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 irreversible .")
```

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 .");
```