H12)) + y_C6H12 / exp(A_C6H12 - B_C6H12 / (T + C_C6H12)) + y_C6H14 / exp(A_C6H14 - B_C6H14 / (T + C_C6H14)) + y_C7H16 / exp(A_C7H16 - B_C7H16 / (T + C_C7H16) ));
endfunction ;
y =fsolve([300],f83) ;
disp(" Example: 8.3    Page no : 370") ;
printf("\n\n              The temperature at which vapour develops the first drop of liquid = %.2f K ",y) ;

```

```
T = y ;
P_sat_C5H12 = exp(A_C5H12 - B_C5H12 / (T + C_C5H12)) ;
p_sat_C6H12 = exp(A_C6H12 - B_C6H12 / (T + C_C6H12)) ;
P_sat_C6H14 = exp(A_C6H14 - B_C6H14 / (T + C_C6H14)) ;
P_sat_C7H16 = exp(A_C7H16 - B_C7H16 / (T + C_C7H16)) ;

x_C5H12 = y_C5H12 * P / P_sat_C5H12 ;
x_C6H12 = y_C6H12 * P / p_sat_C6H12 ;
x_C6H14 = y_C6H14 * P / P_sat_C6H14 ;
x_C7H16 = y_C7H16 * P / P_sat_C7H16 ;

printf("\n\n          x_C5H12 = %f       x_C6H12 = %f\n\n          x_C6H14 = %f       x_C7H16 = %f",x_C5H12,x_C6H12 ,x_C6H14,x_C7H16) ;
```

**Scilab code Exa 8.4** Example 8 4

```
//Engineering and Chemical Thermodynamics
//Example 8.4
//Page no :371

clear ; clc ;
//Given
P_a_sat = 0.53 ;  //[bar]
P_b_sat = 0.16 ; //[bar]
X = 1/3 ;
Y = 1- X ;
x_a_feed = 0.5 ;
x_b_feed = 0.5 ;
a = Y * -(x_a_feed + x_b_feed) + Y^2 ;
b = X * Y *(P_a_sat + P_b_sat) - (x_a_feed * P_b_sat
```

```
    + x_b_feed * P_a_sat)*X ;
c =  P_a_sat * P_b_sat * X^2;

k=poly(0,'k');
P = c + b*k^1 + a*k^2 ;
M = roots(P);

disp(" Example: 8.4   Page no : 371") ;
for i = 1:2
    sign(M(i,1)) ;
        if ans == 1 then
          printf("\n\n      Pressure  = %.2f bar",M(i
             ,1)) ;
          Xa = x_a_feed / (P_a_sat / M(i,1) * X + Y)
              ;//....E8.4D
          Ya = Xa * P_a_sat / M(i,1)  ;//.....E8.4B
          printf("\n\n        Xa = %.2f \n        Ya =
              %.2f\n",Xa,Ya);
        end
end
```

**Scilab code Exa 8.5** Example 8 5

```
//Engineering and Chemical Thermodynamics
//Example 8.5
//Page no :378

clear  ; clc;
//Given
P1_sat = 0.72 ; //[bar]
P2_sat = 0.31 ; //[bar]
A = 3590 ;
B = -1180 ;
R = 8.314 ;
T = 70 + 273 ;//[K]
```

```
function y85 = f85(x1) , y85 = -.48 + ( x1 * exp((A
   + 3*B) * (1 - x1)^2 / (R * T) - 4 * B * (1 - x1)
   ^3  / (R * T)) * P1_sat) / ( x1 * exp((A + 3*B) *
    (1 - x1)^2 / (R * T) -4 * B * (1 - x1)^3  / (R *
    T)) * P1_sat +(1 - x1) * exp((A - 3*B) * x1^2 /
   (R * T) -4 * B * x1^3  / (R * T)) * P2_sat ) ;
endfunction
y = fsolve([0.1],f85);
x1 = y ;
P = ( x1 * exp((A + 3*B) * (1 - x1)^2 / (R * T) - 4
   * B * (1 - x1)^3  / (R * T)) * P1_sat) + (1 - x1)
    * exp((A - 3*B) * x1^2 / (R * T) -4 * B * x1^3
   / (R * T)) * P2_sat ;
disp(" Example: 8.5    Page no : 378") ;
printf("\n      The value of x1 = %.3f\n\n",y) ;
printf("       Pressure = %.2f bar",P) ;
```

**Scilab code Exa 8.6** Example 8 6

```
//Engineering and Chemical Thermodynamics
//Example 8.6
//Page no :378

clear ; clc ;
disp("  Example: 8.6    Page no : 378") ;
disp("            The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression .") ;
```

**Scilab code Exa 8.7** Example 8 7

```
//Engineering and Chemical Thermodynamics
```

```
//Example 8.7
//Page no :385

clear ; clc;
//Given
P = 0.223 ; //[bar]
P_a_sat = 0.156 ; // [bar]
P_b_sat = 0.124 ; //[bar]
R = 8.314 ;
T = 50 + 273 ;
Xa = 0.554 ;
Xb = 1 - Xa ;

gama_a = P / P_a_sat ;
A1 = R * T * log(gama_a) / (Xb^2) * 10^-3 ;
gama_b = P / P_b_sat ;
A2 = R * T * log(gama_b) / (Xa^2) * 10^-3 ;

A = ceil((A1 + A2) / 2) ;
disp(" Example: 8.7    Page no : 385") ;
printf("\n     Value of two suffix Marguels parameter
    = %.1f kJ/mol",A);
```

**Scilab code Exa 8.8** Example 8 8

```
//Engineering and Chemical Thermodynamics
//Example 8.8
//Page no :385

clear ; clc ;
disp("  Example: 8.8    Page no : 385") ;
disp("             The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression .") ;
```

**Scilab code Exa 8.9** Example 8 9

```
//Engineering and Chemical Thermodynamics
//Example 8.9
//Page No:388

clear ; clc ;
//Given
R = 8.314 ;
T = 10 + 273 ; //[K]
A_B = 9.2806 ; // From Appendix A , Table A1.1
B_B = 2788.5 ; // From Appendix A , Table A1.1
C_B = -52.36 ; // From Appendix A , Table A1.1
A_C = 9.1325 ; // From Appendix A , Table A1.1
B_C = 2766.63 ; // From Appendix A , Table A1.1
C_C = -50.50 ; // From Appendix A , Table A1.1

x1 = [0 ,0.0610 ,0.2149 ,0.3187 ,0.4320 ,0.5246
    ,0.6117 ,0.7265 ,0.8040 ,0.8830 ,0.8999 ,1] ; //
    From table E8.9A
P_exp = [6344 ,6590 ,6980 ,7140 ,7171 ,7216 ,7140
    ,6974 ,6845 ,6617 ,6557 ,6073] ; //From table E8
    .9A

P_1_sat = 6072.15 ; //[Pa]
P_2_sat = 6344 ; //[Pa]

A = [1390 ,1391 ,1392 ,1393 ,1394 ,1395 ,1396 ,1397
    ,1398 ,1399 ,1400 ,1401 ,1402 ,1403 ,1404 ,1405
    ,1406 ,1407 ,1408 ,1409 ,1410 ] ;

for k = 1:21
    y = A(1,k) ;
   for i = 1:12
```

```
        P(1,i) = x1(1,i) * exp( y / (R * T ) * (1 -
           x1(1,i))^2) * P_1_sat+(1 - x1(1,i)) * exp
           (y / (R * T ) * x1(1,i)^2) * P_2_sat ;
        C(k,i) = (P(1,i) - P_exp(1,i))^2 ;
    end
end

for k = 1:21
   y = 0 ;
   for i = 1:12
     y = y + C(k,i) ;
   end
    R(1,k) = y ;
end

k = 100000 ;
for i = 1:21
    K = R(1,i) ;
    if K < k then
        k = K ;
    end
end
disp(" Example: 8.9    Page no : 388") ;
for i = 1:21
    if R(1,i) == k then
      printf("\n      The two suffix Margules co-
         efficient is = %g J/mol" ,A(1,i)) ;
    end
end
```

**Scilab code Exa 8.10** Example 8 10

```
//Engineering and Chemical Thermodynamics
//Example 8.10
//Page No:390
```

```
clear ; clc ;
//Given
R = 8.314 ;
T = 10 + 273.15 ; //[K]
A_B = 9.2806 ; // From Appendix A , Table A1.1
B_B = 2788.5 ; // From Appendix A , Table A1.1
C_B = -52.36 ; // From Appendix A , Table A1.1
A_C = 9.1325 ; // From Appendix A , Table A1.1
B_C = 2766.63 ; // From Appendix A , Table A1.1
C_C = -50.50 ; // From Appendix A , Table A1.1

x1 = [0,0.0610 ,0.2149 ,0.3187 ,0.4320 ,0.5246 ,0.6117 ,0.7265 ,0.8040 ,0.8830 ,0.8999 ,1] ; // From table E8.9A
P_exp = [6344 ,6590 ,6980 ,7140 ,7171 ,7216 ,7140 ,6974 ,6845 ,6617 ,6557 ,6073] ; //From table E8.9A

P_1_sat = 6073 ; //[Pa]
P_2_sat = 6344 ; //[Pa]
A = 1390:1410 ;
B = 60:80 ;
w = 1 / (R * T) ;
for k = 1:21
    y = A(k) ;
    for i = 1:21
        z = B(i) ;
        for j = 1:12
        P(1,j) = x1(1,j) * exp((y + 3 * z) * (1 - (x1(1,j)))^2 *w-4*z*(1-x1(1,j))^3* w )* P_1_sat + (1-x1(1,j))*exp((y -3*z)*(x1(1,j))^2 * w + 4 * z * (x1(1,j)^3) * w )* P_2_sat ;
        R(1,j) =(P(1,j) - P_exp(1,j))^2 ;
        end

        m = 0 ;
```

```
        for l = 1:12
            m = m + R(1,l) ;
        end
        S(k,i) = m ;
     end
end
for i = 1:21
    k = S(i,1) ;
    for l = 2:21
        if S(i,l) < k then
           k = S(i,l) ;
        end
    end
        D(1,i) = k ;
end

a = D(1,1) ;
for i = 2:21
    if D(1,i) < a then
        a = D(1,i) ;
    end
end
disp(" Example: 8.10    Page no : 390") ;
for i = 1:21
    if D(1,i) == a then
        for l = 1:21
            if S(i,l) == a then
                printf("\n      A = %g J/mol",A(1,i)) ;
                printf("\n      B = %g J/mol",B(1,l)) ;
            end
        end
    end
end
```

**Scilab code Exa 8.11** Example 8 11

```
//Engineering and Chemical Thermodynamics
//Example 8.11
//Page No:390

clear ; clc ;
//Given
R = 8.314 ;
T = 10 + 273.15 ; //[K]
x1 = [0 ,0.0610 ,0.2149 ,0.3187 ,0.4320 ,0.5246
    ,0.6117 ,0.7265 ,0.8040 ,0.8830 ,0.8999 ,1] ; //
    From table E8.9A
P_exp = [6344 ,6590 ,6980 ,7140 ,7171 ,7216 ,7140
    ,6974 ,6845 ,6617 ,6557 ,6073 ,6073] ; //From
    table E8.9A
y1 = [ 1 ,0.0953 ,0.2710 ,0.3600 ,0.4453,0.5106
    ,0.5735 ,0.6626 ,0.7312 ,0.8200 ,0.8382, 0 ] ;//
    From table E8.9A
P_1_sat = 6073 ; //[Pa]
P_2_sat = 6344 ; //[Pa]

n = 0 ;
for i = 2:11
    x2(1,i) = 1 - x1(1,i) ;
    y2(1,i) = 1 - y1(1,i) ;
    g_E(1,i) = R * T *( x1(1,i) * log (( y1(1,i) *
        P_exp(1,i)) / (x1(1,i)* P_1_sat)) + x2(1,i) *
         log((y2(1,i) * P_exp(1,i)) / (x2(1,i) *
        P_2_sat)) ) ;
    n = n + g_E(1,i) / ((x1(1,i) * x2(1,i)) * 10) ;
    ydata(1,i-1) = (g_E(1,i)/(x1(1,i)*x2(1,i)));
    xdata(1,i-1) = x1(1,i) - x2(1,i) ;
end
```

```
m= 0 ; n=0 ; o = 0 ; p= 0 ;N = 10 ;
for i = 2:11
    m = m + g_E(1,i) * (2 * x1(1,i) - 1) / ( x1(1,i) * x2(1,i)) ;
    n = n + g_E(1,i) / ( x1(1,i) *  x2(1,i)) ;
    o = o + (2 * x1(1,i) - 1)  ;
    p = p + (2 * x1(1,i) - 1)^2 ;
end
x_bar = o / N ;
y_bar = n / N ;
a1 = (N * m - n * o)/(N * p - o^2) ;
a0 = y_bar - a1 * x_bar ;

for i = 1:10
      ydata2(1,i) = a0 + a1*xdata(1,i) ;
end
plot(xdata,ydata,"+") ;
plot(xdata,ydata2) ;
xtitle("Figure E8.11","x1-x2","g_E/x1*x2") ;
disp(" Example: 8.11    Page no : 390") ;
printf("\n       From average ,  the value of A = %d J/mol\n",n/10) ;
printf("\n       From linear regression best fit line the values of A and B are     %.1f J/mol    &    %.1f J/mol   respectively .",a0 , a1) ;
//Readers can refer figure E8.11 .
```

**Scilab code Exa 8.12** Example 8 12

```
//Engineering and Chemical Thermodynamics
//Example 8.12
//Page no :395

clear ; clc ;
//Given
```

```
H_O2 = 44253.9 ;//[bar] , From table 8.1
p_O2 = 0.21 ; //[bar]

x_O2 = p_O2 / H_O2 ;
v_H2O = 1/(1/0.001 * 1/0.018 * 0.001 );
_O2_ = x_O2 / v_H2O ; //[M]
disp(" Example: 8.12   Page no : 395") ;
printf("\n     Mole fraction of O2 = %g",x_O2 ) ;
printf("\n     Concentration of O2 = %g M ",_O2_) ;
```

**Scilab code Exa 8.13** Example 8 13

```
//Engineering and Chemical Thermodynamics
//Example 8.13
//Page no :396

clear ; clc ;
//Given
P = 300 ; //[bar]
V_bar_inf_N2 = 3.3 * 10^-5 ;
R = 8.314 ;
T = 298 ; //[K]
y_N2 = 1 ; // At 25*C vapour pressure of water is small
H_N2_1 = 87365 ; //[bar]
P_c = 33.8 ; //[bar]
T_c = 126.2 ;// [K]
w = 0.039 ; // From Appendix A.1
log_w_0 = 0.013 ;
log_w_1 = 0.210 ;
H_N2_300 = H_N2_1 * exp((V_bar_inf_N2 * (P -1) * 10^5 )/ (R * T)) ;

k = log_w_0 + w * log_w_1 ;
sai_N2 = 10^k ;
```

```
x_N2 = y_N2 * sai_N2 * P / H_N2_300 ;

disp(" Example: 8.13    Page no : 396")
printf("\n      Solubility of N2 in water = %.5f", x_N2) ;
```

**Scilab code Exa 8.14** Example 8 14

```
//Engineering and Chemical Thermodynamics
//Example 8.14
//Page no :400

clear  ; clc;
disp("  Example: 8.14    Page no : 400") ;
disp("             The problem does not contain any numerical calculation . The readers can go through the text book to get the required answer .")
```

**Scilab code Exa 8.15** Example 8 15

```
//Engineering and Chemical Thermodynamics
//Example 8.15
//Page no :402

clear ; clc;
//Given
R = 8.314 ;
T = 20 + 273 ;//[K]
A = 6000 ; //[J/mol]
B = -384 ; //[J/mol]
x_a = [0.001 ,0.03 ,0.05 ,0.06 ,0.075 ,0.1 ,0.12 , 0.13 ,0.15 ,0.2 ,0.25 ,0.3 ,0.35 ,0.4 ,0.45,0.475
```

```
    ,0.5 ,0.55 ,0.6 ,0.65  ,0.7 ,0.75 ,0.8 ,0.8475
   ,0.85  ,0.9 ,0.925 ,0.95 ,0.975 ,0.999] ;

for i = 1:30
    y_data(1,i) = R * T * ( x_a(1,i) * log(x_a(1,i))
        + (1 - x_a(1,i)) * log(1- x_a(1,i))) + x_a
       (1,i) * (1 - x_a(1,i)) * (A + B * (2*x_a(1,i)
        - 1 )) ;
    y_data2(1,i) = - 82 * x_a(1,i)- 185.6 ;
end

m = min(y_data) ;
for i = 1:30
    if y_data(1,i) == m then
       a = x_a(1,i) ;
    end
end


for i = 1: 30
     y_data2(1,i) = -(R * T *( log(a)  - log(1 - a))
         + A * (1 - 2*a) + B * (6 * a - 1 - 6 * a^2)
        ) * (x_a(1,i) - a) + m ;
end

for i = 1:20
    y_data3(1,i) = y_data(1,i) - y_data2(1,i) ;
end
n = min(y_data3) ;

for i = 1:20
    if y_data3(1,i) == n then
       b = x_a(1,i) ;
    end
end


disp(" Example: 8.15   Page no : 402") ;
```

```
plot(x_a ,y_data) ;
plot(x_a ,y_data2) ;
xtitle(" Figure E8.15","x_a","g - x_a * g_a - x_b *
   g_b") ;

printf("\n\n              The equilibrium composition
    can be found by drawing a line tangent to the
   minima .\n\n                    In this case the
    answer is %.2f and %.1f   ." , a ,b)
```

**Scilab code Exa 8.16** Example 8 16

```
//Engineering and Chemical Thermodynamics
//Example 8.16
//Page no :403

clear ; clc;
//Given
A = 6349 ; //[J/mol]
B = -384 ; //[J/mol]
R = 8.314 ;
T = 20 + 273 ; //[K]

k = 0.000001 ;
disp(" Example: 8.16   Page no : 403") ;
function y816 = f816(x_a) , y816 = R * T * (1/x_a +
   1/(1 - x_a)) - 2 * A +6 * B * (1 - 2 * x_a) + k
endfunction
ans1 = fsolve([0.1],f816) ;
ans2 = fsolve([0.5],f816) ;

printf("\n   %.3f < x_a < %.3f ",ans1,ans2)
```

**Scilab code Exa 8.17** Example 8 17

```
//Engineering and Chemical Thermodynamics
//Example 8.17
//Page no :406
clear  ; clc;
//Given

T = 300 ; //[K]
A = 6235 ; //[J/mol]
P_a_sat = 100 * 10^3 ; //[Pa]
P_b_sat = 50 * 10^3 ; //{Pa}
R = 8.314 ;
w = 1/(R * T) ;
function Z817 = f817(R)
    x_a_a = R(1) ;
    x_a_b = R(2) ;
    Z817(1) = x_a_b * exp(A * (1 - x_a_b) ^ 2 * w) - x_a_a * exp(A * (1 - x_a_a) ^ 2 * w) ; // E8.17A
    Z817(2) = (1 - x_a_b) * exp(A * ( x_a_b) ^ 2 * w) - (1 - x_a_a) * exp(A * (x_a_a) ^ 2 * w ) ; // E8.17B
endfunction
x0 = [0.75 ; 0.1] ;
[z,fxs,m] = fsolve(x0,f817) ;
disp(" Example: 8.17   Page no : 406") ;
printf("\n        The compositions are : x_a_a = %.3f and x_a_b = %.3f",z(1,1), z(2,1)) ;

P = z(1,1) * exp(A * z(2,1) ^ 2 * w) * P_a_sat + z(2,1) * exp(A * z(1,1) ^ 2 * w) * P_b_sat ;
printf("\n        Total pressure = %d kPa",P * 10^-3) ;
y_a = z(1,1) * exp(A * z(2,1) ^ 2 * w) * P_a_sat / P ;
printf("\n             y_a = %.3f" , y_a ) ;
```

**Scilab code Exa 8.18** Example 8 18

```
//Engineering and Chemical Thermodynamics
//Example 8.18
//Page no :418

clear ; clc ;
//Given
T_b = 373.15 ; //[K]
del_h_vap = 2257 ; //[J/g]
MW_salt = 58.5 ; //[g/mol]
MW_water = 18 ; //[g/mol]
w_salt = 3.5 ;
w_water = 100 - w_salt ;
R = 8.314 ;

x_salt = (w_salt / MW_salt) / (w_salt / MW_salt +
    w_water / MW_water) ;
x_b = 2 * x_salt ;// We assume NaCl completely
    dissociates into Na+ & Cl- ions

del_T = R * T_b^2 / (del_h_vap * MW_water)* x_b ;
disp(" Example: 8.18    Page no : 418")
printf("\n    The temperature that sea water boils
    is = %.2f degreeC",100 + del_T);
```

**Scilab code Exa 8.19** Example 8 19

```
//Engineering and Chemical Thermodynamics
//Example 8.19
//Page no :418

```

```
clear ; clc ;
//Given
rho_w = 1000 ; // [kg/m^3]
g = 9.8 ; // [m/s^2]
h = 0.0071 ;//[m]
m_b = 1.93 * 10^-3 ; // [kg]
V = 520 * 10^-6 ; //[m^3]
R = 8.314 ;
T = 298 ;

PI = rho_w * g * h ;
C_b = m_b / V ;
MW_b = R * T * C_b / PI ;

disp(" Example: 8.19   Page no : 418")
printf("\n      The molecular weight of the protein
   = %d kg/mol", MW_b );
```

# Chapter 9

# Chemical reaction Equilibria

**Scilab code Exa 9.1** Example 9 1

```
//Engineering and Chemical Thermodynamics
//Example 9.1
//Page no :440

clear ; clc ;
n_o_CH3OH = 1 ; //[mol]
n_o_H2O = 3 ; //[mol]
S = 0.87 ;
n_CH3OH = 1 - S ;
n_H2O = 2 - S ;
n_CO2 = S ;
n_H2 = 3 * S ;
n_v = n_CH3OH + n_CO2 + n_H2O + n_H2 ;

y_H2 = n_H2 / n_v ;
disp(" Example: 9.1    Page no : 440") ;
printf("\n      No of moles of H2 produced for 1mol
    of CH3OH = %.3f mol" , n_H2)
printf("\n      Mole fraction of H2 = %.2f" , y_H2) ;
```

**Scilab code Exa 9.2** Example 9 2

```
//Engineering and Chemical Thermodynamics
//Example 9.2
//Page no :444

clear ; clc ;
//Given
del_gf_0_CO2 = -394.36 ; //[kJ/mol],From Appendix A.3
del_gf_0_H2 = 0 ; //[kJ/mol],From Appendix A.3
del_gf_0_H2O = -228.57 ; //[kJ/mol],From Appendix A.3
del_gf_0_CH3OH = -161.96 ; //[kJ/mol],From Appendix A.3
n_CO2 = 1 ;
n_H2 = 3 ;
n_CH3OH = 1 ;
n_H2O = 1 ;
T = 298.15 ;//[K]
R = 8.314 ; //[J/molK]

del_g0_rxn = (n_CO2 * del_gf_0_CO2 + n_H2 * del_gf_0_H2 - n_H2O * del_gf_0_H2O - n_CH3OH * del_gf_0_CH3OH) * 10^3 ; // [J/mol]
K_298 = exp( - del_g0_rxn / (R * T)) ;
disp(" Example: 9.2    Page no : 444") ;
printf("\n      The equillibrium constant K298 = %.2f",K_298) ;
```

**Scilab code Exa 9.3** Example 9 3

```
//Engineering and Chemical Thermodynamics
//Example 9.4
//Page no :447

clear ; clc ;
//Given
del_gf_0_CH2O = -110.0 ; //[kJ/mol],From Appendix A
    .2 & A.3
del_gf_0_H2 = 0 ; //[kJ/mol],From Appendix A.2 & A.3
del_gf_0_CH4O = -162.0 ; //[kJ/mol],From Appendix A
    .2 & A.3
del_hf_0_CH2O = -116.0 ; //[kJ/mol],From Appendix A
    .2 & A.3
del_hf_0_H2 = 0 ; //[kJ/mol],From Appendix A.2 & A.3
del_hf_0_CH4O = -200.7 ; //[kJ/mol],From Appendix A
    .2 & A.3n_CH2O = 1 ;
n_H2 = 1 ;
n_CH4O = 1 ;
n_CH2O = 1 ;
T1 = 298 ;//[K]
T2 = 873 ; // [K]
R = 8.314 ; //[J/molK]
Del_A = 3.302 ;
Del_B = -4.776 * 10^-3 ;
Del_C = 1.57 * 10^-6 ;
Del_D = 0.083 * 10^5 ;
//Solution (a)
del_g_rxn_298 = n_CH2O * del_gf_0_CH2O + n_H2 *
    del_gf_0_H2 - n_CH4O * del_gf_0_CH4O ;
K_298 = exp( - del_g_rxn_298 * 10^3 / (R * T1)) ;
disp(" Example: 9.4    Page no : 447") ;
printf("\n     (a) K_298 = %g \n\n    As the
    equilibrium constant is very small very little
    amount of formaldehyde will be formed .\n",K_298)
    ;

//Solution(b)
del_h_rxn_298 = (n_CH2O * del_hf_0_CH2O + n_H2 *
```

```
del_hf_0_H2 - n_CH4O * del_hf_0_CH4O) * 10^3 ;//[J/mol]
K_873 = K_298 * exp((-del_h_rxn_298  * (1/T2 - 1/T1)) / R) ;
printf("\n    (b)\n              (i)   K_873 = %g \n\n",K_873) ;

//Solution(c)
x =  ( -del_h_rxn_298 / R + Del_A * T1 + Del_B / 2 * T1^2 + Del_C /3 * T1^3 - Del_D / T1 ) *(1/T2 - 1/T1) + Del_A * log(T2 / T1) + Del_B / 2 * (T2 - T1) + Del_C / 6 * (T2^2 -T1^2) + Del_D / 2 * (1/(T2^2) -1/(T1^2)) ;
K_873 = K_298 * exp(x) ;
printf("\n              (ii)   K_873 = %g \n\n",K_873) ;
```

**Scilab code Exa 9.4** Example 9 4

```
//Engineering and Chemical Thermodynamics
//Example 9.4
//Page no :447

clear ; clc ;
//Given
del_gf_0_CH2O = -110.0 ; //[kJ/mol],From Appendix A.2 & A.3
del_gf_0_H2 = 0 ; //[kJ/mol],From Appendix A.2 & A.3
del_gf_0_CH4O = -162.0 ; //[kJ/mol],From Appendix A.2 & A.3
del_hf_0_CH2O = -116.0 ; //[kJ/mol],From Appendix A.2 & A.3
del_hf_0_H2 = 0 ; //[kJ/mol],From Appendix A.2 & A.3
del_hf_0_CH4O = -200.7 ; //[kJ/mol],From Appendix A.2 & A.3n_CH2O = 1 ;
```

```
n_H2 = 1 ;
n_CH4O = 1 ;
n_CH2O = 1 ;
T1 = 298 ;//[K]
T2 = 873 ; // [K]
R = 8.314 ; //[J/molK]
Del_A = 3.302 ;
Del_B = -4.776 * 10^-3 ;
Del_C = 1.57 * 10^-6 ;
Del_D = 0.083 * 10^5 ;
//Solution (a)
del_g_rxn_298 = n_CH2O * del_gf_0_CH2O + n_H2 *
    del_gf_0_H2 - n_CH4O * del_gf_0_CH4O ;
K_298 = exp( - del_g_rxn_298 * 10^3 / (R * T1)) ;
disp(" Example: 9.4    Page no : 447") ;
printf("\n     (a) K_298 = %g \n\n    As the
    equilibrium constant is very small very little
    amount of formaldehyde will be formed .\n",K_298)
     ;

//Solution(b)
del_h_rxn_298 = (n_CH2O * del_hf_0_CH2O + n_H2 *
    del_hf_0_H2 - n_CH4O * del_hf_0_CH4O) * 10^3 ;//[
    J/mol]
K_873 = K_298 * exp((-del_h_rxn_298  * (1/T2 - 1/T1)
    ) / R) ;
printf("\n     (b)\n              (i)   K_873 = %g \n\n"
    ,K_873) ;

//Solution(c)
x =  ( -del_h_rxn_298 / R + Del_A * T1 + Del_B / 2 *
     T1^2 + Del_C /3 * T1^3 - Del_D / T1 ) *(1/T2 -
    1/T1) + Del_A * log(T2 / T1) + Del_B / 2 * (T2 -
    T1) + Del_C / 6 * (T2^2 -T1^2) + Del_D / 2 * (1/(
    T2^2) -1/(T1^2)) ;
K_873 = K_298 * exp(x) ;
printf("\n             (ii)   K_873 = %g \n\n",K_873)
    ;
```

**Scilab code Exa 9.5** Example 9 5

```
//Engineering and Chemical Thermodynamics
//Example 9.5:
//Page no :450

clear ; clc ;
disp(" Example: 9.5   Page no : 450") ;
disp("             The problem contains only theory and different substitutions.There is no numerical part involved. Users can go through the book to obtain the required expression .") ;
```

**Scilab code Exa 9.6** Example 9 6

```
//Engineering and Chemical Thermodynamics
//Example 9.6
//Page no :451

clear ; clc ;
del_g0_f_C6H6 = -32.84 ; //[kJ/mol] , From Table E9.6
del_g0_f_C2H4 = 68.15 ; //[kJ/mol] , From Table E9.6
del_g0_f_H2 = 0 ;  //[kJ/mol] , From Table E9.6
del_h0_f_C6H6 = -84.68 ; //[kJ/mol] , From Table E9.6
del_h0_f_C2H4 = 52.26 ; //[kJ/mol] , From Table E9.6
del_h0_f_H2 = 0 ;  //[kJ/mol] , From Table E9.6
T1 = 298.2 ;//[K]
P = 1 ;//[bar]
R = 8.31 ;
```

```
T2 = 1273 ; // [K]
del_g0_f_rxn = del_g0_f_C2H4 + del_g0_f_H2 -
    del_g0_f_C6H6 ;
K_298 = exp ( - (del_g0_f_rxn * 10^3) / (R * T1)) ;

del_h0_f_rxn = (del_h0_f_C2H4 + del_h0_f_H2 -
    del_h0_f_C6H6) * 10^3 ;
K_1273 = K_298 * exp( - del_h0_f_rxn / R * (1/T2 -
    1/T1)) ;

x = sqrt( K_1273 / ( K_1273 + P)) ;

disp(" Example: 9.6    Page no : 451") ;
printf("\n      n_C2H6 = %.2f mol\n\n      n_C2H4 = %
    .2f mol\n\n      n_H2 = %.2f mol",1-x ,x,x) ;
```

**Scilab code Exa 9.7** Example 9 7

```
//Engineering and Chemical Thermodynamics
//Example 9.7
//Page no :453

clear ; clc ;
//Given
del_h0_f_NH3 = -46.11 ; // [kJ/mol],From table E9.7
del_h0_f_N2 = 0 ; // [kJ/mol],From table E9.7
del_h0_f_H2 = 0 ; // [kJ/mol],From table E9.7
del_g0_f_NH3 = -16.45 ; // [kJ/mol],From table E9.7
del_g0_f_N2 = 0 ; // [kJ/mol],From table E9.7
del_g0_f_H2 = 0 ; // [kJ/mol],From table E9.7
n_NH3 = 2 ;
n_N2 = -1 ;
n_H2 = -3 ;
A_NH3 = 3.578 ; B_NH3 = 3.02 * 10^-3 ; D_NH3 =
    -0.186 * 10^5 ;
```

```
A_N2 = 3.280 ; B_N2 = 0.593 * 10^-3 ; D_N2 = 0.040 * 10^5 ;
A_H2 = 3.249 ; B_H2 = 0.422 * 10^-3 ; D_H2 = 0.083 * 10^5 ;
R = 8.314 ;
T = 298 ;
T2 = 773 ;
P = 1 ; //[bat]

Del_h0_rxn = (n_NH3 * del_h0_f_NH3 + n_N2 * del_h0_f_N2 + n_H2 * del_h0_f_H2) * 10^3 ;
Del_g0_rxn = (n_NH3 * del_g0_f_NH3 + n_N2 * del_g0_f_N2 + n_H2 * del_g0_f_H2) * 10^3 ;
del_A = n_NH3 * A_NH3 + n_N2 * A_N2 + n_H2 * A_H2 ;
del_B = n_NH3 * B_NH3 + n_N2 * B_N2 + n_H2 * B_H2 ;
del_D = n_NH3 * D_NH3 + n_N2 * D_N2 + n_H2 * D_H2 ;

K_298 = exp( - Del_g0_rxn / ( R * T)) ;
K_T = K_298 * exp( - Del_h0_rxn / R * (1 / T2 - 1 / T)) ;
A = K_T * P^2 *27 -16 ;
B = 64 - K_T * P^2 * 108 ;
C = -64 + K_T * P^2 * 162 ;
D = -108 * K_T * P^2 ;
E = 27 * K_T * P^2 ;

//(a)
mycoeff =[E , D ,C , B ,A];
p = poly(mycoeff , "x","coeff") ;
M = roots(p);

for i = 1:3
    isreal(M(i,1)) ;
    if ans == %f then
        y = M(i,1) / M(i+1,1) - 1 ;
        sign(y) ;
        if ans == %t then
            x = M(i,1) ;
```

```
        else
            x = M(i+1,1) ;

        end
    end
end
disp(" Example: 9.7   Page no : 453") ;
printf("\n    (a)\n        Extent of reaction = %.3f
    \n",x);

//(b)
X = (-Del_h0_rxn  / R + del_A * T + del_B / 2 * T^2
   - del_D / T) * (1/T2 - 1/T) + del_A * log(T2 / T)
    + del_B / 2 * (T2 - T) + del_D / 2 * (1/(T2^2) -
    1/(T^2) );
K_T = K_298 * exp(X) ;

A = K_T * P^2 *27 -16 ;
B = 64 - K_T * P^2 * 108 ;
C = -64 + K_T * P^2 * 162 ;
D = -108 * K_T * P^2 ;
E = 27 * K_T * P^2 ;

mycoeff =[E , D ,C , B ,A];
p1 = poly(mycoeff , "x","coeff") ;
M1 = roots(p1);

for i = 1:3
    isreal(M1(i,1)) ;
    if ans == %f then
        y = M1(i,1) / M1(i+1,1) - 1 ;
        sign(y) ;
        if ans == %t then
            x1 = M1(i,1) ;
        else
            x1 = M1(i+1,1) ;

        end
```

```
    end
end
printf("    (b)\n         Extent of reaction = %.3f\n
   ",x1);
disp("       Under these conditions we do not expect
   to produce an appreciable amount of ammonia .")
```

**Scilab code Exa 9.8** Example 9 8

```
//Engineering and Chemical Thermodynamics
//Example 9.8
//Page no  :454

clear ; clc ;
disp("  Example: 9.8    Page no : 454") ;
disp("             The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression .") ;
```

**Scilab code Exa 9.9** Example 9 9

```
//Engineering and Chemical Thermodynamics
//Example 9.9
//Page no :454

clear ; clc;
//Given
K_T = 1.51 * 10^-5 ;
P = 300  ; //[bar]
T = 500 + 273.2 ; //[K]
R = 8.314 ;

```

```
function y = f991(k),
    y = ((2 * k)^2 * (4 - 2 * k)^2 / ((1 - k) * (3 - 3*k)^3)) * P^-2 - K_T
endfunction

z1 = fsolve([0.3],f991) ;

disp(" Example: 9.9   Page no : 454") ;
printf("\n   (a)\n        Extent of reaction = %.2f\n",z1);

//(b)
P_c = [111.3 * 101325 , 33.5 * 101325 , 12.8 * 101325] ;
T_c = [405.5 , 126.2 , 33.3] ;

for i = 1:3
    a(1,i) = 27 / 64 * (R * T_c(1,i))^2 / P_c(1,i) ;
    b(1,i) = (R * T_c(1,i)) / (8 * P_c(1,i)) ;

    function y = f992(v) ,
        y = (R * T) / (v - b(1,i)) - a(1,i) / (v^2) - P * 100000 ;
    endfunction

    V(1,i) = fsolve([0.0002],f992) ;

    sai(1,i) = exp( - log((V(1,i) - b(1,i)) * P * 10^5/ ( R * T)) + b(1,i) / (V(1,i) - b(1,i)) - 2 * a(1,i) / (R * T * V(1,i))) ;

end

function y = f993(k),
    y = ((2 * k)^2 * sai(1,1)^2 * (4 - 2 * k)^2 * 3 / ((1 - k) * sai(1,2)* (3 - 3*k)^3 * sai(1,3)^3 ))* P^-2  - K_T
endfunction
```

```
z2 = fsolve([0.3],f993) ;

x = (z1 - z2) / z1 * 100 ;

printf("    (b)\n          Extent of reaction = %.2f \n
   ",z2);
printf("\n  A correction of about   %d%% is observed
    from accounting for nonideal behaviour . ",x)
```

**Scilab code Exa 9.10** Example 9 10

```
//Engineering and Chemical Thermodynamics
//Example 9.10
//Page no :456

clear ; clc ;
//Given
del_g0_f_1 = 31.72 ; //[kJ/mol]
del_g0_f_2 = 26.89 ; //[kJ/mol]
R = 8.314 ;
T = 298 ;//[K]
del_g0_rxn = del_g0_f_2 - del_g0_f_1 ;
K = exp( - del_g0_rxn * 10^3 / (R * T) ) ;
x = K / (1 + K) ;

disp(" Example: 9.10    Page no : 456") ;
printf("\n           x = %.3f \n\n      At equillibrium
    %.1f %% of the liquid exists as cyclohexane.",x
   ,x * 100) ;
```

**Scilab code Exa 9.11** Example 9 11

```
//Engineering and Chemical Thermodynamics
//Example 9.11
//Page no :457

clear ; clc;
// Given
del_g0_f_CaCO3 = -951.25 ;
del_g0_f_CaO = -531.09 ;
del_g0_f_CO2 = -395.81 ;
R = 8.314 ;
T = 1000 ;// [K]
del_g0_rxn = del_g0_f_CaO + del_g0_f_CO2 -
   del_g0_f_CaCO3 ;
K = exp (-del_g0_rxn * 10^3 / (R * T)) ;
p_CO2 = K ;
disp(" Example: 9.11    Page no : 457") ;
printf("\n      Equilibrium pressure = %.3f bar ",
   p_CO2) ;
```

**Scilab code Exa 9.12** Example 9 12

```
//Engineering and Chemical Thermodynamics
//Example 9.12
//Page no :458

clear ; clc ;
//Given
del_g0_f_B = 124.3 ; //[kJ/mol] , From Appendix A.3
del_g0_f_Ac = 209.2 ; //[kJ/mol] , From Appendix A.3
R = 8.314 ;
T = 298 ; // [K]
A = 9.2806 ;
B = 2788.51 ;
C = -52.36 ;
 del_g0_rxn = del_g0_f_B - 3 * del_g0_f_Ac ;
```

```
K = exp( - del_g0_rxn * 10^3 / (R * T)) ;

//We assume no acetylene condenses and no Benzene is
    volatile .
P = 1 / K^(1/3) ;
X = A - B / (T + C) ;
P_b = exp(X) ;
disp(" Example: 9.12   Page no : 458") ;
disp("       At equilibrium , the cylinder is almost
   completely filled with Benzene .")
printf("\n        System pressure = %.3f bar ",P_b)
```

**Scilab code Exa 9.13** Example 9 13

```
//Engineering and Chemical Thermodynamics
//Example 9.13
//Page no :466

clear ; clc ;
//Given
E_0_c = 0.153 ; //[V]
E_0_a = -0.521 ; // [v]
T = 298 ; //[K]
z = 1 ;
F =96485 ; //[C/mol e-]
R =8.314 ; //[J/mol K ]

E_0_rxn = E_0_c + E_0_a ;
del_g_0_rxn = - z * F * E_0_rxn ;

K = exp( - del_g_0_rxn / ( R * T )) ;
disp(" Example: 9.13   Page no : 466") ;
printf("\n                The equilibrium constant =
    %.3g \n",K)
disp("               The equilibrium constant is
```

```
    small . So the etching will not proceed
    spontaneously . However if we apply work through
    application of an electrical potential , we can
    etch the     copper .")
```

**Scilab code Exa 9.14** Example 9 14

```
//Engineering and Chemical Thermodynamics
//Example 9.14
//Page no :466

clear ; clc ;
//Given
E_0_c = 0.34 ; //[V]
E_0_a = -1.23 ; //[V]
T = 298 ; // [K]
pH = 1 ;
z = 2 ;
Cu2 = 0.07 ;
F = 96485 ; //[C/mol e-]
R = 8.314 ;

E_0_rxn = E_0_c + E_0_a ;
E = E_0_rxn + 2.303 * R * T * 2 * pH / (z * F) + R *
    T * log(Cu2) / (z * F) ;
disp(" Example: 9.14    Page no : 466") ;
printf("\n     Del_E_0_rxn = %.2f ",E_0_rxn ) ;
printf("\n\n   We have to apply potential greater
   than %.2f V",-E) ;
```

**Scilab code Exa 9.15** Example 9 15

```
//Engineering and Chemical Thermodynamics
```

```
//Example 9.15
//Page no :468

clear ; clc ;
disp("  Example: 9.15    Page no : 468") ;
disp("           The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression .") ;
```

**Scilab code Exa 9.16** Example 9 16

```
//Engineering and Chemical Thermodynamics
//Example 9.16
//Page no :469

clear ; clc ;
//Given
m = 4 ;
T = 2 ;
Pai = 1 ;
S = 1 ;

R = m - T + 2 - Pai - S ;
disp(" Example: 9.16    Page no : 469") ;
printf("\n     We must specify %g independent
   equations .",R)
```

**Scilab code Exa 9.17** Example 9 17

```
//Engineering and Chemical Thermodynamics
//Example 9.17
//Page no :470
```

```
clear ; clc ;
disp("  Example: 9.17   Page no : 470") ;
disp("            The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression .") ;
```

**Scilab code Exa 9.18** Example 9 18

```
//Engineering and Chemical Thermodynamics
//Example 9.18
//Page no :470

clear ; clc
//Given
del_g_f_CH4 = -50.72 ;
del_g_f_H2 = 0 ;
del_g_f_H2O = -228.57 ;
del_g_f_CO = -137.17 ;
del_g_f_CO2 = -394.36 ;
del_h_f_CH4 = -74.81 ;
del_h_f_H2 = 0 ;
del_h_f_H2O = -241.82 ;
del_h_f_CO = -110.53 ;
del_h_f_CO2 = -393.51 ;

v1_CH4 = -1 ;
v1_H2 = 3 ;
v1_H2O = -1 ;
v1_CO = 1 ;
v1_CO2 = 0 ;
v2_CH4 = -1 ;
v2_H2 = 4 ;
v2_H2O = -2 ;
```

```
v2_CO = 0 ;
v2_CO2 = 1 ;

A_CH4 = 1.702 ;
B_CH4 = 9.08 * 10^-3 ;
C_CH4 = -2.16 * 10^-6 ;
D_CH4 = 0 ;
A_H2 = 3.249 ;
B_H2 = 4.22 * 10^-4 ;
C_H2 = 0 ;
D_H2 = 8.30 * 10^3 ;
A_H2O = 3.47 ;
B_H2O = 1.45 * 10^-3 ;
C_H2O = 0 ;
D_H2O = 1.21 * 10^4 ;
A_CO = 3.376 ;
B_CO = 5.57 * 10^-4 ;
C_CO = 0 ;
D_CO = -3.10 * 10^3 ;
A_CO2 = 5.457 ;
B_CO2 = 1.05 * 10^-3 ;
C_CO2 = 0 ;
D_CO2 = -1.16 * 10^5 ;

M(:,1) = 600:50:1150 ;
R = 8.314 ;
P = 1  ; //[bar]
T_ref = 298.15 ; //[K]

del_g_f_1 = (v1_CO * del_g_f_CO + v1_H2 *del_g_f_H2 + v1_CH4 * del_g_f_CH4 + v1_H2O * del_g_f_H2O) * 1000  ;
del_h_f_1 = (v1_CO * del_h_f_CO + v1_H2 *del_h_f_H2 + v1_CH4 * del_h_f_CH4 + v1_H2O * del_h_f_H2O) * 1000 ;
del_g_f_2 = (v2_CO2 * del_g_f_CO2 + v2_H2 * del_g_f_H2 + v2_CH4 * del_g_f_CH4 + v2_H2O * del_g_f_H2O) * 1000 ;
```

```
del_h_f_2 = (v2_CO2 * del_h_f_CO2 + v2_H2 * del_h_f_H2 + v2_CH4 * del_h_f_CH4 + v2_H2O * del_h_f_H2O) * 1000;
Del_A_1 =  v1_CO * A_CO + v1_H2 * A_H2 + v1_CH4 * A_CH4 + v1_H2O * A_H2O  ;
Del_B_1 =  v1_CO * B_CO + v1_H2 * B_H2 + v1_CH4 * B_CH4 + v1_H2O * B_H2O  ;
Del_C_1 =  v1_CO * C_CO + v1_H2 * C_H2 + v1_CH4 * C_CH4 + v1_H2O * C_H2O  ;
Del_D_1 =  v1_CO * D_CO + v1_H2 * D_H2 + v1_CH4 * D_CH4 + v1_H2O * D_H2O  ;
Del_A_2 = v2_CO2 * A_CO2 + v2_H2 * A_H2 + v2_CH4 * A_CH4 + v2_H2O * A_H2O  ;
Del_B_2 = v2_CO2 * B_CO2 + v2_H2 * B_H2 + v2_CH4 * B_CH4 + v2_H2O * B_H2O  ;
Del_C_2 = v2_CO2 * C_CO2 + v2_H2 * C_H2 + v2_CH4 * C_CH4 + v2_H2O * C_H2O  ;
Del_D_2 = v2_CO2 * D_CO2 + v2_H2 * D_H2 + v2_CH4 * D_CH4 + v2_H2O * D_H2O  ;


K_298_1 = exp( - del_g_f_1 / (R * T_ref)) ;
K_298_2 = exp( - del_g_f_2 / (R * T_ref)) ;
disp(" Example: 9.18   Page no : 470") ;

for i = 1:12
  X = (-del_h_f_1 / R + Del_A_1 * T_ref + Del_B_1 / 2 * T_ref^2 + Del_C_1 /3* T_ref^3- Del_D_1 / T_ref) * (1/M(i,1) - 1/T_ref) + Del_A_1*log(M(i,1) / T_ref)+ Del_B_1 / 2 * (M(i,1) - T_ref) + Del_C_1 / 6 *(M(i,1)^2 - T_ref^2) + Del_D_1 / 2* (1/(M(i,1)^2) - 1/(T_ref^2));

  M(i,2) = K_298_1 * exp(X) ;

  Y = (-del_h_f_2 / R + Del_A_2 * T_ref + Del_B_2 / 2 * T_ref^2 + Del_C_2/3* T_ref^3- Del_D_2 / T_ref) * (1/M(i,1) - 1/T_ref) + Del_A_2 * log(M
```

```
(i,1) / T_ref)+ Del_B_2 / 2 * (M(i,1) - T_ref) + Del_C_2 / 6 *(M(i,1)^2 - T_ref^2) + Del_D_2 / 2* (1/(M(i,1)^2) - 1/(T_ref^2));

  M(i,3) = K_298_2 * exp(Y) ;
 function y = f918(R),
      s1 = R(1) ;
      s2 = R(2) ;
  y(1) = (s1 * (3 * s1 + 4 * s2)^3) / ((5 + 2 * s1 + 2 * s2)^2 * (1 - s1 -s2) * (4 - s1 - 2 * s2)) * P^2 - M(i,2) ;
  y(2) = (s2 * (3 * s1 + 4 * s2)^4) / ((5 + 2 * s1 + 2 * s2)^2 * (1 - s1 -s2) * (4 - s1 - 2 * s2)^2) * P^2 - M(i,3) ;
endfunction
  z = fsolve([0.0001;0.0001],f918)  ;
  M(i,4) = z(1) ;
  M(i,5) = z(2) ;
  M(i,6) = (1 - M(i,4) - M(i,5)) / (5 + 2 * M(i,4) + 2 * M(i,5)) ;
  M(i,7) = (4 - M(i,4) - 2 * M(i,5)) / (5 + 2 * M(i,4) + 2 * M(i,5)) ;
  M(i,8) = (3 * M(i,4) + 4 * M(i,5)) / (5 + 2 * M(i,4) + 2 * M(i,5)) ;
  M(i,9) = M(i,4) / (5 + 2 * M(i,4) + 2 * M(i,5)) ;
  M(i,10) = M(i,5) / (5 + 2 * M(i,4) + 2 * M(i,5)) ;

end

disp("      T                    K1                    K2                    S1                    S2                    y_CH4       y_H2")

for i = 1:10                          // For convenient display of solution .
    for j = 1:7
        n1(i,j) = M(i,j) ;
    end
```

```
end
for i = 1:10                              // For convenient display of solution .
    for j = 1:3
        n2(i,j) = M(i,j+7) ;
    end
end
disp(n1) ;
disp("      y_H20              y_CO              y_CO2   ") ;
disp(n2) ;
for i = 1:10
    for j = 1:10
        N(i,j) = M(i,j) ;
    end
end

plot(N(:,1) , N(:,4),"+") ;
plot(N(:,1), N(:,5),".") ;
xtitle("Figure E9.18    Extent of reaxn vs temp","Temperature(K)","S") ;
legend("S1","S2") ;

h = figure(1) ;
clf() ;
set(h,"background",35) ;
plot(N(:,1) , N(:,6), "o-") ;
plot(N(:,1) , N(:,7), "s-");
plot(N(:,1) , N(:,8), "^-") ;
plot(N(:,1) , N(:,9), "x-") ;
plot(N(:,1) , N(:,10), ".-") ;
legend("y_CH4 ","y_H2 ","y_H2O ","y_CO ","y_CO2") ;

xtitle("Figure E9.18     mole fractn vs temp","Temp","mole fraction") ;
```

**Scilab code Exa 9.19** Example 9 19

```
//Engineering and Chemical Thermodynamics
//Example 9.19
//Page no :472

clear ; clc
//Given
del_g_0_f_SiCl2 = - 216012 ;
del_g_0_f_SiCl4 = - 492536 ;
del_g_0_f_SiCl3H = -356537 ;
del_g_0_f_SiCl2H2 = -199368 ;
del_g_0_f_SiClH3 = -28482 ;
del_g_0_f_SiH4 = -176152 ;
del_g_0_f_HCl = -102644 ;
del_g_0_f_H2 = 0 ;
del_g_0_f_Si = 0 ;
R = 8.314 ;
T = 1300 ; //[K]
Del_g_rxn_1 = del_g_0_f_SiCl2 + 2 * del_g_0_f_HCl -
    del_g_0_f_SiCl4 - del_g_0_f_H2 ;
Del_g_rxn_2 = del_g_0_f_SiCl3H + del_g_0_f_HCl -
    del_g_0_f_SiCl4 - del_g_0_f_H2 ;
Del_g_rxn_3 = del_g_0_f_SiCl2H2 + del_g_0_f_HCl -
    del_g_0_f_SiCl3H - del_g_0_f_H2 ;
Del_g_rxn_4 = del_g_0_f_SiClH3 + del_g_0_f_HCl -
    del_g_0_f_SiCl2H2 - del_g_0_f_H2 ;
Del_g_rxn_5 = del_g_0_f_SiH4 + del_g_0_f_HCl -
    del_g_0_f_SiCl3H - del_g_0_f_H2 ;
Del_g_rxn_6 = del_g_0_f_Si + 4 * del_g_0_f_HCl -
    del_g_0_f_SiCl4 - 2 * del_g_0_f_H2 ;

M(1,1) = exp( - Del_g_rxn_1 / (R * T)) ;
M(2,1) = exp( - Del_g_rxn_2 / (R * T)) ;
M(3,1) = exp( - Del_g_rxn_3 / (R * T)) ;
M(4,1) = exp( - Del_g_rxn_4 / (R * T)) ;
M(5,1) = exp( - Del_g_rxn_5 / (R * T)) ;
M(6,1) = exp( - Del_g_rxn_6 / (R * T)) ;
```

```

S = [0.0763 ;0.1979 ;0.0067 ;0.0001 ;0.0000 ;-0.0512] ;
K_cal = [.00137 ;0.0457 ;0.00644 ;0.00181 ;0.000752 ;0.000509] ;
disp(" Example: 9.19    Page no : 472") ;
disp("        K_i                    S           K_i_cal          K_i - K_i_cal") ;
for i = 1:6
    M(i,2) = S(i,1) ;
    M(i,3) = K_cal(i,1) ;
    M(i,4) = M(i,1) - M(i,3) ;
end
disp(M)
// Readers can refer figure E9.19 .
```

**Scilab code Exa 9.20** Example 9 20

```
//Engineering and Chemical Thermodynamics
//Example 9.20
//Page no :476

clear ; clc
//Given
del_g_0_f_CH4 = -2.057 ; //[J/mol]
del_g_0_f_H2O = -192.713 ; //[J/mol]
del_g_0_f_CO = -182.494 ; //[J/mol]
del_g_0_f_CO2 = -203.595 ; //[J/mol]
del_g_0_f_H2 = 0 ; //[J/mol]
R = 8.314 ;
T = 800 ; //[K]
w = 1 / (R * T) ;
function Z920 = F920(R)
    m = R(1) ,
    n = R(2) ,
```

```
    o = R(3) ,
    a = R(4), // n_CH4
    b = R(5), // n_H2O
    c = R(6), // n_H2
    d =  R(7), // n_CO
    e = R(8), // n_CO2

Z920(1) = a + d + e - 1 ;
Z920(2) = 4 * a + 2 * b + 2 * c - 12 ;
Z920(3) = b + d + 2 * e - 4 ;
Z920(4) = del_g_0_f_CH4 * w + log(a) - log(a + b + c
     + d + e) + m  + 4 * o ;
Z920(5) = del_g_0_f_H2O * w + log(b) - log(a + b + c
     + d + e) + 2 * o + n ;
Z920(6) = del_g_0_f_H2 * w + log(c)- log(a + b + c
   + d + e) + 2 * o ;
Z920(7) = del_g_0_f_CO * w + log(d) - log(a + b + c
    + d + e) + m  + n ;
Z920(8) = del_g_0_f_CO2 * w + log(e) - log(a + b + c
     + d + e) + m  + 2 * n ;

endfunction ;


function [J] = jacob(X)

    m = X(1) ,
    n = X(2) ,
    o = X(3) ,
    a = X(4), // n_CH4
    b = X(5), // n_H2O
    c = X(6), // n_H2
    d = X(7), // n_CO
    e = X(8), // n_CO

    J(1,1) = 0 ;  J(1,2) = 0 ; J(1,3) = 0 ; J(1,4) =
        1 ; J(1,5) = 0 ;
    J(1,6) = 0 ; J(1,7) = 1 ; J(1,8) = 1 ;
```

```
    J(2,1) = 0 ;  J(2,2) = 0 ; J(2,3) = 0 ; J(2,4) = 4 ; J(2,5) = 2 ;
    J(2,6) = 2 ; J(2,7) = 0 ; J(2,8) = 0 ;
    J(3,1) = 0 ;  J(3,2) = 0 ; J(3,3) = 0 ; J(3,4) = 0 ; J(3,5) = 1 ;
    J(3,6) = 0 ; J(3,7) = 1 ; J(3,8) = 2 ;
    J(4,1) = 1 ;  J(4,2) = 0 ; J(4,3) = 4 ; J(4,4) = (b+c+d+e)/(a*(a+b+c+d+e)) ; J(4,5) = -1/(a+b+c+d+e) ; J(4,6) = -1/(a+b+c+d+e) ; J(4,7) = -1/(a+b+c+d+e); J(4,8) = -1/(a+b+c+d+e);
    J(5,1) = 0 ; J(5,2) = 1 ; J(5,3) = 2 ; J(5,4) = -1/(a+b+c+d+e) ;
    J(5,5) = (a+c+d+e)/(b*(a+b+c+d+e)) ; J(5,6) = -1/(a+b+c+d+e) ;
    J(5,7) = -1/(a+b+c+d+e) ; J(5,8) = -1/(a+b+c+d+e) ;
    J(6,1) = 0 ; J(6,2) = 0 ; J(6,3) = 2 ; J(6,4) = -1/(a+b+c+d+e) ;
    J(6,5) = -1/(a+b+c+d+e) ; J(6,6) = (a+b+d+e)/(c*(a+b+c+d+e)) ;
    J(6,7) = -1/(a+b+c+d+e) ; J(6,8) = -1/(a+b+c+d+e) ;
    J(7,1) = 1 ; J(7,2) = 1 ; J(7,3) = 0 ; J(7,4) = -1/(a+b+c+d+e) ;
    J(7,5) = -1/(a+b+c+d+e) ; J(7,6) = -1/(a+b+c+d+e) ;
    J(7,7) = (a+b+c+e)/(d*(a+b+c+d+e)) ; J(7,8) = -1/(a+b+c+d+e) ;
    J(8,1) = 1 ; J(8,2) = 2 ; J(8,3) = 0 ; J(8,4) = -1/(a+b+c+d+e) ;
    J(8,5) = -1/(a+b+c+d+e) ; J(8,6) = -1/(a+b+c+d+e) ;
    J(8,7) = -1/(a+b+c+d+e) ; J(8,8) = (a+b+c+d)/(e*(a+b+c+d+e)) ;
endfunction

// We will use newton Raphson Method to solve the set of equations.
```

```
// Reference : www.infoclearinghouse.com/files/
   scilab/scilab6a.pdf

function [x] = newtonm(x0,f,J)
    N = 1000 ;
    epsilon = 1*10^-10 ;
    maxval = 1000 ;
    xx = x0 ;

    while(N>0)
        JJ = J(xx)
       // disp(abs(det(JJ)))
        if abs(det(JJ))<epsilon then
            error('newtonm-Jacobian is singular- try
                new x0')
            abort ;
        end ;
        xn = xx -inv(JJ) * f(xx) ;
     //   disp(abs(f(xn)))
        if abs(f(xn))<epsilon then
            x = xn ;
          //  disp(100-N) ;
          //  disp((x))
            return(x) ;
        end ;

        if abs(f(xn))>maxval then
           disp(1000-N) ;
           error('Solution diverges') ;
           abrot ;
        end ;
        N = N -1 ;
        xx = xn ;
 end ;
endfunction ;

x1 = [1 ; 1 ; 1 ; 1 ; 1 ; 1 ; 1 ; 1 ] ; // Initial
   guess .
```

```

[z] = newtonm(x1,F920,jacob) ;

disp("Example 9.20     Page no:476") ;
printf("\n\n    L_c/RT = %f  ,\n    L_o/RT = %f  ,\n
    L_h/RT = %f  ,\n    n_CH4 = %f  ,\n    n_H2O = %f  ,\n
        n_H2   = %f  ,\n    n_CO = %f  ,\n    n_CO2 = %f"
    ,z(1),z(2),z(3),z(4),z(5),z(6),z(7),z(8)) ;
//The solutions given in the text book does not
    satisfy E9.20D, E9.20E,
// E9.20F and so on .
```

**Scilab code Exa 9.21** Example 9 21

```
//Engineering and Chemical Thermodynamics
//Example 9.21
//Page no :485

clear ; clc ;
disp("  Example: 9.21   Page no : 485") ;
disp("            The problem contains only theory
    and different substitutions.There is no numerical
    part involved. Users can go through the book to
    obtain the required expression .") ;
```

**Scilab code Exa 9.22** Example 9 22

```
//Engineering and Chemical Thermodynamics
//Example 9.22
//Page no :487

clear ; clc ;
disp("  Example: 9.22   Page no : 487") ;
```

```
disp("            The problem contains only theory
   and different substitutions.There is no numerical
    part involved. Users can go through the book to
   obtain the required expression .") ;
```