Scilab Textbook Companion for Introduction To Chemical Engineering Thermodynamics by J. M. Smith, H. C. Van Ness And M. M. Abbott¹

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Book Description

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

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

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

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

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Chapter 1

Introduction

Scilab code Exa 1.1 Find the Astronaut Mass and Weight on moon

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
  endfunction
10 //Example 1.1
11 //Caption : Program To find the Astronaut's Mass and
       Weight on moon.
12
13 //Given values
14
15 F = 730; // Force(N)
16 g_texas=9.792; // Acceleration of gravity in Houston,
      Texas(m/s^2).
17 g_moon=1.67; // Acceleration of gravity at moon(m/s^2)
```

```
18
19 //Solution
20
21 m=approx(F/g_texas,2);//Mass of Astronaut(Kg)
22 F_moon=approx(m*g_moon,2);//Force on Moon(N)
23 disp('Kg',m,'Mass of Astronaut');
24 disp('N',F_moon,'Force on Moon');
25
26 //End
```

Scilab code Exa 1.2 Find Gauge Pressure and absolute Pressure

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
10 //Example 1.2
11 //Caption : Program To Find Gauge Pressure and
      absolute Pressure
12
13
  //Given values
14
15 d=0.01; // Diameter (m)
16 m=6.14; //Mass(Kg)
17 g=9.82; // Acceleration of gravity
18 Pb=748; // Barometric Pressure (Torr)
19
```

Scilab code Exa 1.3 Find Pressure in a Manometer

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
9
10 //Example 1.3
11 //Caption : Program To Find Pressure in a Manometer
12
13 // Given Values
14
15 T=300.15; //\text{Temp}=300.15\text{K}(27\text{ 'C})
16 h=60.5*(10^-2); // Height=60.5cm
17 rho=13530; // Density(Kg/m^3)
18 g=9.784; // Acceleration of gravity (m/s^2)
```

```
19
20  //Solution
21
22  P=approx(h*rho*g,0);
23  disp('KPa',P/1000, 'Pressure in KPa');
24  disp('bar',P/100000, 'Pressure in bar');
25
26  //End
```

Scilab code Exa 1.4 Find the velocity and Energy

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8
  endfunction
10 //Example 1.4
11 //Caption : Program to find the velocity and Energy
12
13 //Given values
14
15 M = 2500; //Mass = 2500 Kg
16 h1=10; // height1=10m
17 h2=100; //height2=100m
18 g=9.8; // Acceleration of gravity (m/s^2)
19
20 //Solution
21 / (a)
22 PE1=M*h1*g; //(J)
```

```
23 disp('J', PE1, '(a) Potential energy of the elevator in
       its Initial Position')
24
25 //(b)
26 \text{ W=M*g*integrate}('1','l',h1,h2);//(J)
27 disp('J', W, '(b) Work Done in Raising the Elevator')
28
29 //(c)
30 PE2=M*g*h2; //(J)
31 disp('J', PE2, '(c) Potential energy of the elevator in
       its Highest Position')
32
33 / (d)
34 \text{ KE2=0};
35 \text{ PE3=0};
36 KE3=PE2; // (J) // Conservation Of Mechanical Energy
37 u=approx((2*KE3/M)^(1/2),2);//(m/s)
38 disp('m/s',u,'(d) Velocity of the Elevator')
39 disp('J', KE3, '(d) Kinetic Energy of the Elevator')
40
41 // (e)
42 PE_Spring=KE3; //(J)
43 disp('J', PE_Spring, '(e) Potential energy of
      compressed spring ')
44
45 //(f)
46 TE = PE1 + W;
47 disp('J', TE, '(f) Total Energy of the System')
48
49 //End
```

Chapter 2

The First Law And Other Basic Concepts

Scilab code Exa 2.1 Find Energy in a Waterfall

```
clear;
clc;

//Example 2.1
//Caption : Program to find Energy in a Waterfall

//Given values
H=100;//height=100m
M=1;//Mass of water=1Kg
g=9.8066;//Acceleration due to gravity(m/s^2)

//Solution
//Del(Energy of the system)=0
//hence,del(U)+del(KE)+del(PE)=0
```

```
18 //(a)
19 PE1=M*H*g; //(J)
20 disp('J', PE1, '(a) Potential energy of Water at the
      Top ');
21
22 //(b)
23 \text{ del_U=0};
24 \text{ KE1=0};
25 \text{ PE2=0};
26 KE2=PE1; //(J)
27 disp('J', KE2, '(b) Kinetic energy of Water');
28
29 //(c)
30 \text{ del_U=KE2};
31 disp('J',del_U,'(c)Change in Internal energy when 1
      kg Water added');
32
33 / End
```

Scilab code Exa 2.3 Find the energy change in a System

Scilab code Exa 2.4 Find the Heat flow in the Path

```
1 clear;
2 clc;
3
4 //Example 2.4
5 // Caption: Program to find the Heat flow in the
      Path
6
7 // Given values
8 \text{ W_acb=40;} //J
9 Q_acb=100; //J
10 W_aeb=20; //J
11 W_bda=30; //J
12
13 // Solution
14
15 del_U_ab=Q_acb-W_acb;
16
17 //(a)
18 Q_aeb=del_U_ab-W_aeb; //J
```

```
19 disp('J',Q_aeb,'(a)Heat Flow in acb')
20
21 //(b)
22 del_U_ba=-del_U_ab;//J
23 Q_bda=del_U_ba-W_bda;
24 disp('J',Q_bda,'(b)Heat Flow in bda')
25
26 //End
```

Scilab code Exa 2.5 Find The degree of freedom for the various systems

```
1 clear;
2 clc;
3
4 // Example 2.5
5 // Caption: Program To Find The degree of freedom
      for the various systems
  //Formula To be Used F=2-#+N (Where, #(pi)-no of
      phases, N-number of chemical species)
8
9 //(a)-Liquid Water in equllibrium with its vapour.
10 N = 1;
11 pi=2;
12 \quad F=2-pi+N;
13 disp(F, '(a) Degree Of freedom is');
14
15 //(b)-Liquid Water in equllibrium with a mixture of
      vapour and nitrogen.
16 N = 2;
17 pi=2;
18 F = 2 - pi + N;
19 disp(F, '(b) Degree Of freedom is ');
```

Scilab code Exa 2.6 Find the work done by gas

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
9
10 //Example 2.6
11 //Caption: Program to find the work done by gas
12
13 //Given values
14 P=14; // Pressure=14bar
15 V1=0.03; // Initial volume=0.03m<sup>3</sup>
16 V2=0.06; // Final Volume
17 // Process is isothermal
18 //(a)-To find the work done by gas in moving the
      External force
19 //(b)-To find the work done by gas if external force
       is suddenly reduced to half its initial value
```

```
20
21 //Solution
22 //(a)
23 K=P*V1*(10^5); //J
24 W1=approx(-K*integrate('1/V','V',0.03,0.06),0);//J
25 P2=K/V2; // Final Pressure (Pa)
26 \text{ P2=P2/(10^5)}; // \text{bar}
27 disp('J', W1, '(a) The work done by gas in moving the
      External Force is')
28
29 //(b)
30 W2=-P2*(10^5)*integrate('1','V',0.03,0.06)
31 n=approx((W2/W1)*100,1);//Efficiency
32 disp('J', W2, '(b) The work done by gas if external
      force is reduced to half is')
  disp('%',n,'Hence the efficiency is')
33
34
35 / End
```

Scilab code Exa 2.7 Find the Energy Changes in the Process

```
1 clear;
2 clc;
3
4 //Example 2.7
5 //Caption : Program to find the Enegy Changes in the Process
6
7 //Given values
8 P=7;//pressure=7bar
9 m=45;//Mass of cube
10 mt=23;//mass of piston, piston rod, pan
11 x=0.5;//Distance moved=0.5m
```

```
12 g=9.8; // Acceleration Due to gravity (m/s^2)
13
14 // Solution
15
16 // Acc to Eqn del_U_sys+del_U_surr+del_PE_surr=0
17 del_PE_surr=(m+mt)*g*x;
18 // ans=del_U_sys+del_U_surr
19 disp('J',-del_PE_surr, 'Energy Changes in the Process')
20
21 // End
```

Scilab code Exa 2.8 Find Change in Enthalpy and Internal Energy

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
      funcprot(0)
   endfunction
9
10 //Example 2.8
11 //Caption: Program to find Change in Enthalpy and
      Internal Energy
12
13 //Given values
14 m=1; //1 kg of water
15 T=373.15; //\text{Temp}=373.15\text{K}(100 \, ^{\circ}\text{C})
16 P=101.325; // Pressure=101.325KPa
17 V2=1.673; // Final Volume [m<sup>3</sup>]
18 V1=0.00104; // Initial Volume [m<sup>3</sup>]
```

```
19 Sv_liqiud=0.00104; // Specific Volume of Liqiud
20 Sv_vapour=1.673; // Specific Volume of Vapour
21 del_H=2256.9; // Heat Added(KJ)
22
23 // Solution
24 Q=del_H;
25 del_V=V2-V1;
26 W=P*del_V; // KJ
27 del_U=approx(del_H-(P*del_V),1);
28 disp('KJ',del_H,'Change in Enthalpy');
29 disp('KJ',del_U,'Change in Internal energy');
30 // End
```

Scilab code Exa 2.9 Find Work Heat del U and del H

```
1 clear;
2 clc;
3
4 //Example 2.9
   //Caption : Program To Find Work, Heat, del U and del
      Η
7 // Given values
8 // Initial
9 P1=1; // Pressure=1bar
10 T1=298.15; //\text{Temp}=298.15\text{K}(25\text{ 'C})
11 V1=0.02479; // \text{Molar Volume} = 0.02479 \text{m}^3/\text{mol}
12 // Final
13 P2=5; // Pressure=5bar
14 Cv = 20.78; //J/mol/K
15 Cp=29.10; //J/mol/K
16
17 //to Find del_U, del_H by two processes
```

```
18 V2=V1*(P1/P2); //m^3(1 \text{ mol})
19 disp('m<sup>3</sup>', V2, 'Final Volume')
20
21 // Solution
22
23 //(a)-Cooling at const pressure followed by heating
      at const Volume
24 T2=T1*(V2/V1); //K
25 disp('K',T2, 'Final Temperature')
26 del_H=round(Cp*(T2-T1));//J
27 Q1=del_H; //J
28 del_U1=round(del_H-(P1*(10^5)*(V2-V1)));//J
29 //Second Step
30 del_U2=round(Cv*(T1-T2)); //J
31 Q2=del_U2;
32 Q = Q1 + Q2;
33 del_U=0;
34 \text{ W=del_U-Q;}//J
35 del_H=0;//const Temperature
36
37 disp('(a) Cooling at const Pressure Followed by
      Heating at const Volume')
38 disp('J',Q,'Heat Required')
39 disp('J',W,'Work Required')
40 disp('J',del_H,'Change in enthalpy')
41 disp('J',del_U,'Change in Energy')
42 //(b)-heating at Const Volume Followed by cooling at
       const Pressure
43 T2=T1*(P2/P1); //K
44 del_U1=round(Cv*(T2-T1)); //J
45 \quad Q1=del_U1;
46 del_H=round(Cp*(T1-T2)); //J
47 Q2=del_H;
48 del_U2=round(del_H-(P2*(10^5)*(V2-V1))); //J
49 Q = Q1 + Q2;
50 \text{ del_U=0};
51 W=del_U-Q;//J
52 del_H=0; // const Temperature
```

Scilab code Exa 2.10 Find change in Internal Energy and Enthalpy

```
1 clear;
2 clc;
4 //To find Approx Value
  function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
  endfunction
9
10 //Example 2.10
11 //Caption: Program to Find change in Internal
      Energy and Enthalpy
12
13 //Given values
14
15 // Initial values
16 T1=277; //\text{Temp}=277\text{K}
```

```
17 P1=10; // Pressure=10bar
18 V1=2.28; // \text{molar Volume} = 2.28 \text{m}^3/\text{Kmol}
19
20 //Final value
21 T2=333; //\text{Temp}=333K
22 P2=1; // Pressure=1atm
23
24 Cv = 21; //KJ/Kmol/K
25 Cp=29.3; //KJ/Kmol/K
26
27 // Solution
\frac{28}{a} //(a)-Cooled at const Vol to the final pressure
29 //(b)-Heated at const Pressure to final temperature
30 T_{=}T1*(1/10); //Intermediate temperature
31 \text{ del}_{Ta}=T_{-}T1;
32 \text{ del_Tb=T2-T_};
33 del_Ua=Cv*del_Ta; //KJ/Kmol
34 \text{ del_Ha=del_Ua+(V1*(P2-P1)*(10^5)/(10^3));} //KJ/Kmol}
35 V2=(V1*P1*T2)/(P2*T1); //m^3/kmol
36 del_Hb=Cp*del_Tb;
37 del_Ub=del_Hb-(P2*(V2-V1)*(10^5)/(10^3));//KJ/Kmol
38
39 del_U=approx(del_Ua+del_Ub,0);
40 del_H=approx(del_Ha+del_Hb,0);
41 disp('KJ/Kmol',del_U,'Change In Internal Energy')
42 disp('KJ/Kmol',del_H,'Change In Enthalpy')
43
44 //End
```

Scilab code Exa 2.13 Find the time for a certain Temperature Drop

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

```
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
     funcprot(0)
8
  endfunction
9
10 / \text{Example } 2.13
11 //Caption: Program to Find the time for a certain
      Temperature Drop
12
13 //Given values
14 M=190; //Mass=190Kg
15 T0=333.15; //Temperature=333.15K(60 'C)
16 m=0.2; //Steady rate of mass (Kg/s)
17 T=308.15; // Temperature=308.15K(35 °C)
18 T1=283.15; // Temperature=283.15K(10 °C)
19
20 //Solution
21 // Using the Eqn (2.29)
22 t=approx(-(M/m)*\log((T-T1)/(T0-T1)),1);//s
23 disp('s',t,'Time Taken for temperature of water to
     drop from 333.15K to 308.15K')
24 t=round(t/60);//min
25 disp('min',t,'Time Taken for temperature of water to
       drop from 333.15K to 308.15K')
26
27 //End
```

Scilab code Exa 2.14 Find the Enthalpy of Steam

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

```
4  //Example 2.14
5  //Caption : Program to find the Enthalpy of Steam
6
7  //Given values
8
9  rQ=4.15; //[g/s] flow rate
10  rQ2=12740; //Rate of Heat addition from resistance heater
11
12  //Solution
13  //del_z and del_u*2 are negligible if Ws and H1=0... then H2=Q
14  H2=round(rQ2/rQ); //[J/g]
15  disp('J/g',H2,'Enthalpy of Steam')
16
17  //End
```

Scilab code Exa 2.15 Find the Heat to be Removed during Compression

```
1 clear;
2 clc;
3
4 //Example 2.15
5 //Caption : Program To find the Heat to be Removed during Compression
6
7 //Given values
8
9 V=600; // [m/s]
10 W_compression=240; // [KJ/Kg]
11
12 //Solution
```

```
// Using Eqn(2.32a)
Q=(1/2*(V*V)/1000)-W_compression;

disp('KJ/kg',-Q,'Thus Heat Removed from each KG of air compressed is')
//End
```

Scilab code Exa 2.16 Find the Heat to be Removed during Compression

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
10 //Example 2.15
11 //Caption: Program to Find the Temperature in the
      second Tank
12
13 //Given values
14
15 R=3.15*10^-3; //[m^3/s] Rate of pumping
16 rH=-700; // [KW] Rate of Heat lost
17 h=15; // [m] Height
18 rW=1.5; // [KW]
19 rho=958; // [Kg/m^3] at 366.65K
20 g=9.805;
21 \text{ gc} = 1000;
22 \text{ del_z=h};
```

```
23
24 //Solution
25
26 rm=approx(R*rho,3);//[Kg/s]
                                   Mass flow rate
27 Q=approx(rH/rm,1); //[KJ/Kg]
28 W=approx(rW/rm,3);//[KJ/Kg]
                                   Shaft Work
29 K=approx(g/gc*del_z,3);
30
31 // using Eqn(2.32b)
32 \text{ del}_H=Q+W-K;
33
34 //From Steam tables for water at 366.65K
35 H1=391.6; //[KJ/Kg]
36 \text{ H2=del_H+H1};
37 disp('KJ/Kg', H2, 'Enthalpy')
38 //From Steam Tables temp at this enthalpy is
39 T = 311.35; //[K]
40 disp('K',T,'Temperature in the Second tank')
41
42 //End
```

Chapter 3

Volumetric Properties Of Pure Fluids

Scilab code Exa 3.1 Find Volume Change and Pressure generated

```
17 k=62*10^{(-6)}; //isothermal compressibility (bar^{-1})
18 V1=1.287*10^(-3); //Volume(m^3 kg^-1)
19
20 //Solution
21 / (a)
\frac{22}{\sqrt{\text{Find}}} \left(\frac{dP}{dT}\right) v??
\frac{23}{\sqrt{\text{Using eq.}(3.4)}}, V constant hence dV=0
24 ans_a=round(Beta/k);
25 \operatorname{disp}('K^-1', \operatorname{ans_a}, '(a)) The value of (\operatorname{dp/dT}) v is ')
26
27 //(b)
28 //Find Pressure when acetone heated at const. Vol
        from T1(1 bar) to T2.
29 T2_b=30; //\text{Temp2}=303.15\text{K}(30 \, ^{\circ}\text{C})
30 del_P = ans_a * (T2_b - T1);
31 ans_b=P1+del_P;
32 disp('bar',ans_b,'(b)The pressure is ')
33
34 //(c)
35 //Find vol. change when acetone changed from T1(P1)
        to T2(P2)
36 T2_c=0; //\text{Temp2}=273.15\text{K}(0 \, ^{\circ}\text{C})
37 P2=10; // pressure=10 bar
\frac{38}{\text{solve using Eq.}} (3.5)
39 \ln_{\text{value}} = (\text{Beta}*(\text{T2}_{\text{c}}-\text{T1})) - (\text{k}*(\text{P2}-\text{P1})); //\ln(\text{V2}/\text{V1})
40 ratio=exp(ln_value); //taking antilog, V2/V1
41 V2=ratio*V1;
42 \text{ del_V=approx}(V2-V1,6)
43 disp('(X 10^-3) m^3 kg^-1', del_V*1000, '(c) The change
         in Volume is ')
44
45 / End
```

Scilab code Exa 3.2 Find Work Heat del H del H

```
1 clear;
2 clc;
 3
 4 //Example 3.2
 5 // Caption: Program to Find Work, Heat, del H, del H
 7 //Given Values for the Gas
 9 // Figure
10 P = [1 5];
11 V = [25 \ 25];
12 plot2d(V,P,style=1)
13
14 \quad V = 5:0.5:25;
15 P = 25 * V^- - 1;
16 plot2d(V,P,style=2)
17 P=P<sup>1</sup>.4;
18 plot2d(V,P,style=3)
19 P = [5 \ 9.52];
20 \quad V = [5 \quad 5];
21 plot2d(V,P,style=3,rect=[0,0,30,10])
22 xtitle ("Diagram for Ex.3.2", "V x 10^3 (m<sup>3</sup>)", "P(bar)"
23 legend("(a)","(b)","(c)")
24 P = [5 5];
25 \quad V = [5 \quad 25];
26 plot2d(V,P,style=1)
27
28 clear;
29 //Initial Stage
30 P1=1; // Pressure=1bar
31 T1=298.15; //\text{Temp1}=298.15\text{K}(25\text{ 'C})
32
33 //Final Stage
34 P2=5; // Pressure=1bar
35 //Temp same as Temp1(Isothermal)
```

```
36
37 R=8.314; //J/Mol/K
38 Cv = (5/2) *R; //J/Mol/K
39 Cp = (7/2) *R; //J/Mol/K
40
41 / (a)
42 //Const Vol follwd by const Pressure
43 T2=T1*(P2/P1);
44 / By Eq 2.23
45 \text{ del}_T=T2-T1;
46 Q1=Cv*(T2-T1); // Heat at const Vol
47 Q2=Cp*(T1-T2);//Heat at const pressure
48
49 Q_a=round(Q1+Q2);
50 \text{ W_a=-Q_a}; //\text{W=del_U-Q}, \text{here del_U=0}
                 (a) Heating at constant volume Followed
       by cooling at constant Pressure')
52 disp('J', W_a, 'work done by heating at const vol
      followed by const Pressure ')
53
54 disp('J',Q_a,'Heat Transferred Q')
55
56 disp('change in Internal Energy and enthalpy = 0')
57
58 //(b)
59 //Isothermal Compression
60 / \text{By Eq.} (3.26)
61 Q_b = round(R*T1*log(P1/P2));
62 \quad W_b = -Q_b;
63 disp('
                 (b) Isothermal compression')
64
65 disp('J', W_b, 'work done by Isothermal compression')
66 disp('J',Q_b, 'Heat Transferred Q')
67 disp('change in Internal Energy and enthalpy = 0')
68
69 //(c)
70 // Adiabatic compression
71 gama=Cp/Cv;
```

```
72 V1 = (R*T1)/(P1^(10^5));
73 V2=V1*(P1/P2);
74 T2_c=T1*((V1/V2)^(gama-1)); // Kelvin(K)
75 P2_c=P1*((V1/V2)^gama);//bar
76 //Using Eq. (3.31)
77 W_c=round(Cv*(T2_c-T1)); //W=Cv*del_T(Joules)
78 Q_c = -W_c;
79
                 (c) Adiabatic compression followed by
80 disp('
      cooling at constant Volume')
81
  disp('J', W_c, 'work done by Adiabatic compression
      Followed by Cooling at const Vol ')
83
84 disp('J',Q_c,'Heat Transferred Q')
85 disp('change in Internal Energy and enthalpy = 0')
86
87 / End
```

Scilab code Exa 3.3 Find W Q del U and del H for the Figure

```
1 clear;
2 clc;
3
4 //Example 3.3
5 //Caption : Program to Find W,Q, del U and del H for the Figure
6
7 //Figure
8 V=2083:0.5:2853;
9 P=2853*V^-1;
```

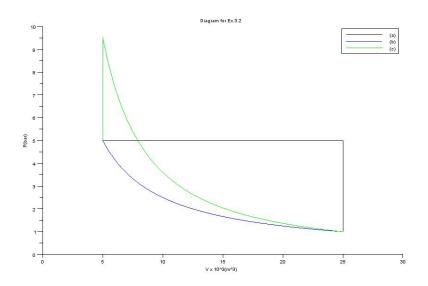


Figure 3.1: Find Work Heat del H del H

```
10 P=P^1.67;
11 plot2d(V,P,style=1)
12 P = [1.698 1.698];
13 V = [1690 \ 2083];
14 plot2d(V,P,style=2)
15 V = 1690:0.5:2853;
16 P = 2853 * V^-1;
17 plot2d(V,P,style=3,rect=[1500,0.8,3000,2])
18 xtitle("Diagram for Ex.3.3", "V", "P")
19 legend("(a)","(b)","(c)")
20 clear;
21
22
23 //Given Values for the Ideal Gas
24 R=8.314; //J/Mol/K
25 Cv = (3/2) *R; //J/Mol/K
26 Cp=(5/2)*R; //J/Mol/K
27 gama=Cp/Cv;
28
```

```
29 // Solution
30
31 //(a)
32 // Adiabatic Compression
33 P1=1; // Pressure=1bar
34 T1=343.15; //\text{Temp1}=343.15\text{K}(70 \text{ 'C})
35 T2=423.15; //\text{Temp2}=423.15\text{K}(150 \text{ °C})
36 Q_a=0; // Adiabatic Compression
37 del_U_a=round(Cv*(T2-T1));
38 W_a=del_U_a;
39 \text{ del_H_a=} \text{round} (Cp*(T2-T1));
40 //Using Eq. (3.29b)
41 P2=P1*((T2/T1)^(gama/(gama-1))); //bar
42
43 // (b)
44 //cooled form 150 °C to 70 °C at Const pressure
45 // Using Eq. (3.27)
46 Q_b = round(Cp*(T1-T2));
47 \text{ del_H_b=Q_b};
48 //for Ideal Gas
49 del_U_b=round(Cv*(T1-T2));
50 //by First law
51 \text{ W_b=del_U_b-Q_b}; // \text{Joules}
52
53 //(c)
54 //Expanded Isothermally to original state
55 \text{ del_U_c=0}; // \text{isothermal}
56 \text{ del_H_c=0}; // \text{isothermal}
57 Q_c=round(R*T1*log(P2/P1));
58 W_c = -Q_c;
59
60 //Entire process
61 Qt = Q_a+Q_b+Q_c;
62 \text{ Wt} = W_a+W_b+W_c;
63 del_Ut=del_U_a+del_U_b+del_U_c;
64 del_Ht=del_H_a+del_H_b+del_H_c;
65
66
```

```
67 // PartII (Irreversible)
68 eta=.80; // Efficiency = 80\%
69
70 //(a)
71 Wm_a=round(W_a/eta);
72 Qm_a=del_U_a-Wm_a; //del_U remains same (by First Law
73
74 //(b)
75 Wm_b=round(W_b/eta);
76 Qm_b=del_U_b-Wm_b; //del_U remains same (by First Law
77
78 //(c)
79 Wm_c=round(W_c*eta);
80 Qm_c=del_U_c-Wm_c;//del_U remains same (by First Law
81
82 //Entire Process
83 Qmt = Qm_a+Qm_b+Qm_c;
84 \text{ Wmt} = \text{Wm}_a + \text{Wm}_b + \text{Wm}_c;
85
86
87 del_U_rev=[del_U_a,del_U_b,del_U_c];
88 del_H_rev=[del_H_a,del_H_b,del_H_c];
89 Qrev=[Q_a,Q_b,Q_c];
90 Wrev=[W_a, W_b, W_c];
91 Sumr = [del_Ut, del_Ht, Qt, Wt];
92
93 del_U_irev=del_U_rev;
94 del_H_irev=del_H_rev;
95 Qirev=[Qm_a,Qm_b,Qm_c];
96 Wirev=[Wm_a, Wm_b, Wm_c];
97 Sumi = [del_Ut, del_Ht, Qmt, Wmt];
98
99
100 disp('
                (a) Adiabatic Compression')
101 disp('
                (b) Cooled form 150 °C to 70 °C at Const
```

```
pressure')
102 disp('
              (c) Expanded Isothermally to original
      state')
103
104 disp(' Mechanically reversible');
105
106 Ans_rev=[del_U_rev',del_H_rev',Qrev',Wrev'];
107
   disp(Sumr, 'Sum', Ans_rev, ' del U
                                          del H
                                                    Q
108
109
110 disp('
                  Irreversible ');
111
112 Ans_irev=[del_U_irev',del_H_irev',Qirev',Wirev'];
113
114 disp(Sumi, 'Sum', Ans_irev,' del U
                                           del H
                                                     Q
             W')
115
   //End
116
```

Scilab code Exa 3.4 Find Q W del U and del H in a PV Diagram

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
```

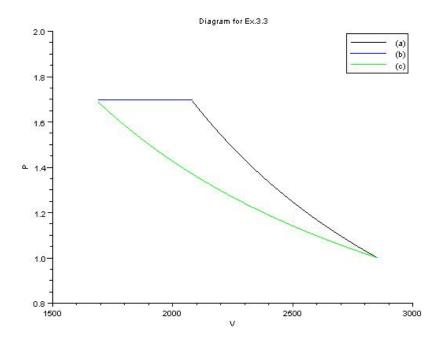


Figure 3.2: Find W Q del U and del H for the Figure

```
10 //Example 3.4
11 //Caption : Program To find Q,W,del_U and del_H in a
       PV Diagram
12
13 // Figure
14 P = [1.35 1.35];
15 \quad V = [0.24 \quad 0.264];
16 plot2d(V,P,style=2)
17 V = 0.12 : 0.001 : 0.24;
18 P=0.324*V^-1;
19 plot2d(V,P,style=5)
20 P = [2.7 2.97];
V = [0.12 \ 0.12];
22 plot2d(V,P,style=9,rect=[0.1,0.5,0.3,3])
23 xtitle ("Diagram for Ex.3.4", "V(m^3)", "P(bar)")
24 legend("(a)","(b)","(c)")
25 P = [2.97 2.97];
26 \quad V = [0 \quad 0.12];
27 plot2d(V,P,style=4)
28 P = [2.7 \ 2.7];
29 \quad V = [0 \quad 0.12];
30 plot2d(V,P,style=4)
31 P = [1.35 1.35];
32 \quad V = [0 \quad 0.24];
33 plot2d(V,P,style=4)
34 P = [0 2.7];
35 \quad V = [0.12 \quad 0.12];
36 plot2d(V,P,style=4)
37 P = [0 1.35];
38 \quad V = [0.24 \quad 0.24];
39 plot2d(V,P,style=4)
40 P = [0 1.35];
41 V = [0.264 \ 0.264];
42 plot2d(V,P,style=4)
43
44 clear;
45
46 // Given Values for Nitrogen Gas
```

```
47 m = 0.4; //Kg
48 M=28; // Molecular Mass Of Nitrogen
49 T1=300.15; //\text{Temp}=300.15\text{K}(27 \, ^{\circ}\text{C})
50 Pn=0.35; // Pressure of nitrogen = 0.35 \,\mathrm{bar}
51 Pa=1; //Atm Pressure = 1bar
52 R=8.314; //J/Mol/K
53 Cv = (5/2) *R; //J/Mol/K
54 Cp = (7/2) *R; //J/Mol/K
55 \text{ gama} = \text{Cp/Cv};
56
57 n = (m/M) * 1000; //moles
58
59 // Solution
60
61 //(a)
62 //Immersed In ice/water bath
63 T2=273.15; //\text{Temp}=273.15\text{K}(0 \text{ 'C})
64 W_a=-round(n*R*(T2-T1)); // Joules
65 del_H_a=approx(Cp*(T2-T1),0);
66 Q_a=round(n*del_H_a);
67 del_U_a = approx((Q_a+W_a)/n,0);
68 disp('(a) Immersed In ice/water bath')
69 disp('J', W_a, 'work done ')
70 disp('J',Q_a,'Heat Transferred Q = ')
71 disp('J',del_U_a,'change in Internal Energy ')
72 disp('J',del_H_a,'change in enthalpy ')
73
74
75 //(b)
76 //Isothermal Compression
77 del_U_b=0; //Isothermal
78 del_H_b=0; //Isothermal
79 W_b = -round(n*R*T2*log(1/2)); //W = nRTln(V3/V2), here V3
      /V2 = 0.5 (Given)
80 \quad Q_b = -W_b;
81 disp('(b) Isothermal Compression')
82 disp('J', W_b, 'work done by Isothermal Compression')
83 disp('J',Q_b,'Heat Transferred Q = ')
```

```
84 disp('J',del_U_b,'change in Internal Energy')
85 disp('J', del_H_b, 'change in enthalpy')
86
87
88 //(c)
89 //constant Vol Process
90 W_c=0; //const Vol
91 del_H_c = approx((Cp*(T1-T2))/n,0);
92 del_U_c = approx(Cv*(T1-T2),0);
93 Q_c=round(n*del_U_c);
94 disp('(c) Constant Vol Process')
95 disp('J', W_c, 'work done by Const Vol Process')
96 disp('J',Q_c,'Heat Transferred Q = ')
97 disp('J',del_U_c,'change in Internal Energy')
98 disp('J', del_H_c, 'change in enthalpy')
99
100
101 / End
```

Scilab code Exa 3.6 Find Change in KE and Temperature

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
9
```

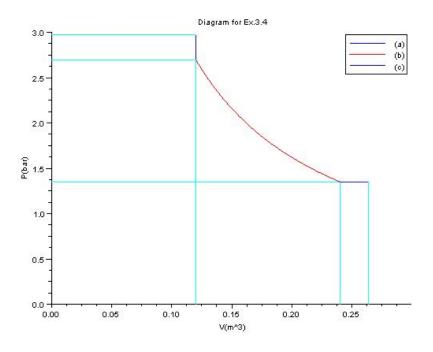


Figure 3.3: Find Q W del U and del H in a PV Diagram

```
11 //Example 3.6
12 //Caption : Program To find (a) Kinetic energy Change
       (b) change in temperature
13
14 //Given values
15 n=1; // Molar Rate(mol/s)
16 D=5; //inner Diameter (cm)
17 R=83.14;
18 Cp = (7/2) *R;
19 M=29*10^-3; // Molar mass(g/mol)
20 T=293.15; // temperature=293.15K(20 °C)
21 P1=6; // Upstream Pressure
22 P2=3; //Downstream Pressure
23
24 // Solution
25 // from Eq. (2.24b)
26 A = (\%pi/4) * ((D*10^-2)^2); //Area(m^2)
27 //upstream molar Volume
28 V1=(R*T/P1)*10^-6; //m^3/mol
29 u1=n*V1/A; //velocity(m/s)
30 V2 = 2 * V1;
31 u2=2*u1;
32 del_KE=approx(n*M*((u2^2)-(u1^2))/2,3);//J/s(W)
33 del_T=approx(-del_KE/(Cp*0.1),4);/K
34 \operatorname{disp}(\mathrm{`W\ or\ J/s',del_KE,'Change\ in\ KE'})
35 disp('K',del_T,'Change in Temperature')
36
37 / End
```

Scilab code Exa 3.7 Find V and Z for isopropyl vapor

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

```
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
     funcprot(0)
8 endfunction
9
10 //Example 3.7
11 //Caption: Program to Find V and Z for isopropyl
      vapor
12
13 //Given Values
14 T=473.15; //\text{Temp}=473.15 \text{ k} (200 \text{ C})
15 P=10; // Pressure=10bar
16 B=-0.388; // Viral Coefficient (m<sup>3</sup>/Kmol)
17 C = -26*(10^{(-3)}); // Viral Coefficient (m^6/(kmol)^2)
18 // Calculate V and Z for isopropyl vapor
19
20 //Solution
21
22 R=83.14*(10^(-3)); //m^3bar/Kmol/K
23
24 / (a)
25 //Ideal Gas equation
V_a = approx((R*T)/P,3);
27 Z_a=1; //Ideal Gas
28 disp('(a) By Ideal gas Equation')
29 disp('m^3/kmol', V_a, 'V = ')
30 \text{ disp}(Z_a, Z = ')
31
32 //(b)
33 //Using Eqution 3.37 \rightarrow Z=PV/RT=1+BP/RT
34 \ V_b = approx((R*T/P)+B,3);
35 Z_b = approx(P*V_b/(R*T), 4);
36 \operatorname{disp}('(b) \text{ Using Eqution } 3.37 \rightarrow Z=PV/RT=1+BP/RT')
37 \text{ disp}('m^3/kmol', V_b, 'V = ')
38 \text{ disp}(Z_b, 'Z = ')
39
```

```
40 //(c)
41 //Using Equation 3.39 \rightarrow Z=PV/RT=1+(B/V)+(C/(V<sup>2</sup>))
42 // Iterations
43 a=V_a; //Initial
44 i = -1;
45 \text{ while}(i==-1)
       b=((R*T/P)*(1+(B/a)+(C/(a^2))));
46
       c = abs(b-a)
47
       if (c<=0.0001)
48
49
          i=1;
50
          break;
51
       end
52
       a=b;
53 end
54
V_c = approx(b,3);
Z_c = approx(P*V_c/(R*T), 4);
57 //Ans
58 disp('(c) Using Equation 3.39 \rightarrow Z=PV/RT=1+(B/V)+(C)
       /(V^2)),
59 \operatorname{disp}(\mathrm{'m^3/kmol'}, V_c, \mathrm{'V} = \mathrm{'})
60 \operatorname{disp}(Z_c, Z = ')
61
62 / End
```

Scilab code Exa 3.8 Find Molar Volume of nButane

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
6 A = round(V*10^n)/10^n; //V-Value n-To what place
```

```
funcprot(0)
8
  endfunction
9
10 //Example 3.8
11 //Caption : Program to Find Molar Volume of n-Butane
12
13 //Given Values
14 T=350; //\text{Temp}=350\text{K}(76.85 ^{\circ}\text{C})
15 P=9.4573; // Pressure = 9.4573 bar
16 R=83.14;
17
18 Tc = 425.1; //App B
19 Pc = 37.96; //App B
20 \text{ Tr=T/Tc};
21 \text{ Pr=P/Pc};
22 // Parameters for RK
23 \text{ si} = 0.42748;
24 \text{ omega=0.08664};
25 epsilon=0;
26 \text{ sigma=1};
27 a = Tr^-0.5;
28
29 // Solution
30
31 // \text{Using Eq}(3.51)
32 q=si*a/(omega*Tr);
33 Beta=omega*Pr/Tr;
34
35 disp('The Following Results given By Redlich/Kwong
       Equation')
36 //(a)
37 Z=1; //initial
38 \quad a=Z;
39 \text{ for } i=0:10
      b=1+Beta-((q*Beta)*(a-Beta)/(a*(a+Beta)));
40
       if((b-a) == 0.0001)
41
42
         break;
43
       end
```

```
44
       a=b;
45
       i=i+1;
46 \, \text{end}
47 \quad Z = approx(b, 4)
48 V=round(Z*R*T/P);
49 disp('cm^3/mol', V, 'Molar Volume of saturated Vapor
      is ');
50
51 //(b)
52 Z=Beta; //initial
53 a=Z;
54 \text{ for } i=0:20
     b=Beta+(a*(a+Beta)*(1+Beta-a)/(q*Beta));
55
       if((b-a) == 0.0001)
56
57
         break;
58
       end
59
       a=b;
60
       i=i+1;
61 end
62 \quad Z = approx(b,5)
63 V=approx(Z*R*T/P,1);
64 disp('cm^3/mol', V, 'Molar Volume of Saturated Liquid
      is ');
65
66 //Given Values
67 T=350; //\text{Temp}=350\text{K}(76.85 ^{\circ}\text{C})
68 P=9.4573; // Pressure=9.4573 bar
69 R=83.14;
70
71 Tc=425.1; //App B
72 Pc = 37.96; //App B
73 Tr=T/Tc;
74 Pr=P/Pc;
75 // Parameters for eqns [vdW, RK, SRK, PR]
76 si = [27/64, 0.42748, 0.42748, 0.45724];
77 omega=[1/8,0.08664,0.08664,0.07779];
78 epsilon=[0,0,0,(1-sqrt(2))];
79 sigma=[0,1,1,(1+sqrt(2))];
```

```
80 w = 0.2; //App B
81 aSRK=(1+((0.480+(1.574*w)-(0.1768*w^2))*(1-Tr^0.5)))
82 aPR=(1+((0.37464+(1.54226*w)-(0.26992*w^2))*(1-Tr)
       ^0.5)))^2;
83 a=[1,Tr^-0.5,aSRK,aPR];
84
85 // Solution
86
                 By All Equations')
87 disp('
88 // \text{Using Eq} (3.51)
89 q=si.*a./(omega.*Tr);
90 Beta=omega.*Pr./Tr;
91
92 //disp('The Following Results given By Redlich/Kwong
        Equation ')
93 //(a)
94 \text{ for } j=1:4
95
96
        Z=1; // initial
97
        A = Z;
        for i = 0:10
98
          b=1+Beta(j)-((q(j)*Beta(j))*(A-Beta(j))/((A+(
99
              epsilon(j)*Beta(j)))*(A+(sigma(j)*Beta(j)))
             ));
            if((b-A) == 0.0001)
100
101
              break;
102
            end
103
            A = b;
104
            i=i+1;
105
106
        z(j) = approx(b,4);
107 end
108 V=round(z.*R*T/P);
109 disp('Molar Volume(Vv) of Saturated Vapor');
110 disp(V','
                  vdW
                            RK
                                     SRK
                                                 PR')
111
112 //(b)
```

```
113 for j=1:4
114
         Z=Beta(j); // initial
115
        A = Z;
116
        for i=0:20
117
           b=Beta(j)+((A+(epsilon(j)*Beta(j)))*(A+(sigma(
              j)*Beta(j)))*(1+Beta(j)-A)/(q(j)*Beta(j)));
            if((b-A) == 0.0001)
118
119
              break;
120
            end
121
            A = b;
122
            i=i+1;
123
124
         z(j) = approx(b,5);
125 end
126 V=approx(z*R*T/P,1);
127 disp('Molar Volume(VI) of Saturated Liquid');
128 disp(V','
                   vdW
                             RK
                                       SRK
                                                  PR')
129
130 disp('Note: Exp Value is Vv = 2482 cm<sup>3</sup>/mol and Vl
       = 115 \text{ cm}^3/\text{mol}
131
132 / End
```

Scilab code Exa 3.9 Find Molar Volume of n Butane by Various Eqn

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
```

```
9
10 //Example 3.9
11 //Caption : Program to Find Molar Volume of n-Butane
       by Various Eqn
12 // Given Values
13 T=510; //Temp=510K
14 P=25; // Pressure=25bar
15 R = 0.08314;
16
17 //(a)
18 //By the Ideal-gas Equation
19
20 V=approx(R*T/P,4);//m^3/kmol
21 disp('(a)By the Ideal-gas Equation')
22 disp('m^3/kmol', V, 'The Molar Volume is ')
23
24 //(b)
25 //The Generalized compressibility-factor Correlation
26 Tc=425.1; //From App.B
27 Pc=37.96; //From App.B
28 Tr = approx(T/Tc, 1);
29 Pr=approx(P/Pc,3)
30 //Interpolation in Tables E.1 and E.2 then provides
31 \quad Z0 = 0.865;
32 \quad Z1 = 0.038;
33 \quad w = 0.200;
34 Z = Z0 + (w * Z1);
35 V = \operatorname{approx}(Z * R * T / P, 2); //m^3 / \operatorname{kmol}
36 disp('(b) The Generalized compressibility - factor
      Correlation')
37 disp('m^3/kmol', V, 'The Molar Volume is ')
38
39 //(c)
40 //The Generalized Virial-coefficient Correlation
41 B0=0.083-(0.422/(Tr^1.6)); //Eqn (3.61)
42 B1=0.139-(0.172/(Tr^4.2)); //Eqn (3.62)
43 K = approx(B0 + (w*B1), 3) / K = BPc/RTc By Eqn (3.59)
44 //By Eqn(3.58)
```

Scilab code Exa 3.10 Find Pressure generated for methane

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
10 //Example 3.10
11 //Caption : Program To Find Pressure generated for
      methane
12
13 // Given Values
14 T=323.15; //\text{Temp}=323.15\text{K}(50 \, ^{\circ}\text{C})
15 V = 0.125; //Volume = 0.125m<sup>3</sup>
16 R = 0.08314;
17
18 //(a)
19 //By Ideal-gas equation,
20 P=approx(R*T/V,1);//in bar
21 disp('(a)By Ideal-gas equation')
22 disp('bar',P,'Pressure is ')
```

```
23
24 //(b)
25 //for Redlich/Kwong equation
26 Tc=190.6; //App B
27 \text{ Tr}=T/Tc;
28 \text{ si} = 0.42748;
29 \text{ omega} = 0.08664;
30 Pc = 45.99; //App B
31 a = approx(si*((Tr^(-0.5))*(R^2)*(Tc^2))/Pc,3)/Eqn
      (3.42) Units of a(T) bar m^6
32 b=approx(omega*R*Tc/Pc,5)//Eqn (3.43) Units of b m<sup>3</sup>
33 // Using eqn (3.41)
34 / P=RT/(V-b)-a(T)/(V+Eb)(V+b), E-epsilon, ->sigma
35 \text{ epsilon=0};
36 \text{ sigma=1};
37 P=approx(((R*T/(V-b))-(a/((V+(epsilon*b))*(V+(sigma*
      b))))),2);
38 disp('(b) for Redlich/Kwong equation')
39 disp('bar',P,'Pressure is ')
40
41 //(c)
42 //A generalized Correlation
43 Z0=0.887; // from Table E.3 and E.4
44 Z1=0.258; //from Table E.3 and E.4
45 \quad w = 0.012;
46 \quad Z = Z0 + (w * Z1);
47 P=approx(Z*R*T/V,1);//bar
48 disp('(c)A generalized Correlation')
49 disp('bar',P,'Pressure is ')
50
51 / End
```

Scilab code Exa 3.11 Find Pressure generated for ammonia

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
  endfunction
8
9
10 //Example 3.11
11 //Caption : Program to Find Pressure generated for
      ammonia
12
13 // Given Values
14 T=338.15; //\text{Temp}=338.15\text{K}(65 \text{ 'C})
15 Vt=0.03; //Volume=0.03m^3
16 R=0.08314;
17 m=0.5; //mass in Kg
18 M=17.02; // Molecular Mass
19 V=Vt/(m/M); // n=m/M(moles)
20
21 / (a)
22 //By Ideal-gas equation,
23 P=approx(R*T/V,2);//in bar
24 disp('(a)By Ideal-gas equation')
25 disp('bar',P,'Pressure is ')
26
27 //(b)
28 //A generalized correlation
29 Tc=405.7; //App B
30 \text{ Tr}=T/Tc;
31 Pc = 112.8; //App B
32 B0=0.083-(0.422/(Tr^1.6)); //Eqn (3.61)
33 B1=0.139-(0.172/(Tr<sup>4</sup>.2)); //Eqn (3.62)
34 //Substituting in eq(3.59)
35 \quad w = 0.253;
36 K=B0+(w*B1); //K=BPc/RTc
37 B=K*R*Tc/Pc; //m^3 kmol^-1
```

```
38 //solving eq.(3.37)
39 P=approx(R*T/(V-B),2);
40 disp('(b)A generalized Correlation')
41 disp('bar',P,'Pressure is ')
42
43 //End
```

Scilab code Exa 3.12 Find density for ammonia

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
  endfunction
8
9
10 //Example 3.12
11 //Caption: Program to Find density for ammonia
12
13 //Given Values
14 T=310; //\text{Temp}=310\text{K}(36.85 ^{\circ}\text{C})
15 \quad M = 17.02;
16
17 // Solution
18
19 //(a)
20 //saturated liquid
21 Tc = 405.7; //App B
22 Vc = 0.07247; //App B
23 Zc = 0.242; //App B
24 Vsat=approx(Vc*(Zc^{((1-Tr)^0.2857)}),5);/m^3kmol^-1
```

```
25 rho=approx(M/Vsat,2);
26 disp('(a) Saturated liquid')
27 disp('m^3/kmol', Vsat, 'Volume is')
28 disp('kmol/m<sup>3</sup>',rho,'Density is')
29
30 //(b)
31 //Liquid at 100bar
32 P=100; // Pressure = 100 bar
33 Pc = 112.8; //App B
34 \text{ Pr=P/Pc};
35 \text{ rho\_r=2.38;} //\text{From Graph}
36 V=Vc/rho_r;
37 //but this Gives large error
38 rho_r1=2.34;
39 V_new=approx(V*rho_r1/rho_r,5);
40 //In exceptance with Experimental Value
41
42 rho=approx(M/V_new,2);
43 disp('(b) For Liquid at 100 bar')
44 disp('m^3/kmol', V_new, 'Volume is')
45 disp('kmol/m<sup>3</sup>',rho,'Density is ')
46
47 //End
```

Chapter 4

Heat Effects

Scilab code Exa 4.2 Find Heat Required to Heat Methane gas

```
1 clear;
    2 clc;
    4 //To find Approx Value
    5 function[A] = approx(V,n)
                                 A=round(V*10^n)/10^n;//V-Value n-To what place
                                  funcprot(0)
                  endfunction
 10 function[Q]=ICPH(TO,T,A,B,C,D)
11
                                 t=T/T0;
                                 Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D(C/3) * T0 * T0 * ((t^2) + t+1)) + (D(C/3) * ((t^2) + t+1)) + (D
12
                                                    /(t*T0*T0)))*(T-T0)
                                 funcprot(0);
13
14 endfunction
15
16
17 //Example 4.2
18 //Caption : Program to find Heat Required to Heat
```

```
Methane gas
19
20 //Given values for methane
21 R=8.314;
22 \quad T0 = 533.15;
23 T=873.15;
24 \quad A = 1.702;
25 B=9.081*(10^-3);
26 \quad C = -2.164*(10^-6);
27 D = 0;
28
29
30 //Solution
31 Q=approx(R*ICPH(T0,T,A,B,C,D),0);
32 disp('J',Q,'Heat Required')
33
34 / End
```

Scilab code Exa 4.3 Find the Final Temperature with Heat Given

```
12
13
14 // Given values for Ammonia
15 R=8.314;
16 \quad T0 = 533.15;
17 A=3.578;
18 B=3.020*(10^-3);
19 C = 0;
20 D = -0.186*(10^5);
21 \quad Q = 422*(10^3);
22 n=11.3;
23 del_H=Q/n;
24
25 //Solution
26 i = -1;
27 a=round(T0);//Initial
28 while (i==-1)
29
     b=R*MCPH(TO,a,A,B,C,D);
30
     c=b*(a-T0);
     flag=del_H-c;
31
32
     if(flag<=100) then</pre>
33
       T=a-1;
34
        i=1;
35
     else
36
        a=a+1;
37
        i = -1;
38
     end
39 end
40
41
42 disp('K',T,'Temperature Required(Approx)')
43
44 //End
```

Scilab code Exa 4.4 Find the Latent Heat

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
9
10 //Example 4.4
11 //Caption : Program to find the Latent Heat
12
13 del_H1=2257;//latent Heat of Vapourisation of water
     at 373.15K(100 °C) [KJ/Kg]
14 Tr1=373.15/647.1;
15 Tr2=573.15/647.1;
16
17 del_H2=approx(del_H1*((1-Tr2)/(1-Tr1))^0.38,0);/KJ/
     Kg
18 disp('KJ/Kg',del_H2,'latent Heat at 573.15K')
19
20 disp('Note: The Value as given in steam tables at
     573.15K is 1406 KJ/Kg')
21
22 //End
```

Scilab code Exa 4.5 Find the Standard Heat at 298K

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

```
4 //Example 4.5
5 // Caption: Program to Find the Standard Heat at
      298.15K
6
7 //4HCL + O2 \longrightarrow 2H2O + 2C12
8 del_H_HCL=-92.307; //KJ Heat Of Formation
9 del_H_H20=-241.818; //KJ
10
11 //4HCL \longrightarrow 2H2 + 2C12
12 del_H_298_HCL=4*(-1)*del_H_HCL;
13 / 2H2 + O2 \longrightarrow 2H2O
14 del_H_298_H20=2*del_H_H20;
15 //Final
16 del_H_298=del_H_298_HCL+del_H_298_H20;
17
18 disp('KJ',del_H_298, 'Standard Heat')
19
20 //End
```

Scilab code Exa 4.6 Find the Standard Heat of Methanol Synthesis

```
12
13 function [Q] = IDCPH(TO, T, dA, dB, dC, dD)
14
     t=T/T0;
15
     Q = (dA + ((dB/2) * T0 * (t+1)) + ((dC/3) * T0 * T0 * ((t^2) + t+1))
         +(dD/(t*T0*T0)))*(T-T0)
16
      funcprot(0);
17 endfunction
18
19
20 //Methanol Synthesis @ 1073.15K(800 °C)
21 / CO + 2H2 \longrightarrow CH3OH
22 del_H_CO=-110.525//@298K from Table C.4
23 del_H_CH30H_g=-200.660; //@298K from Table C.4
24 del_H_298=((1)*del_H_CH3OH_g)-((1)*del_H_CO); //KJ/
      mol
25 \quad T0 = 298.15;
26 \quad T = 1073.15;
27 R=8.314;
28 // Moles (CH3OH, CO, H2)
29 n = [1; -1; -2];
30 //A..from Table C.1
31 A = [2.211; 3.376; 3.249];
32 //B.. from Table C.1
33 B=(10^-3)*[12.216;0.557;0.422];
34 //C.. from Table C.1
35 \quad C = (10^-6) * [-3.450; 0; 0];
\frac{36}{D}. From table C.1
37 D = (10^5) * [0; -0.031; 0.083];
38
39 \text{ del_A=0};
40 \text{ del_B=0};
41 del_C=0;
42 \, del_D=0;
43 for (i=1:3)
44
     del_A=del_A+n(i,1)*A(i,1);
45
     del_B = del_B + n(i, 1) * B(i, 1);
     del_C=del_C+n(i,1)*C(i,1);
46
     del_D=del_D+n(i,1)*D(i,1);
47
```

```
48 end
49
50 I=IDCPH(T0,T,del_A,del_B,del_C,del_D);
51 del_H=approx(del_H_298+(R*I/10^3),3);
52
53 disp('KJ',del_H,'Standard Heat Of Enthalpy');
54
55 //End
```

Scilab code Exa 4.7 Find Max Temperature reached in Combustion of CH4

```
1 clear;
2 clc;
3
4 //Example 4.7
  //Caption : Program To Find Max Temperature reached
      in Combustion of Methane
7
  function[Q]=MCPH(TO,T,A,B,C,D)
8
     t=T/T0;
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
        /(t*T0*T0)))
10
     funcprot(0);
11 endfunction
12
13
14 // Combustion Of methane
15 / CH4 + 2O2 \longrightarrow CO2 + 2H2O
16 R=8.314;
17 del_H_C02 = -393509; //from table C.4
18 del_H_02 = -241818; // from table C.4
19 del_H_CH4 = -74520; //from table C.4
```

```
20 del_H_298=del_H_CO2+(2*del_H_O2)-del_H_CH4;
21 del_Hp=-del_H_298;
22 //moles of reactants
23 n_CH4=1;
24 n_02=2+(0.2*2); //20\% Excess
25 n_N2=n_02*(79/21);
26 // Moles Of Products.. (CO2, H2O, O2, N2)
27 \text{ np} = [1; 2; 0.4; 9.03];
28 //A.. from Table C.1
29 A = [5.457; 3.470; 3.639; 3.280];
30 //B.. from Table C.1
31 B=(10^-3)*[1.045;1.450;0.506;0.593];
32 //C.. from Table C.1
33 C=(10^-6)*[0;0;0;0];
34 //D.. From table C.1
35 D=(10^5)*[-1.157;0.121;-0.227;0.040];
36
37 \quad E_A = 0;
38 E_B = 0;
39 E_C = 0;
40 E_D = 0;
41 for (i=1:4)
     E_A = E_A + np(i,1) * A(i,1);
42
43
     E_B=E_B+np(i,1)*B(i,1);
44
     E_C = E_C + np(i,1) * C(i,1);
45
     E_D=E_D+np(i,1)*D(i,1);
46 end
47
48 \quad T0 = 298.15;
49 a=round(TO); // Initial
50 i = -1
51 while (i==-1)
     b=R*MCPH(T0,a,E_A,E_B,E_C,E_D);
52
53
     c=b*(a-T0);
54
     flag=del_Hp-c;
55
     if (flag <= 100) then
56
       T=a-1;
57
        i=1;
```

```
58     else
59         a=a+1;
60         i=-1;
61         end
62     end
63     disp('K',T,'Temperature Required(Approx)')
64     //End
```

Scilab code Exa 4.8 Find the Heat Requirement for the Reactor

```
1 clc;
2 clear;
4 //Example 4.8
5 // Caption: Program to Find the Heat Requirement for
       the Reactor
6
  //To find Approx Value
8 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
10
     funcprot(0)
11
  endfunction
12
13
  function[Q]=MCPH(TO,T,A,B,C,D)
14
     t=T/T0;
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
15
        /(t*T0*T0)))
     funcprot(0);
16
17 endfunction
18
19
20 / CH4 + H2O \longrightarrow CO + 3H2 (A)
21 / CH4 + 2H2O \longrightarrow CO2 + 4H2
```

```
22 \text{ del}_H_A = 205813; //J
23 del_H_B=164647; //J
24 //0.87 \text{ mol of CH4 for (A)} (1-0.87) \text{ mol of CH4 for (B)}
25 \text{ del}_H_298 = (0.87*\text{del}_H_A) + (0.13*\text{del}_H_B);
26 R=8.314;
27 \quad T0 = 298.15;
28 T_A = 600; // Cooled
29 T_B = 1300; //Heated
30 // Moles of reactants (CH4, H2O)
31 nr=[1;2];
32 //Moles of Products (CO, H2, CO2, H2O)
33 np = [0.87; 3.13; 0.13; 0.87];
34 //For Reactants
35 // for CH4
36 \quad \text{I1=MCPH} (\text{T0}, \text{T_A}, 1.702, 9.081*(10^-3), -2.164*(10^-6), 0)
37 //For H2O
38 I2=MCPH(T0,T_A,3.470,1.450*(10^-3),0,0.121*(10^5));
39 del_Hr=R*((nr(1,1)*I1)+(nr(2,1)*I2))*(T0-T_A);//J
40 //For Products
41 // for CO
42 I1=MCPH(T0, T_B, 3.376, 0.557*(10^-3), 0, -0.031*(10^5));
43 / For H2
44 I2=MCPH(T0,T_B,3.249,0.422*(10^-3),0,0.083*(10^5));
45 / for CO2
46 I3=MCPH(T0, T_B, 5.457, 1.045*(10^-3), 0, -1.157*(10^5));
47 //For H2O
48 I4=MCPH(T0,T_B,3.470,1.450*(10^{-3}),0,0.121*(10^{5}));
49 del_{Hp}=R*((np(1,1)*I1)+(np(2,1)*I2)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(np(3,1)*I3)+(
                  (4,1)*I4))*(T_B-T0);//J
50 // del_H
51 del_H=del_H_298+del_Hr+del_Hp;
52 Q=approx(del_H,-1);
53 disp('J',Q,'Heat Required');
54
55 //End
```

Chapter 5

The Second Law Of Thermodynamics

Scilab code Exa 5.1 Find the Heat discarded to the River

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
9
10 //Example 5.1
11 //Caption : Program To Find the Heat discarded to the River
12
13 //Given Values
14 Tc=295;//K
15 Th=585;//K
16 W=800000;//KW
```

```
17  n_max=1-(Tc/Th);
18  n=approx(0.7*n_max,3)
19  Qc=approx(((1-n)/n)*W,-2);
20  disp('KW',Qc,'Heat required');
21
22  //End
```

Scilab code Exa 5.3 Find the Final Temperature

```
1 clear;
2 clc;
3
4 //Example 5.3
5 // Caption: Program to Find the Final Temperature in
       Reversible Adiabatic Expansion
  function[Q]=MCPS(TO,T,A,B,C,D)
8
     t=T/T0;
     Q = (A) + (((B*T0) + (((C*T0*T0) + (D/(t*t*T0*T0)))*(t+1))
        /2))*((t-1)/log(t)))
10
     funcprot(0);
11 endfunction
12
13
14 // Given values
15 P2=1; //bar
16 P1=5; // bar
17 T0=550; //K
18 A=1.702;
19 B=9.081*(10^-3);
20 C = -2.164*(10^-6);
21 D=0;
22
```

```
23 //Equation to be used
24 //(<Cp>s/R) ln (T2/T1)=ln (P2/P1) since del_S=0
25 // let I = (\langle Cp \rangle s / R)
26
27 / T2 = \exp(\log(1/5)/I);
28 a=T0-1; // Initial
29 i = -1;
30 while (i==-1)
     b=MCPS(TO,a,A,B,C,D);
31
32
     c = (log(1/5))/(log(a/T0));
     flag=c-b;
33
     if (flag <= 0.0001) then
34
35
        T=a;
36
        i=1;
37
     else
38
        a=a-.01;
39
        i = -1;
40
      end
41 end
42
43 disp('K',T,'Final Temperature')
44
45 / End
```

Scilab code Exa 5.4 Find the change in entropy in a steel Casing

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
```

```
8 endfunction
9
10 //Example 5.4
11 //Caption : Program To Find the change in entropy in
       a steel Casing
12
13 //Given Values
14
15 //For Casting
16 Cp_Casting=0.5; // [KJ/Kg/K]
17 T1=723.15; //[K]
18 T0 = 298.15; //[K]
19 M_Casting=40; //[Kg]
20 //For Oil
21 Cp_0il=2.5; //[KJ/Kg/K]
22 \text{ M_Oil=150; // [Kg]}
23
24 //Formula M1Cp1dT'=M2Cp2dT
25 //40*0.5*(T-723.15) = 150*2.5*(298.15-T)
26 //Whence
27 T = ((T1*M_Casting*Cp_Casting) + (T0*M_Oil*Cp_Oil))/((
      M_Casting*Cp_Casting)+(M_Oil*Cp_Oil));
28
29 //(a)-change in entropy For casting
30 del_S_Casting=approx(M_Casting*Cp_Casting*integrate(
      '1/T', 'T', T1, T), 2);
31
  disp('KJ/K',del_S_Casting,'(a)Change In Entropy of
      Casting')
33
34 //(b)-change in entropy For Oil
35 \text{ del_S_Oil=approx}(M_Oil*Cp_Oil*integrate('1/T', 'T', TO))
      ,T),2);
36
37 disp('KJ/K',del_S_Oil,'(b)Change In Entropy of Oil')
38
39 //(c) - Total
40 del_S_total=del_S_Casting+del_S_Oil;
```

```
41 disp('KJ/K',del_S_total,'(c)Total entropy change')
42
43 //End
```

Scilab code Exa 5.5 Find the Rate of Heat Transfer and Entropy

```
1 clear;
2 clc;
3
4 //Example 5.5
  //Caption : Program to Find the Rate of Heat
      Transfer and Entropy
  //Given Values
7
8
9 //Gas A
10 rn_A=1; // rate [mol/s]
11 T_A = 600; //[K]
12
13 //Gas B
14 rn_B=2; //rate[mol/s]
15 T_B=450; //[K]
16
17 //product
18 rn=rn_A+rn_B; //[mol/s]
19 T = 400; //[K]
20 R=8.314;
21 Cp = (7/2) *R;
22 T_s = 300; // Temperature [K]
23
24 //By equation (2.30) rQ=rn*H-rn_A*H_A-rn_B*H_B=rn_A
      H-H_A)+rn_B*(H-H_B) Rate of heat transfer
25 rQ=(rn_A*Cp*(T-T_A))+(rn_B*Cp*(T-T_B)); //[J/s] or
```

Scilab code Exa 5.6 Find the Feasibility of a Process

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8
  endfunction
10 //Example 5.6
11 //Caption : Program to Find the Feasibility of a
      Process
12
13 // Given Values
14 //Saturated Steam
15 / At T = 373.15K
16 H1=2676; // [KJ/Kg] from Steam table (App F)
17 S1=7.3554; //[KJ/Kg/K] from steam table (App F)
18 //At T=273.15K Liquid water
19 H2=0;
```

```
20 S2=0;
21
22 T_sigma = 273.15; //[K]
23 T_r = 473.15; //[K]
24 Q_r = -2000; // [KJ]
25
26 \text{ del}_H=H2-H1;
27 \quad Q=del_H;
28 Q_sigma = Q - Q_r;
29
30 \text{ del_S=S2-S1};
31 //For Heat Reservoir at 473.15K
32 del_St_T_r = (-Q_r/T_r); // [KJ/K]
33 //For Heat reservoir provided by cooling water at
      273.15K
34 del_St_T_sigma = -Q_sigma/T_sigma;
35 del_S_total=del_S+del_St_T_r+del_St_T_sigma;
36 disp('Since del_S_total < 0 Process not feasible')
37
38 // Actual
39 Q_r = approx((T_r/(T_r-T_sigma))*(del_H-(T_sigma*del_S))
40 disp('KJ/Kg',Q_r,'Actual Heat transfer')
41
42 //End
```

Scilab code Exa 5.7 Find the Maximum Work obtained

```
1 clear;
2 clc;
3 4
5 //Example 5.7
```

```
6 // Caption: Program to Find the Maximum Work
      obtained in a Steady state Flow
7
8
9 //To find Approx Value
10 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
11
     funcprot(0)
12
13 endfunction
14
15 function [Q] = ICPH (TO, T, A, B, C, D)
     t=T/T0;
16
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
17
         /(t*T0*T0)))*(T-T0)
18
     funcprot(0);
19 endfunction
20
21 function[Q]=ICPS(TO,T,A,B,C,D)
22
     t=T/T0;
23
     Q = ((A) * \log(t)) + (((B*T0) + (((C*T0*T0) + (D/(t*t*T0*T0)))))
        ))*(t+1)/2))*(t-1))
24
     funcprot(0);
25 endfunction
26
27
28 //Given Values
29 P1 = 50; //bar
30 P2=1.013; //bar
31 T1 = 800; //[K]
32 \text{ T2=300; } //[K]
33 R=8.314;
34
35 //del_H=intergral(CpdT) in the limits T1 and T2
36 \quad A = 3.280;
37 B=0.593*(10^-3);
38 C=0;
39 D=0.040*(10^5);
40 del_H=R*ICPH(T1,T2,A,B,C,D); //[J/mol]
```

Scilab code Exa 5.8 Find the Maximum Possible Work for Ideal Condition

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
9
10 //Example 5.8
11 // Caption : Program To Find the Maximum Possible
     Work for Ideal Condition
12
13 // Given Values
14 //Saturated Steam
15 / At T = 373.15K
16 H1=2676; // [KJ/Kg] from Steam table (App F)
17 S1=7.3554; //[KJ/Kg/K] from steam table (App F)
18 //At T=273.15K Liquid water
19 H2=0;
```

```
20 S2=0;
21
22 T_sigma=273.15; // [K]
23 T_r=473.15; // [K]
24
25 del_H=H2-H1;
26 del_S=S2-S1;
27 W_ideal=del_H-(T_sigma*del_S); // [KJ/Kg]
28 Q=approx(abs(W_ideal*(T_r/(T_sigma-T_r))),1); // [KJ]
29 disp('KJ',Q,'Maximum Possible Work')
30
31 // End
```

Scilab code Exa 5.9 Find the Lost Work in Heat Exchangers

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
     funcprot(0)
8 endfunction
9
10 //Example 5.9
11 //Caption : Program to find the Lost Work in Heat
      Exchangers
12
13 //Given Values
14
15 T_H1 = 400; //[K]
16 T_H2=350; //[K]
17 T_C1 = 300; //[K]
```

```
18 T_{sigma}=300; //[K]
19 rn_H=1; //[mol/s]
20 R=8.314;
21 Cp = (7/2) *R;
22
23 T_C2_a = T_H2 - 10;
24 T_C2_b=T_H1-10;
25
26 // Figure
27 mtlb_axis('auto');
28 subplot(1,2,1);
29 X = [0, 1];
30 Y = [T_C1, T_C2_a];
31 plot2d(X,Y);
32 Y = [T_H1, T_H2];
33 plot2d(X,Y,style=3,rect=[0,290,1,410]);
34 legend('Tc', 'Th')
35 \quad X = [1, 1];
36 \quad Y = [290, 410];
37 plot2d(X,Y);
38 \quad X = [0, 0.25];
39 Y = [T_C1, T_C1];
40 plot(X,Y,'--');
41 Y = [T_H1, T_H1];
42 plot(X,Y,'--');
43 X = [0.75, 1];
44 Y = [T_C2_a, T_C2_a];
45 plot(X,Y,'--');
46 Y = [T_H2, T_H2];
47 plot(X,Y,'--');
48 xtitle("(a) Case 1, Cocurrent", "Qc", "T");
49
50 subplot(1,2,2);
51 \quad X = [0, 1];
52 Y = [T_C1, T_C2_b];
53 plot2d(X,Y);
54 Y = [T_H2, T_H1];
55 plot2d(X,Y,style=3,rect=[0,290,1,410]);
```

```
56 legend('Tc', 'Th')
57 X = [1, 1];
58 Y = [290, 410];
59 plot2d(X,Y);
60 \quad X = [0, 0.25];
61 Y = [T_C1, T_C1];
62 plot(X,Y,'--');
63 Y = [T_H2, T_H2];
64 plot(X,Y,'--');
65 \quad X = [0.75, 1];
66 Y = [T_C2_b, T_C2_b];
67 plot(X,Y,'--');
68 Y = [T_H1, T_H1];
69 plot(X,Y,'--');
70 xtitle("(b) Case 2, Countercurrent", "Qc", "T");
71
72 //Solution
73 //Equation to be used
74 / (rn_H *Cp(T_H2-T_H1)) + (rn_C *Cp(T_C2-T_C1)) = 0 Eq(A)
75 // del_r S = rn_H * Cp * (ln (T_H2/T_H1) + kln (T_C2/T_C1)) k =
                   rn_C/rn_H r\longrightarrow Rate
                                                                                     Eqn(B)
76 / rW_lost = T_sigma*del_rS Eqn(C)
77
78 //(a)-Cocurrent
79 / \text{by Eqn}(A)
80 T_C2_a=T_H2-10;
81 k=(T_H1-T_H2)/(T_C2_a-T_C1);//k=rn_C/rn_H
82 //By Eqn(B)
83 del_rS=approx(rn_H*Cp*(log(T_H2/T_H1)+(k*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_H2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*log(T_C2_a/T_L2)+(h*
                   T_C1)),3);//[J/K/s]
84 //By Eqn (C)
85 rW_lost=approx(T_sigma*del_rS,1); //[J/s] or [W]
86 disp('(a)-Cocurrent')
87 disp('J/K/s',del_rS,'Rate Of change of entropy')
88 disp('J/s or W',rW_lost,'Lost Work')
89
90 //(b)-Countercurrent
91 T_C2_b=T_H1-10;
```

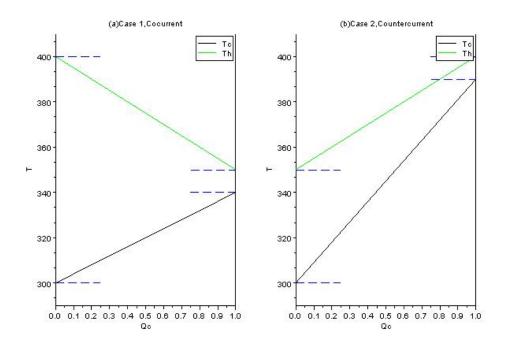


Figure 5.1: Find the Lost Work in Heat Exchangers

```
92 k=(T_H1-T_H2)/(T_C2_b-T_C1); //k=rn_C/rn_H
93 //By Eqn(B)
94 del_rS=approx(rn_H*Cp*(log(T_H2/T_H1)+(k*log(T_C2_b/T_C1))),3); //[J/K/s]
95 //By Eqn(C)
96 rW_lost=approx(T_sigma*del_rS,1); //[J/s] or [W]
97 disp('(b)-Countercurrent')
98 disp('J/K/s',del_rS,'Rate Of change of entropy')
99 disp('J/s or W',rW_lost,'Lost Work')
100
101 //End
```

Chapter 6

Thermodynamic Properties Of Fluids

Scilab code Exa 6.1 Find the Changes in enthalpy and entropy

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
9
10 //Example 6.1
11 //Caption : Program To find the Changes in enthalpy and entropy
12
13 //Given Values
14
15 //At Temp T1=298.15K
16 T1=298.15;//[K]
```

```
17 P1=1; //[bar]
18 P2=1000; // [bar]
19 Cp_T1 = 75.305; // [KJ Kmol/K]
20 V1_T1=18.071*10^-3; // [m^3/Kmol]
21 V2_T1=18.012*10^-3; //[m^3/Kmol]
22 beta1_T1=256*10^-6; //[1/K]
23 beta2_T1=366*10^-6; //[1/K]
24
25 / \text{At Temp T2} = 323.15 \text{K}
26 T2 = 323.15; //[K]
27 P1=1; // [bar]
28 P2=1000; // [bar]
29 Cp_T2=75.314; // [KJ Kmol/K]
30 V1_T2=18.234*10^-3; // [m^3/Kmol]
31 V2_T2=18.174*10^-3; //[m^3/Kmol]
32 beta1_T2=458*10^-6; //[1/K]
33 beta2_T2=568*10^-6; //[1/K]
34
35 // Solution
36
37 //Formula to be used
38 //Eqn (6.28) del_H = ((Cp)(T2-T1)) - ((V)(1-(beta)(T2))
      P2-P1))
39 //Eqn (6.29) del_S = ((Cp) ln (T2/T1) - ((beta) (V) (P2-P1))
40
41 // For P=1
42 Cp = (Cp_T1 + Cp_T2)/2;
43 //For T=323.15K
44 V = (V1_T2 + V2_T2)/2;
45 beta_T=(beta1_T2+beta2_T2)/2;
46
47 \text{ del}_{H=approx}((Cp*(T2-T1))+(V*(1-(beta_T*T2))*(P2-P1)
      *10^5*10^-3),0);
   del_S = approx((Cp*(log(T2/T1))) - (beta_T*V*(P2-P1))
      *10^5*10^-3),2);
49
50 \mathtt{disp}(\ 'KJ/Kmol',\mathtt{del_H},\ 'Change\ In\ Enthalpy')
51 disp('KJ/Kmol/K',del_S,'Change In Entropy')
```

```
52
53 //End
```

Scilab code Exa 6.3 find Entropy and Enthalpy of Saturated isobutane

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
10 function [Q] = ICPS (TO, T, A, B, C, D)
11
     t=T/T0;
12
     Q = ((A) * \log(t)) + (((B*T0) + (((C*T0*T0) + (D/(t*t*T0*T0))
        ))*(t+1)/2))*(t-1))
13
     funcprot(0);
14 endfunction
15
16 function [Q] = ICPH(TO,T,A,B,C,D)
17
     t=T/T0;
18
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
        /(t*T0*T0)))*(T-T0)
19
     funcprot(0);
20 endfunction
21
22 //Example 6.3
23 //Caption: Program to find Entropy and Enthalpy of
      Saturated isobutane Vapor
24
25 // Given Values
```

```
26
27 \text{ T0=300; } //[K]
28 T=360; //[K]
29 R=8.314;
30 P=15.14; // [bar]
31 \quad A=1.7765;
32 B=33.037*10^{-3};
33 C=0;
34 D = 0;
35 H0=18115; //J/mol
36 \text{ SO} = 295.976; //J/mol/K
37
38 //Graph
39 \quad X = [0, 0.10, 0.50, 2, 4, 6, 8, 10, 12, 14, 15.41];
40 Y1
      =[1.780,1.700,1.514,1.293,1.290,1.395,1.560,1.777,2.073,2.432,2.7
      //[(dZ/dT)p/P]
  Y2
41
      =[2.590,2.470,2.186,1.759,1.591,1.544,1.552,1.592,1.658,1.750,1.8
      //[-(Z-1)/P]
42 subplot(1,2,1);
43 plot2d(Y1,X);
44 xgrid();
45 xtitle("(a)","P(bar)","[(dZ/dT)p/P]X10^4(K^-1 bar
       (-1)");
46 subplot(1,2,2);
47 plot2d(Y2,X);
48 xgrid();
49 xtitle ("(b)", "P(bar)", "[-(Z-1)/P]X10^2(bar^-1)");
50
51
52 // Area Under the Curve (a)
53 \quad Y1 = Y1 * 10^-4;
54 \quad A1 = 0;
55 for i=2:11;
     A1 = A1 + ((X(i-1) - X(i)) * Y1(i));
56
57 end
58 disp('(X 10^-4) K^-1', A1*10000, 'Area under the graph)
```

```
(a)')
59 //Area Under the Curve (b)
60 \quad Y2 = Y2 * 10^{-2};
61 \quad A2 = 0;
62 \text{ for } i=2:11;
63
     A2=A2+((X(i-1)-X(i))*Y2(i));
64 end
65 disp(approx(A2,4), 'Area under the graph(b)')
66
67
68 K=A1*T; //Hr/RT
69 //From Eqn (6.47)
70 Hr=R*T*(K); //[J/mol]
71 //From Eqn (6.48)
72 Sr=R*(K-(A2)); //[J/mol/K]
73
74 //From Eqn (6.49) and Eqn (6.50)
75 H1=R*ICPH(T0,T,A,B,C,D);
76 S1=R*ICPS(TO,T,A,B,C,D);
77
78 H = HO + H1 + Hr;
79 S=approx(S0+S1+Sr-(R*log(P)),3);
80
81 disp('J/mol',H,'Enthalpy')
82 disp('J/mol/K',S,'Entropy')
83 disp('Note: The Answer is different with that of the
       Book because the Method Used to find the Area
      under the Graph is done by finding the area of
      small
                   Rectangles')
84
  //End
85
```

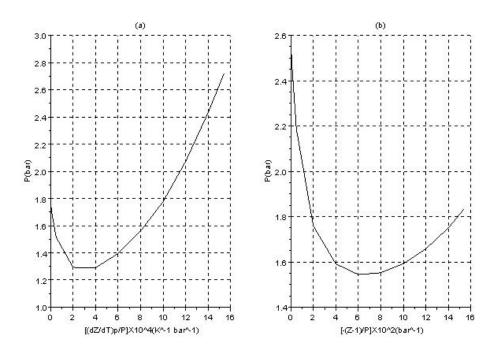


Figure 6.1: find Entropy and Enthalpy of Saturated isobutane

Scilab code Exa 6.4 Find the Residual Enthalpy and Residual Entropy

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
9
10 //Example 6.4
11 //Caption : Program to Find the Residual Enthalpy
      and Residual Entropy
12
13 // Given Values and values from Table (3.1)
14 T=500; //[K]
15 R=8.314;
16 Tc = 425.1; //[K]
17 P=50; // [bar]
18 Pc = 37.96; // [bar]
19 omega=0.08664;
20 \text{ si=0.4636};
21 \text{ Tr=T/Tc};
22 \text{ Pr=P/Pc};
23 alpha_Tr=Tr^(-0.5); //a(Tr)
24 // Using Eqn(3.50)
25 Beta=omega*(Pr/Tr);
26 // \text{Using Eqn} (3.51)
27 q=si*alpha_Tr/(omega*(Tr^1.5));
28
29 / using eqn(3.49)
30 / Z=1+beta-q*beta*((Z-beta)/((Z+(epsilon*beta))*(Z+(epsilon*beta)))
      sigma*beta)))
31
32 //calculation of Z
33 Z=1; // Initial
34 \quad a=Z;
```

```
35 \text{ for } i=0:10
     b=1+Beta-(q*Beta*((a-Beta)/(a*(a+Beta))));
36
     if((b-a) == 0.0001)
37
38
         break;
39
      end
40
      a=b;
41
      i=i+1;
42 end
   Z=approx(b,3)
43
44
  //\operatorname{Using} \operatorname{Eqn}(6.64) and \operatorname{eqn}(6.65)
45
  //(Hr/RT)=Z-1+[(d ln(alpha_Tr)/d ln Tr)-1]qI
                                                          I=ln
      ((Z+beta)/Z) d ln(alpha_Tr)/d ln Tr=-0.5
  //Sr/R = ln (Z-beta) + [d ln (alpha_Tr)/d ln Tr] qI
                                                          I=ln
      ((Z+beta)/Z) d ln(alpha_Tr)/d ln Tr=-0.5
48 I = log((Z + Beta)/Z);
49 Hr = approx(R*T*(Z-1+((-0.5-1)*q*I)),0);
50 Sr=approx(R*(log(Z-Beta)+(-0.5*q*I)),3);
51
52 disp('Using Redlich/Kwong Equation')
53 disp('J/mol', Hr, 'Residual Enthalpy')
54 disp('J/mol/K',Sr,'Residual Entropy')
55
56 / End
```

Scilab code Exa 6.6 Find the State of Steam at the Exit Nozzle

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
6 A = round(V*10^n)/10^n; //V-Value n-To what place
```

```
funcprot(0)
8
  endfunction
10 //Example 6.6
11 //Caption: Program to Find the State of Steam at
      the Exit Nozzle
12
13 //Given values
14 P1=1000; // [KPa]
15 T=533.15; //[K]
16 P2=200; // [KPa]
17 \text{H1=2965.2;} // [\text{KJ/kg}] from Steam tables
18 S1=6.9680; //[KJ/Kg/K] From steam tables
19 S2=S1;
20 S_1=1.5301; // [KJ/Kg/K] Entropy Of Saturated Liquid
      @ 200KPa
                             Entropy Of Saturated vapor
21 S_v = 7.1268; //[KJ/Kg/K]
     @ 200KPa
22 H_1 = 504.7; //[KJ/Kg]
                             Enthalpy Of saturated liquid
       @ 200KPa
23 H_v = 2706.7; //[KJ/Kg]
                             Enthalpy Of saturated vapor
     @ 200KPa
24
25
26 //Solution
27 //find x_v from the eqn S=(1-x_v)S_l+x_c*S_v
28 \text{ x_v=approx}((S1-S_1)/(S_v-S_1),4);
29
30 //From Eqn (6.73 a)
31 H2 = ((1-x_v)*H_1)+(x_v*H_v);
32 del_H=approx(H2-H1,0); //[KJ/Kg]
33
34 disp('%',x_v*100,'Percent vapor')
35 disp('%',(1-x_v)*100, 'Percent Liquid')
36 disp('KJ/Kg',del_H,'Change In Enthalpy')
37
38 / End
```

Scilab code Exa 6.7 Find how much Energy must be Transferred

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
9
10 //Example 6.7
11 //Caption : Program to Find how much Energy must be
      Transferred to the Tank
12
13 //Given values (from steam tables)
14 H=293; //[KJ/Kg]
                    at 343.15K
15 H_{liquid} = 419.1; // [KJ/Kg]
                                at 373.15K
16 H_vapor=2676; //[KJ/Kg] at 373.15K
17 V_{vapor}=1.5; // [m^3]
18 m1_liquid=500; // [Kg]
19 rho_liquid=0.001044; //[m^3/Kg]
20 rho_vapor=1.673; // [m^3/Kg]
21 del_m=750; //[Kg]
22
23 //using the eqn Q=(m2H2) tank - (m1H1) tank - (H*del_m)
24 m1_vapor=(V_vapor-(m1_liquid*rho_liquid))/rho_vapor;
25 / \text{Term} 2 = ((\text{m}1\text{H}1) \text{tank})
26 Term2=(m1_liquid*H_liquid)+(m1_vapor*H_vapor);
27 mT=m1_liquid+del_m+m1_vapor;
28 //Solving Eqn By matrix Method
```

```
29 //m_vapor+m_liquid=mT and (rho_vapor*m_vapor)+(
      rho_liquid *rho_vapor)=V_vapor
30 A=[1,1;rho_vapor,rho_liquid];
31 B=[mT; V_vapor];
32 \quad X = inv(A) *B;
33 \text{ m2\_vapor} = X(1,1);
34 m2_liquid=X(2,1);
35
36 Term1=(m2_liquid*H_liquid)+(m2_vapor*H_vapor);
37 Q=approx(Term1-Term2-del_m*H,0);
38
39 disp('KJ',Q,'Heat Required')
40 disp('Note: The Answer Varies With That of The Book
      because the calculations as in Book do not give
      the Answer the Book results')
41 / End
```

Scilab code Exa 6.8 Find V U S and H fo 1 butene

```
1 clear;
2 clc;
3
4 //Example 6.8
5 //Caption: Program to Find V U S and H fo 1-butene
6
7 //To find Approx Value
8 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
9
10
     funcprot(0)
11 endfunction
12
13 function [Q] = SRB (Tr, Pr, omega)
14
     B0=0.083-(0.422/(Tr^1.6));
```

```
15
     diffr_B0=0.675/(Tr^2.6);//dB0/dTr
16
     B1=0.139-(0.172/(Tr^4.2));
     diffr_B1=0.722/(Tr^5.2);//dB0/dTr
17
     Q=-Pr*(diffr_B0+(omega*diffr_B1));
18
19
     funcprot(0);
20 endfunction
21
22 function[H]=HRB(Tr,Pr,omega)
23
     B0=0.083-(0.422/(Tr^1.6));
24
     diffr_B0=0.675/(Tr^2.6);//dB0/dTr
     B1=0.139-(0.172/(Tr^4.2));
25
     diffr_B1=0.722/(Tr^5.2);//dB0/dTr
27
     H=Pr*(B0-(Tr*diffr_B0)+(omega*(B1-(Tr*diffr_B1))))
28
     funcprot(0);
29 endfunction
30
31 function[Q]=ICPS(T0,T,A,B,C,D)
32
     t=T/T0;
     Q = ((A) * \log(t)) + (((B*T0) + (((C*T0*T0) + (D/(t*t*T0*T0)))))
33
        ))*(t+1)/2))*(t-1))
34
     funcprot(0);
35 endfunction
36
37 \quad function[Q] = ICPH(TO, T, A, B, C, D)
38
     t=T/T0;
39
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
        /(t*T0*T0)))*(T-T0)
     funcprot(0);
40
41 endfunction
42
43 //Example 6.8
44 //Caption : Program to Find V U S and H fo 1-butene
45
46 // Given values (from steam tables)
47 Tc = 420; //[K]
48 Pc = 40.43; // [bar]
49 \text{ omega=0.191};
```

```
50 \text{ Tn} = 266.9; //[K]
51 \quad A0 = 1.967;
52 B0=31.630*10^-3;
53 \quad C0 = -9.837 * 10^{-6};
54 D0 = 0;
55 \text{ T1} = 473.15; //[K]
56 P = 70; // [bar]
57 R=8.314;
58 //From Table (E.3) And Table (E.4)
59 \quad Z0 = 0.485;
60 \quad Z1 = 0.142;
61
62 \text{ Tr}=\text{T1}/\text{Tc};
63 \text{ Pr=P/Pc};
64 \quad Z=Z0+(omega*Z1);
65 V = approx((Z*R*T1*10^-2)/P,4); // [m^3/Kmol]
66
67 //step(a) vaporization at T1 and P1=P_saturated
68 //using eqn (6.70) ln P_sat=A-(B/T)
69 // Solving eqn \ln (1.0133) = A - (B/266.9) and \ln (40.43) = A
       -(B/420)
70 a=[1,(-1/266.9);1,(-1/420)];
71 b = [\log(1.0133); \log(40.43)];
72 x = (a^-1*b);
73 A = x(1,1);
74 B=x(2,1);
75 // using eqn(4.12)
                          del_H n / RTn = 1.092 * (ln Pc - 1.013)
       /(0.930 - Tr_n)
76 Tr_n=Tn/Tc;
77 del_Hn=R*Tn*(1.092*(\log(Pc)-1.013)/(0.93-Tr_n));//[J
      /mol]
78 T2=273.15; //[K]
79 Tr=T2/Tc;
80 //Using Eqn (4.13) del_H/del_Hn = ((1-Tr)/(1-Tr_n))
       ^0.38
81 del_H_a=del_Hn*((1-Tr)/(1-Tr_n))^0.38;
82 del_S_a=approx(del_H_a/T2,2);
83
```

```
84 //Step(b) transition to ideal gas State at (T1, P1)
 85 P_{\text{sat}} = \exp(A - (B/273.15));
 86 Pr=P_sat/Pc;
 87 \text{ Tr}=T2/Tc;
 88 Hr_b=approx(R*Tc*HRB(Tr,Pr,omega),0)//[J/mol]
 89 Sr_b = approx(R*SRB(Tr, Pr, omega), 2) // [J/mol/K]
 90
 91 //Step(c) Change to (T2, P2) in ideal-gas state
 92
 93 H_c=approx(R*ICPH(T2,T1,A0,B0,C0,D0),0); //[J/mol]
 94 S=R*ICPS (T2, T1, A0, B0, C0, D0); //[J/mol/K]
 95 del_S_c=approx(S-(R*log(P/P_sat)),2); //[J/mol/K]
 96
 97 //Step(d) Transition to actual final state at (T2, P2)
98 //Using eqn (6.76) and eqn (6.77)
99 //Hr/RTc=Hr0/RTc+(omega*Hr1/RTc)
100 //Sr/R = Sr0/R + (omega*Sr1/R) Sr0, Sr1 from Tables (E.5)
101 \text{ Tr}=T1/Tc;
102 \text{ Pr=P/Pc};
103 Hr_d=R*Tc*(-2.294+(omega*-0.713));
104 \text{ Sr_d=R*(-1.566+(omega*-0.726))};
105
106 \text{ H=approx}(del_H_a-Hr_b+H_c+Hr_d,0);
107 S=approx(del_S_a-Sr_b+del_S_c+Sr_d,2);
108 U = approx(H - (P*V*10^2), 0);
109
110 \operatorname{disp}('\operatorname{m}^3/\operatorname{Kmol}', V, '\operatorname{Volume}(V)=')
111 \operatorname{disp}('J/\operatorname{mol}', U, '\operatorname{Internal energy}(U)=')
112 \operatorname{disp}('J/\operatorname{mol}', H, '\operatorname{Enthalpy}(H)=')
113 \operatorname{disp}('J/\operatorname{mol}/K',S,'\operatorname{Entropy}(S)=')
114
115
    disp ('Note: The Answer here Slightly Varies with
        That of Book because of the different
        approximation')
116
117 / End
```

Scilab code Exa 6.9 Find Residual Enthalpy and Entropy and V

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
7
     funcprot(0)
   endfunction
9
10
11 //Example 6.9
12 //Caption : Program to Find Residual Enthalpy and
      Entropy and V by Lee/Kesler
13
14
15 //Given Values
16 T=450; //[K]
17 P=140; // [bar]
18
19 //pseudo parameters
20 Tc1=304.2; //[K]
21 Tc2=369.8; //[K]
22 Pc1=73.83; // [bar]
23 Pc2=42.48; //[bar]
24 Tpc = (0.5*Tc1) + (0.5*Tc2);
25 Ppc = (0.5*Pc1) + (0.5*Pc2);
26
27 Tpr=T/Tpc;
28 Ppr=P/Ppc;
29
```

```
30 \quad Z0 = 0.697;
31 \quad Z1 = 0.205;
32
33 \text{ omega1=0.224};
34 \text{ omega2=0.152};
35 omega=(0.5*omega1)+(0.5*omega2);
36
37 \quad Z=Z0+(omega*Z1);
38
39 V = approx(Z*R*T*10/P,1); //[cm^3/mol]
40
41 //(H/RT)0 = -1.73 (H/RT)1 = -0.169
42 H=approx(R*Tpc*(-1.73+(omega*-0.169)),0);//[J/mol]
43 S=approx(R*(-0.967+(omega*-0.330)),2);//[J/mol/K]
44
45 \operatorname{disp}(\operatorname{'cm}^3/\operatorname{mol'}, V, \operatorname{'Volume}(V)=\operatorname{'})
46 disp('J/mol', H, 'Residual Enthaply(H)=')
47 \operatorname{disp}('J/\operatorname{mol}/K',S,'\operatorname{Residual Entropy}(S)=')
48
49 //End
```

Chapter 7

Applications Of Thermodynamics To Flow Process

Scilab code Exa 7.2 Find the Ratio of Area in a Nozzle

```
15 T=573.15; //[K]
16 P = [700,600,500,400,300,200]; // [KPa]
17 // values for H, V, S for various P from steam tables
18 H=[3059.8,3020.4,2975.71,2923.5,2859.9,2777.35];//[
      KJ/Kg]
19 V = [371.39, 418.25, 481.26, 571.23, 711.93, 970.04]; // [cm]
      ^3/g
20 S=7.29997*ones(1,6); //[KJ/Kg/K] Isentropic
21 u0=30; //[m/s]
22 \ u=zeros(1,6);
23
24 // Using Eq (7.3)
25 / u^2 = u1^2 - 2(H-H1)
u = approx(sqrt((u0^2-2*(H-H(1))*10.^3)),1);
27
28 // \text{Using Eq}(2.27)
29 //A/A1 = u1 *V/V1 * u;
30 c=u(1)./V(1);
31 K = approx((c*V./u),3); //K = A/A1 c = u1/V1
32
33 Ans=[P',V',u',K'];
34 disp(Ans, 'P/[KPa] V/[cm^3/g] u/[m/s] A/A1')
35
36 / End
```

Scilab code Exa 7.3 Find Critical Pressure and Discharge Pressure

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
6 A = round(V*10^n)/10^n; //V-Value n-To what place
```

```
funcprot(0)
7
8
   endfunction
9
10
11 //Example 7.3
12 //Caption : Program to Find the Critical Pressure
      and the Discharge Pressure
13
14 //Given Values
15 T1 = 573.15; //[K]
16 R=8314;
17 P1=700; // [KPa]
18 \quad M = 18.015;
19 Gamma=1.3;
20 \text{ u0=30; } //[\text{m/s}]
21
22 / (a)
23 // \text{Using Eqn} (7.12)
24 / K = P2/P1 = (2/(Gamma+1)) (Gamma/(Gamma-1))
25 K = approx((2/(Gamma+1))^(Gamma/(Gamma-1)), 2); //
      rounding to 2 decimal places
26
27 P1V1=round (R*T1/M); //\text{m}^2/\text{s}^2
28 // \text{Using Eqn} (7.11)
29 //u_throat^2=u^2+2(Gamma)(P1V1)/(Gamma-1)[1-(P2/P1)]
      ((Gamma-1)/Gamma))
30 u_{throat} = approx(sqrt(u0^2+((2*Gamma*P1V1/(Gamma-1)))
      *(1-(K^((Gamma-1)/Gamma))))),2);
31
32 disp(K, '(a) Critical Pressure ratio (P2/P1)')
33 disp(' m/s',u_throat,' Velocity at the throat')
34
\frac{35}{(b)} Mach No 2.0
36 \quad u=2*u\_throat;
37 K=(1-((u^2-u0^2)*(Gamma-1)/(2*Gamma*P1V1)))^(Gamma/(
      Gamma-1)); //K=P2/P1
38 P2=round(K*P1);
39
```

Scilab code Exa 7.4 Find the final Temperature and its Entropy change

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
  endfunction
8
10 function[H]=HRB(Tr,Pr,omega)
11
     B0=0.083-(0.422/(Tr^1.6));
12
     diffr_B0=0.675/(Tr^2.6); //dB0/dTr
     B1=0.139-(0.172/(Tr^4.2));
13
     diffr_B1=0.722/(Tr^5.2); //dB0/dTr
14
     H=Pr*(B0-(Tr*diffr_B0)+(omega*(B1-(Tr*diffr_B1))))
15
16
     funcprot(0);
17 endfunction
18
19 function[Q]=SRB(Tr,Pr,omega)
20
     B0=0.083-(0.422/(Tr^1.6));
21
     diffr_B0=0.675/(Tr^2.6);//dB0/dTr
     B1=0.139-(0.172/(Tr^4.2));
22
23
     diffr_B1=0.722/(Tr^5.2);//dB0/dTr
24
     Q=-Pr*(diffr_B0+(omega*diffr_B1));
     funcprot(0);
25
```

```
26 endfunction
27
28 //Example 7.4
29 //Caption: Program to Find the final Temperature
      and its Entropy change
30
31 //Given Values
32 P1=20; // [bar]
33 T=400; //[K]
34 P2=1; //[bar]
35 R=8.314;
36
37 // Solution
38
39 // using Eq(6.84)
40 // del_H = Cp(T2-T1) + Hr2 - Hr1 = 0 but Hr2 = 0
41 //T2 = Hr1/Cp + T1
42 Tc=369.8; //[K]
43 Pc = 42.48; //[bar]
44 \text{ omega=0.152};
45 \text{ a=T}; //Initial
46 \text{ for } i=1:2
47
     Tr=a/Tc
     Pr=P1/Pc;
48
49
     Hr1=R*Tc*HRB(Tr,Pr,omega);//[J/mol]
     Cp=R*(1.213+(28.785*10^-3*a)-(8.824*10^-6*a*a));//
50
         [J/mol/K]
     T2=(Hr1/Cp)+a;
51
     Tm = (a+T2)/2;
52
53
     i=i+1;
54
     a = Tm;
55 end
56 \text{ Tm}=a;
57 T2 = round(Tm) / [K]
58 \text{ Tr}=T/Tc;
59 Sr=R*SRB(Tr,Pr,omega);
60
61 del_S=approx((Cp*log(T2/T))-(R*log(P2/P1))-Sr,2);
```

```
62
63 disp('J/mol/K',del_S, 'Entropy')
64 disp('Positive Entropy represents the
        irreversibility of Throttling Process')
65 disp('K',T2, 'Final Temperature')
66
67 //End
```

Scilab code Exa 7.6 Find the state of Steam at Discharge and Mass Rate

```
1 clear;
2 clc;
4 //To find Approx Value
  function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
  endfunction
10 //Example 7.6
11 //Caption: Program to Find the state of Steam at
      Discharge & Mass Rate of Flow
12
13 // Given Values
14 P1=8600; // [KPa]
15 T1 = 773.15; //[K]
16 //values of Enthalpy and Entropy from Steam tables
17 H1=3391.6; //[KJ/Kg]
18 S1=6.6858; //[KJ/Kg/K]
19 eta=0.75;
20 P2=10000; // [KPa]
21 rW=56400; // [KW] or [KJ/s]
22 S2i=S1; // Isentropic
```

```
23
24 S2_liquid=0.6493;
25 S2_vapor=8.1511;
26 H2_liquid=191.8;
27 H2_vapor=2584.8;
28
29 x2=(S2i-S2_liquid)/(S2_vapor-S2_liquid);
30
31 H2i=H2_liquid+(x2*(H2_vapor-H2_liquid));
32 \text{ del_Hs=H2i-H1;} // [KJ/Kg]
33 del_H=eta*del_Hs;
34
35 H2=approx(H1+del_H,0);//[KJ/Kg]
36 \text{ x2}=(\text{H2}-\text{H2}\_\text{liquid})/(\text{H2}\_\text{vapor}-\text{H2}\_\text{liquid});
37 \quad S2=approx(S2\_liquid+(x2*(S2\_vapor-S2\_liquid)),4);
38
39 rm=approx(-rW/(H2-H1),2);//[Kg/s]
40 disp('KJ/Kg', H2, 'Enthalpy')
41 disp('KJ/Kg/K',S2,'Entropy')
42 disp('Kg/s',rm,'Rate of mass change')
43
44 / End
```

Scilab code Exa 7.7 Find the isentropic Work Produced

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
```

```
9
10 function [Q] = MCPS (TO, T, A, B, C, D)
     t=T/T0;
11
     Q = (A) + (((B*T0) + (((C*T0*T0) + (D/(t*t*T0*T0))) * (t+1)
12
        /2))*((t-1)/log(t)))
13
     funcprot(0);
14 endfunction
15
16 function[Q]=MCPH(TO,T,A,B,C,D)
     t=T/T0;
17
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
18
        /(t*T0*T0)))
19
     funcprot(0);
20 endfunction
21
22 function[H]=HRB(Tr,Pr,omega)
     B0=0.083-(0.422/(Tr^1.6));
23
24
     diffr_B0=0.675/(Tr^2.6); //dB0/dTr
     B1=0.139-(0.172/(Tr^4.2));
25
     diffr_B1=0.722/(Tr^5.2);//dB0/dTr
26
27
     H=Pr*(B0-(Tr*diffr_B0)+(omega*(B1-(Tr*diffr_B1))))
28
     funcprot(0);
29 endfunction
30
31 function [Q] = SRB (Tr, Pr, omega)
32
     B0=0.083-(0.422/(Tr^1.6));
33
     diffr_B0=0.675/(Tr^2.6);//dB0/dTr
34
     B1=0.139-(0.172/(Tr^4.2));
     diffr_B1=0.722/(Tr^5.2);//dB0/dTr
35
     Q=-Pr*(diffr_B0+(omega*diffr_B1));
36
37
     funcprot(0);
38 endfunction
39
40 //Example 7.7
41 //Caption : Program to Find the isentropic Work
      Produced
42
```

```
//Given Values
44
45 T1=573.15; //[K]
46 P1=45; //[bar]
47 P2=2; // [bar]
48 Tc = 282.3; //[K]
49 Pc = 50.4; //[bar]
50 \text{ omega} = 0.087;
51 \quad A = 1.424;
52 B=14.394*10^{-3};
53 C = -4.392*10^{-6};
54 D = 0;
55 R=8.314;
56
57 // \text{Using Eqn} (6.84)
58 // del_H = Cp + (T2-T1) + Hr2 - Hr1
59 // Using Eqn(6.85)
60 // del_S = Cp > s ln (T2/T1) - R*ln (P2/P1) + Sr2 - Sr1
61
62 //(a) equations for Ideal gas
63 //No residuals terms, whence
64
65 / del_H = Cp > h(T2-T1)
66 // del_S = Cp > s ln (T2/T1) - R*ln (P2/P1)
67
68 del_S=0//isentropic
69 //Whence K = \langle Cp \rangle s / R \ln (T2/T1) = \ln (P2/P1)
70 K = log(P2/P1);
71 // let c = \langle Cp \rangle s / R
72 //T2 = \exp(K/c + \ln(T1))
73 i = -1;
74 a=round(T1); // Initial
75 while (i==-1)
     b=MCPS(T1,a,A,B,C,D);
76
     temp = exp((K/b) + log(T1));
77
78
     flag=a-temp;
      if(flag<=0.1) then</pre>
79
80
        T2=a;
```

```
81
         i=1;
 82
       else
 83
         a=temp-0.1;
 84
         i = -1;
 85
       end
 86 \text{ end}
 87 disp('(a)by Equations for an Ideal gas')
 88 \operatorname{disp}('K', \operatorname{approx}(T2, 1), 'Temp = ')
 89 Cp_h=R*MCPH(T1, T2, A, B, C, D);
 90 del_Hs=Cp_h*(T2-T1);
 91 Ws_a=approx(del_Hs,0);
 92 disp('J/mol', Ws_a, 'Work')
93
 94 //(b)-Appropriate Generalized correlations
95
96 \text{ Tr1=T1/Tc};
97 Pr1=P1/Pc;
98
99 Hr1=R*Tc*HRB(Tr1,Pr1,omega); //[J/mol]
100 Sr1=R*SRB(Tr1,Pr1,omega); //[J/mol/K]
101
102 \text{ Tr}2=T2/Tc;
103 \text{ Pr2=P2/Pc};
104
105 \text{ Sr2=R*SRB}(\text{Tr2},\text{Pr2},\text{omega});
106
107 // \text{Using Eqn} (6.85)
108 // del_S = Cp > s ln (T2/T1) - R*ln (P2/P1) + Sr2 - Sr1
109 // del_S = 0 isentropic
110 / K = Cp > s ln (T2/T1) = Rln (P2/P1) - Sr2 + Sr1
111 K=R*log(P2/P1)-Sr2+Sr1;
112 //T2 = \exp((K/\langle Cp \rangle s) + \ln T1)
113 i = -1;
114 a=round(T1);//Initial
115 while (i == -1)
       b=R*MCPS(T1,a,A,B,C,D);
116
117
       temp = exp((K/b) + log(T1));
118
       flag=a-temp;
```

```
119
      if(flag<=0.1) then</pre>
120
        T2=a;
121
        i=1;
122
      else
123
        a=temp-0.1;
124
        i = -1;
125
      end
126 end
127
128 disp('(b)by Appropriate generalized correlations')
129 disp('K', approx(T2,1), 'Temp = ')
130 \text{ Tr}2=T2/Tc;
131
132 Sr2=R*SRB(Tr2,Pr2,omega);//[J/mol/K]
133 Hr2=R*Tc*HRB(Tr2,Pr2,omega);//[J/mol]
134 Cp_h=R*MCPH(T1,T2,A,B,C,D);
135 \text{ del_Hs=Cp_h*(T2-T1)+Hr2-Hr1;}
136 Ws_b=approx(del_Hs,-1);
137 disp('J/mol', Ws_b, 'Work')
138
139 //End
```

Scilab code Exa 7.8 Find the Work Required and Properties of Steam

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
```

```
10 //Example 7.8
11 //Caption: Program to Find the Work Required and
      Properties of Discharge Steam
12
13
  //Given Values
14
15 P1=100; //[KPa] (Tsat/tsat)=327.78K/99.63 'C)
16
17 //From Steam Tables @ 100KPa
18 S1=7.3598; //[KJ/Kg/K]
19 H1 = 2675.4; //[KJ/Kg]
20
21 P2=300; // [KPa]
22 //From Steam Tables @ 300KPa
23 S2=S1; // Isentropic
24 H2i=2888.8; //[KJ/Kg]
25
26 eta=0.75; // Efficiency
27
28 del_H=H2i-H1;
29 del_H=del_H/eta;
30 H2=approx(H1+del_H,1); //[KJ/Kg]
31
32 //From Steam Tables w.r.t H2
33 T2=519.25; //[K]
34 S2=7.5019; //[KJ/Kg/K]
35
36 Ws=approx(del_H,1); //[KJ/Kg]
                                   Work Reqd
37
38 disp('KJ/Kg', H2, 'Enthalpy')
39 disp('KJ/Kg/K',S2, 'Entropy')
40 disp('K',T2, 'Temperature')
41 disp('KJ/Kg', Ws, 'Work Done')
42
43 / End
```

Scilab code Exa 7.9 Find Work Required and Discharge Temperature

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
7
  endfunction
8
10 function[Q]=MCPH(TO,T,A,B,C,D)
11
     t=T/T0;
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
12
        /(t*T0*T0)))
13
     funcprot(0);
14 endfunction
15
16 function [Q] = MCPS (TO, T, A, B, C, D)
17
     t=T/T0;
18
     Q = (A) + (((B*T0) + (((C*T0*T0) + (D/(t*t*T0*T0)))*(t+1))
        /2))*((t-1)/log(t)))
19
     funcprot(0);
20 endfunction
21
22 //Example 7.9
23 //Caption : Program to Find Work Required and
      Discharge Temperature of Methane
24
25 // Given Values
26
27 R=8.314;
```

```
28 T1 = 293.15; //[K]
29
30 \text{ P1=140; } // \text{ [KPa]}
31 P2=560; // [KPa]
32
33 eta=0.75; // [Efficiency]
34 \quad A = 1.702;
35 B=9.081*10^{-3};
36 \quad C = -2.164*10^-6;
37 D=0;
38
39 i = -1;
40 a=round(T1);//Initial
41 while (i==-1)
42
     b = MCPS(T1,a,A,B,C,D);
43
     b=b^{-1};
     c=T1*((P2/P1)^b);
44
45
     flag=c-a;
     if (flag <= 0.0001) then
46
47
        T2i=a;
        i=1;
48
49
      else
50
        a=a+0.01;
51
        i = -1;
52
     end
53 end
54
55 Cps=R*MCPS(T1,T2i,A,B,C,D);
56 \text{ Cph=approx}(R*MCPH(T1,T2i,A,B,C,D),3);
57
58 / \text{from Eqn}(7.19)
59 Ws=approx(Cph*(T2i-T1),0)//[J/mol]
60 Ws=approx(Ws/eta,0)//Actual work
61 del_H=Ws;
62
63 //From eqn (7.21) Actual discharge Temperature
64 / T2 = T1 + (del_H/Cph)
65 i = -1;
```

```
66 a=round(T2i);//Initial
67 \text{ chk=1};
68 while (i==-1)
     b=R*MCPH(T2i,a,A,B,C,D);
69
70
     c=del_H/(a-T1);
71
     flag=c-b;
72
     if(flag<=0.001) then</pre>
73
         T2=a;
74
         i=1;
75
     else
76
         a=a+0.001;
77
         i = -1;
78
     end
79 end
80 Cph_T2=approx(R*MCPH(T2i,T2,A,B,C,D),2);
81 disp('K',T2, 'Temperature')
82 disp('J/mol/K',Cph_T2, 'Enthalpy')
83 disp('J/mol', Ws, 'Actual Work')
84
85 disp('Note: The answer in the Book varies with that
      of this code because the Calculation in the Book
      does not leads to the answer given')
86
87 / End
```

Scilab code Exa 7.10 Find Work Temperature Change and Entropy Change

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
```

```
funcprot(0)
8 endfunction
9
10 //Example 7.10
11 // Caption: Program to Find Work, Temperature Change
      and Entropy Change in Pump
12
13 //Given Values
14 T1=318.15; //[K]
15 P1=10; // [KPa]
16 P2=8600; // [KPa]
17 eta=0.75; // Efficiency
18
19 // Properties of saturated liquid water @ 318.15K
20 V = 1010; //[cm^3/Kg]
21 V=1010*10^{-6}; //[m^3/Kg]
22 Beta=425*10^-6; //[K^-1]
23 Cp=4.178; //[KJ/Kg/K]
24
25 //From Eqn (7.24)
26 Ws=V*(P2-P1); // [KPa m<sup>3</sup>/Kg]
27 del_H=Ws;
28 / \text{From Eqn}(7.17)
29 del_H=del_H/eta;
30 \text{ Ws=approx}(\text{del_H}, 2);
31
32 / \text{From Eqn} (7.25)
33 del_T=approx((del_H-(V*(1-(Beta*T1))*(P2-P1)))/Cp,2)
34
35 / \text{From Eqn} (7.26)
36 \quad T2=T1+del_T;
37 \text{ del_S=approx}(Cp*log(T2/T1)-(Beta*V*(P2-P1)),3);
38
39 disp('KJ/Kg', Ws, 'Work Done')
40 disp('K', del_T, 'Change in Temperature')
41 disp('KJ/Kg/K',del_S,'Change in Entropy')
42
```

43 //End

Chapter 8

Production Of Power From Heat

Scilab code Exa 8.1 Find the Thermal efficiency in a Steam Turbine

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
9
10 //Example 8.1
11 //Caption : Program to Find the Thermal efficiency in a Steam Turbine
12
13 //Given Values
14 //(a)-As in Example(7.6)
15 P1=8600;//[KPa]
16 T1=773.15;//[K]
```

```
17 //values of Enthalpy and Entropy from Steam tables
18 H1=3391.6; //[KJ/Kg]
19 S1=6.6858; //[KJ/Kg/K]
20
21 P2=10; // [KPa]
22 S2i=S1; // Isentropic
23
24 S2_liquid=0.6493;
25 S2_vapor=8.1511;
26 H2_liquid=191.8;
27 H2_vapor=2584.8;
28
29 x2=(S2i-S2_liquid)/(S2_vapor-S2_liquid);
30
31 H2i=H2\_liquid+(x2*(H2\_vapor-H2\_liquid));
32 del_Hs_1=approx((H2i-H1),1); //[KJ/Kg]
33 Ws=del_Hs_1;
34 H3i=H2i;
35 \text{ H4=H2\_liquid};
36 //Applying Eqn(8.2)
37 Q_condenser=approx((H4-H3i),1);//heat Of condenser
      |KJ/Kg|
38 //From Example (7.10)
39 // Properties of saturated liquid water @ 318.15K
40 V = 1010; // [cm^3/Kg]
41 V=1010*10^{-6}; //[m^3/Kg]
42 Beta=425*10^-6; //[K^-1]
43 Cp=4.178; //[KJ/Kg/K]
44
45 //From Eqn (7.24)
46 Ws_2=approx((V*(P1-P2)),1)//[KPa m^3/Kg]
47 \text{ del_Hs}_2 = Ws_2;
48 H1=H4+del_Hs_2;
49 //Enthalpy Of saturated steam at 8600KPa and 773.15K
50 H2=3391.6; //[KJ/Kg]
51 / Applying Eqn(8.2)
52 Q_boiler=H2-H1;
53
```

```
54 Ws_Rankine=-Q_boiler-Q_condenser;
55 eta=approx((abs(Ws_Rankine)/Q_boiler),3);
56 disp('(a) Rankine Cycle')
57 disp(eta, 'Thermal Efficiency')
58
59 //(b)
60
61 \text{ eta_b=0.75};
62
63 \text{ del_H_1=del_Hs_1*eta_b};
64 Ws_turbine=del_H_1;
65 \text{ H3=H2+del_H_1};
66 Q_condenser=H4-H3;
67
68 //By Example 7.10 for the pump
69 Ws_pump=del_Hs_2/eta_b;
70 del_H_2=Ws_pump;
71 Ws_net=Ws_turbine+Ws_pump;
72 \text{ H1=H4+del_H_2};
73
74 \quad Q_boiler=H2-H1;
75 efficiency=approx(abs(Ws_net)/Q_boiler,4);
76 disp('(b) Practical cycle with 0.75 efficiency')
77 disp(efficiency, 'Thermal Efficiency')
78
79 //(c)
80 //By rating of Power Cycle
81 rWs_net=-80000; //[KJ/s] Power Rating
82 rm=approx(rWs_net/Ws_net,2);
83
84 rQ_boiler=approx(rm*Q_boiler/1000,1); // [MW]
85 rQ_condenser=approx(rm*Q_condenser/1000,1); // [MW]
86 disp('(c)By rating of Power Cycle');
87 disp('kg/s',rm,'Steam Rate')
88 disp('MW',rQ_boiler,'Heat Transfer rate in boiler')
89 disp('MW',rQ_condenser,'Heat Transfer rate in
      condenser')
90
```

Scilab code Exa 8.4 Find the Efficiency in a Gas Turbine

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8
  endfunction
10 //Example 8.4
11 //Caption : Program to Find the Efficiency in
      Various Cycles in a Gas turbine
12
13 //Given Values
14 K=6; //Pb/Pa
15 T1 = 298.15; //[K]
16 Tmax = 1033.15; //[K]
17 Gamma=1.4;
18
19 / (a)
          Gamma = 1.4
20 //From Eqn (8.12)
21 eta_a=approx(1-((1/K)^((Gamma-1)/Gamma)),1);
22 disp('(a) Efficiency of an ideal air cycle')
23 disp(eta_a, 'Efficiency')
24
25 //(b)  eta_c = 0.83
                      eta_t = 0.86
26 \text{ eta_c=0.83};
27 eta_t=0.86;
28 K2=Tmax/T1;
```

```
29 alpha=(K)^((Gamma-1)/Gamma);
30
31 //Using Eqn(8.13)
32 eta_b=approx(((eta_t*eta_c*K2*(1-(1/alpha)))-(alpha_-1))/((eta_c*(K2-1))-(alpha-1)),3);
33 disp('(b)Thermal efficiency of an air cycle if the Compressor and Turbine Operate adiabatically')
34 disp(eta_b,'Thermal efficiency')
35
36 //End
```

Chapter 9

Refrigerator And Liquifaction

Scilab code Exa 9.1 Find the COP of a Refrigerator

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
  endfunction
10 / \text{Example } 9.1
11 //Caption : Program to Find the COP of a
      Refrigerator
12
13 //Given Values
14 T1=261.15; //[K]
                    Temgerature of refrigerated space
15 T2 = 294.15; //[K]
                    Temperature of cooling water
16 dT = 5.6; //[K]
                    Temperature Difference
17 Qc=35.2; //[kW]
                    Refrigerant Capacity
18 eta=0.8; // Efficeincy (b)
```

```
19
20 //(a) Carnot Refrigerator
21 \text{ Tc=T1-dT};
22 Th = T2 + dT;
23 // \text{Using Eqn} (9.3)
24 w=approx(Tc/(Th-Tc),2);
25 disp(w,'(a) Coefficient of Performance for Carnot
      Refrigerator')
26
           Vapor Compression Cycle
27 //(b)
28
29 //From Table (9.1)
30 / @ Tc = 255.55K
31 H2=388.13; //[KJ/Kg]
32 S2=1.7396; //[KJ/Kg/K]
33
34 / @ Th = 299.75K
35 H4 = 236.76; //[KJ/Kg]
36
37 S3=S2; // Isentropic
38 //Hence
39 H3=420.27; //[KJ/Kg]
40 / \text{Step } 2 \longrightarrow 3
41 del_Hs=H3-H2;
42 //But Compressor Efficiency = 0.80
43 del_Hs=del_Hs/eta
44 / \text{Step } 1 \longrightarrow 4
45 H1=H4; //isenthalpic
46 w=approx((H2-H4)/del_Hs,2);
47 disp(w, '(b) Coefficient of Performance for Vapor
      Compression Cycle')
48 rm=approx(Qc/(H2-H4),4);//[Kg/s]
49 disp('kg/s',rm,'Circulation rate');
50
51 / End
```

Scilab code Exa 9.2 Find Power Requirement For Various seasons

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
9
10 / \text{Example } 9.2
11 //Caption : Program to Find Power Requirement For
      Various seasons
12
13 // Given Values
14 Qh_Winter=30; // [KW]
15 Qc_Summer=60; // [KW]
16 Tc_Winter=283.15; //[K]
17 Th_Winter=303.15; //[K]
18 Tc_Summer = 278.15; //[K]
19 Th_Summer = 298.15; //[K]
20
21 // For WINTER's
22 // Using Eqn (5.7)
23 Qc_Winter=Qh_Winter*(Tc_Winter/Th_Winter);
24 // Using Eqn(9.1)
25 W_Winter=approx((Qh_Winter-Qc_Winter),2);//[KW]
26 disp('KW', W_Winter, 'Power Requirement for WINTER''s'
      )
27
28 //For SUMMER's
```

Scilab code Exa 9.3 Find the Temperature of the High Pressure steam

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
  endfunction
10 //Example 9.3
11 //Caption: Program to Find the Temperature of the
     High Pressure steam
12
13
  //Given Values
14
15 x = 0.25;
16 //For Superheated Methane
17 //By Perry and Green by linear interpolation
18 H4=1140; // [KJ/Kg] @ 300K and 60 Bar
19 H15=1188.9; // [KJ/Kg] @ 295K and 1 Bar
20 //By interpolation based on lnP
21 T_sat=111.5; //[K]
22 H9 = 285.4; //[KJ/Kg]
                        Saturated Liquid
```

```
23 H12=769.9; // [KJ/Kg] Saturated Vapor
24 S12=9.521; // [KJ/Kg/K] Saturated vapor
25
26 T5 = 253.6; //[K]
27 H5=1009.8; // [KJ/Kg] @ 60 Bar
28
29 //From Eqn (9.7)
30 z=((x*(H12-H5))+H4-H15)/(H9-H15);
31
32 H14 = ((H5 - H4)/(1-z)) + H15; //[KJ/Kg]
33 //Whence
34 T14=227.2; // [K] @ 1Bar
35
36 \text{ H7=H5-((1-z)/(1-x)*(H14-H12));}/[KJ/Kg]
37 T7=197.6; //[K] @ 60Bar
38
39 //From Eqn (9.8)
40 z=approx((H4-H15)/(H9-H15),4);
41
42 H7 = H4 - ((1-z)*(H15-H12));
43 T7=206.6; //[K]
44
45 disp('%',z*100, 'Fraction of methane liquefied')
46 disp('K', T7, 'Temperature of High Pressure steam
      entering the throttle valve')
47
48 / End
```

Chapter 10

Vapor Liquid Equillibrium Introduction

Scilab code Exa 10.1 Plot the Graphs of P vs x1 y1 and t vs x1 y1

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
10 //Example 10.1
11 //Caption : Program to Plot the Graphs of P vs x1, y1
       and t vs x1, y1
12
13 // Antoinie Equations
14
15 //\ln P1_sat = 14.2724 - (2945.47/(T-49.15))
                                               [KPa]
16 //\ln P2_sat = 14.2043 - (2972.64/(T-64.15))
                                               [KPa]
```

```
17
   //(a) Graph Showing P vs x1 and P vs y1 for T=348.15
18
      K
19 T = 348.15; //[K]
20 //using BUBL P calculations
21
22 // Calculation of P1_sat and P2_sat at T=348.15K
23 P1_sat=approx(exp(14.2724-(2945.47/(T-49.15))),2)
      //KPa
24 P2_sat=approx(exp(14.2043-(2972.64/(T-64.15))),2)
       //KPa
25
26 //U \operatorname{sing} \operatorname{Eqn} P = P2 \operatorname{sat} + (P1 \operatorname{sat} - P2 \operatorname{sat}) x1
27
28 \quad x = [0:0.2:1];
29 P=approx(P2_sat+((P1_sat-P2_sat)*x),2);
30 \text{ y=approx}(x*P1\_sat./P,4);
31
32 disp('Explanations Of graph')
33
34 Ans=[x', y', P'];
35 disp(Ans, 'x1
                                       P/PKa')
                             y1
36
37 \text{ y} 1 = 0.6;
38 y2=1-y1;
39 P_{dew=approx}(1/((y1/P1_sat)+(y2/P2_sat)),2)
40 	ext{ x1=approx}(y1*P_dew/P1_sat,4)
41
42 // Plotting the graph
43 subplot (1,2,1);
44 T = 348.15; //[K]
45
46 P1_sat=approx(exp(14.2724-(2945.47/(T-49.15))),2)
      //KPa
47 P2_sat=approx(exp(14.2043-(2972.64/(T-64.15))),2)
       //KPa
48
49 x = [0:0.2:1];
```

```
50 P=approx(P2\_sat+((P1\_sat-P2\_sat)*x),2);
51 \text{ y=approx}(x*P1\_sat./P,4);
52
53 mtlb_axis('auto');
54 plot(x,P,'g-') //P vs x1
55 plot(y,P,'b-') //P vs y1
56 x = [0, 0.1];
57 P=[P2_sat, P2_sat];
58 plot(x,P,'--') //P2_sat
59 x = [0.9, 1];
60 P=[P1_sat,P1_sat];
61 plot(x,P,'r--') //P1_sat
62
63 \times 1 = 0.6;
64 P_b=approx(P2_sat+((P1_sat-P2_sat)*x1),2);
65 y1=approx(x1*P1_sat/P_b,4);
66 x = [x1, y1];
67 P = [P_b, P_b];
68 plot(x,P,'bo-') //b-b'
69
70 y1=0.6;
71 y2=1-y1;
72 P_c = approx(1/((y1/P1_sat)+(y2/P2_sat)),2)
73 x1=approx(y1*P_c/P1_sat,4)
74
75 x = [x1, y1];
76 P = [P_c, P_c];
77 plot(x,P,'ro-') //c'--c
78
79 P = [(P_b+10), P_b, P_c, (P_c-10)];
80 x = [0.6, 0.6, 0.6, 0.6];
81 plot(x,P,'go-') //a-b-c-d-0.6
82
83 P = [(P_c - 10), 30];
84 x = [0.6, 0.6];
85 plot(x,P,'yo—')
86
87 P = [110, 80];
```

```
88 x = [0.6, 0.6];
89 plot(x,P,'w')
90 legend('P vs x1(Liquid)', 'P vs y1(Vapor)', 'P2_sat', '
       P1_sat', "b--b'', ", "c'', -c", 'a--b--c--d--0.6')
91 xtitle ('(a)T/t=348.15K', 'x1,y1', 'P/Kpa')
92
93 disp("This is the liquid-phase composition at point
      c', ")
94
95 //(b) Graph showing (t vs x1) and (t vs y1) for a
       pressure of 70KPa
96 //Example 10.2(b)
97 P=70; // [KPa]
98
99 T1_sat = approx(2945.47/(14.2724 - log(P)) + 49.15, 2);
100 T2_{sat} = approx(2972.64/(14.2043 - log(P)) + 64.15, 2);
101
102 T=[T1_sat,347.15,351.15,355.15,359.15,T2_sat];
103
104 P1_sat=approx(exp(14.2724-(2945.47./(T-49.15))),2);
       //KPa
105 P2_{sat} = approx(exp(14.2043 - (2972.64./(T-64.15))), 2);
        //KPa
106
107 \text{ x=approx}((P-P2\_sat)./(P1\_sat-P2\_sat),3);
108 y=approx((x.*P1_sat)/P,3);
109
110 Ans=[x',y',T'];
111 disp(Ans, 'x1
                      y1 T/t(K/C')')
112
113 // at x1 = 0.6;
114 x1_b=0.6;
115 x2_b=1-x1_b;
116
117 T_a=347.15; // Intermediate Temperature (Point a in
       graph)
118 P1_sat_a=approx(exp(14.2724-(2945.47./(T_a-49.15)))
       ,2); //KPa
```

```
119 P2_{sat_a=approx(exp(14.2043-(2972.64./(T_a-64.15)))}
       ,2); //KPa
120 alpha=P1_sat_a/P2_sat_a; //Initial
121 a = T_a;
122 i = -1;
123 while (i==-1)
124
     P2_sat_b=P/((x1_b*alpha)+x2_b);
      b = approx(2972.64/(14.2043 - log(P2_sat_b)) + 64.15, 2);
125
126
      dT = abs(a-b);
127
      if(dT==0)
128
        i=0;
129
        T_b=b;
130
131
      alpha = exp(0.0681 - (2945.47/(b-49.15)) + (2972.64/(b-49.15))
         -64.15))); //Eqn C
132
      a=b;
133 end
134 P1_sat_b=approx(exp(14.2724-(2945.47./(T_b-49.15)))
       ,2); //KPa
135 y1_b = approx((x1_b*P1_sat_b)/P,4); //b
136
137 disp('K', T_b, 'Hence by iteration Temp(Temp at b) at
      x1 = 0.6 is ')
138 disp('KPa', P1_sat_b, 'Hence by iteration P1_sat at x1
       =0.6 is ')
139 disp(y1_b, 'Composition of Vapor(b') at x1=0.6')
140
141
142 / At y1 = 0.6
143 y1_c=0.6;
144 y2_c=1-y1_c;
145 T_d=355.15; // Intermediate Temperature (Point a in
       graph)
146 P1_sat_d=approx(exp(14.2724-(2945.47./(T_d-49.15)))
       ,2); //KPa
147 P2_sat_d=approx(exp(14.2043-(2972.64./(T_d-64.15)))
       ,2); //KPa
148 alpha=P1_sat_d/P2_sat_d; //Initial
```

```
149 d = T_d;
150 i = -1;
151 while (i==-1)
      P1_sat_c=P*(y1_c+(y2_c*alpha));
152
153
      c = approx(2945.47/(14.2724 - log(P1_sat_c)) + 49.15, 2);
154
      dT = abs(d-c);
      if(dT==0)
155
156
        i=0;
157
        T_c=c;
158
      alpha = exp(0.0681 - (2945.47/(c-49.15)) + (2972.64/(c-49.15)))
159
         -64.15))); //Eqn C
160
      d=c;
161 end
162 P1_sat_c=approx(exp(14.2724-(2945.47./(T_c-49.15)))
       ,2); //KPa
163 x1_c = approx((y1_c*P)/P1_sat_c, 4); //c
164
165 disp('K', T_c, 'Hence by iteration Temp(Temp at b) at
       y1 = 0.6 \text{ is '}
166 disp('KPa', P1_sat_c, 'Hence by iteration P1_sat at y1
       =0.6 \text{ is '}
167 disp(x1_c, 'Composition of liqud(c') at y1=0.6')
168
169 // Graph
170 subplot (1,2,2);
171 T=linspace(T1_sat, T2_sat, 10);
172
173 P1_sat=approx(exp(14.2724-(2945.47./(T-49.15))),2);
        //KPa
174 P2_{sat} = approx(exp(14.2043 - (2972.64./(T-64.15))), 2);
        //KPa
175
176 \text{ x=approx}((P-P2\_sat)./(P1\_sat-P2\_sat),3);
177 y = approx((x.*P1_sat)/P,3);
178
179 plot(x,T,'g-');
180 plot(y,T,'b-');
```

```
181
182 xsat = [0,0.1];
183  T2sat = [T2_sat, T2_sat];
184 plot(xsat, T2sat, '---') // T2_sat
185
186 \text{ xsat} = [0.9, 1];
187  T1sat = [T1_sat, T1_sat];
188 plot(xsat, T1sat, 'r—') // T1_sat
189
190 Tcc = [T_c, T_c];
191 xc = [x1_c, y1_c];
192 plot(xc,Tcc,'ro-') //c—c'
193
194 Tbb=[T_b, T_b];
195 xb = [x1_b, y1_b];
196 plot(xb, Tbb, 'bo-') //b—b'
197
198 Tabcd=[T_d, T_c, T_b, T_a];
199 xabcd = [0.6, 0.6, 0.6, 0.6];
200 plot(xabcd, Tabcd, 'go-') //a—b—c—d--0.6
201
202 Tao=[T_a,340];
203 \text{ xao} = [0.6, 0.6];
204 plot (xao, Tao, 'yo—')
   legend('T vs x1(Liquid)', 'T vs y1(Vapor)', 'T2_sat','
205
       T1_sat', "c''--c", "b--b'', ", 'd--c--b--a--0.6')
    xtitle('(b)P=70KPa', 'x1, y1', 'T(K)')
206
207
208 //End
```

Scilab code Exa 10.2 Find the Composition of the vapor and Liquid phase

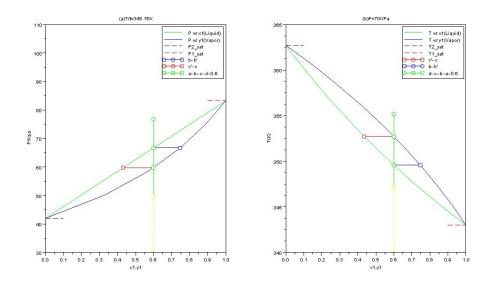


Figure 10.1: Plot the Graphs of P vs x1 y1 and t vs x1 y1

```
1 clear;
2 clc;
4 //To find Approx Value
  function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
   endfunction
9
10 //Example 10.2
11 // Caption: Program to Find the Composition of the
      vapor and Liquid phases
12
13 //Taking CO2 as Species 1 and Water as Species 2
14 H=990; // [Bar] Henry's Law const
15 T = 283.15; //[K]
16 P2_sat=0.01227; // [Bar] from Steam Tables
17 x1 = 0.01; //Assumed
18 	 x2=1-x1;
```

```
19 y1=1;
20 P=approx((x1*H)+(x2*P2_sat),3);
21 x1=approx((y1*P)/H,4);
22 x2=1-x1;
23 y2=approx((x2*P2_sat)/P,4);
24 y1=1-y2;
25 disp(x1, 'Composition in liquid Phase')
26 disp(y1, 'Composition in vapor Phase')
27 disp('Bar',P,'Pressure Exerted on Can')
28 disp('Hence Vapor phase chosen is nearly pure')
29
30 //End
```

Scilab code Exa 10.3 Find Pressure Temperature and Composition

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
10 //Example 10.3
11 //Caption : Program to Find Pressure, Temperature and
       Composition for a system
12
13 //Equations to be Used
14 // \ln v1 = A*(x2^2) \ln v2 = A*(x1^2) Where A
      =2.771-0.00523T
15
16 // Antoine Equations
```

```
17 / \ln P1_sat = 16.59158 - (3643.31/(T-33.424))
18 / \ln P2_sat = 14.25326 - (2665.54/(T-53.424))
19 / P = E(xi * Vi * Pi_sat) E—Summation
                                                         Eqn
      10.6
20 //P = 1/E(yi / (vi * Pi_sat)) E—Summation
                                                         Eqn
      10.7
21
\frac{22}{(a)} Calculate P and (yi), for T=318.15K and x1
      =0.25
23
24 //BULB P Calculation
25 T=318.15; // [K] Given
26 \text{ x1=0.25}; //Given
27 \times 2 = 1 - \times 1;
28 P1_sat = approx(exp(16.59158-(3643.31/(T-33.424)))
      ,2);//[KPa]
29 P2_sat = approx(exp(14.25326-(2665.54/(T-53.424)))
      ,2);//[KPa]
30 A = approx(2.771 - (0.00523*T), 3);
31 v1 = approx(exp(A*(x2^2)), 3);
32 v2=approx(exp(A*(x1^2)),3);
33
34 / \text{Form Eqn} (10.6)
35 P_a = approx((x1*v1*P1_sat)+(x2*v2*P2_sat),2); // [KPa]
36 \text{ y1}_a = \operatorname{approx}((x1*v1*P1_sat)/P_a,3);
37 \text{ y2}_a=approx((x2*v2*P2_sat)/P_a,3);
38
39 disp('(a)P) and [vi] for T=318.15K and x1=0.25')
40 disp('BUBL P calculations')
41 disp('KPa', P_a, 'P = ')
42 \text{ disp}(y1_a, 'y1 = ')
43 disp(y2_a, y2 = ')
44
45 //(b) Calculate P and (xi), for T=318.15K and y1
      =0.60
46
47 //DEW P calculation
48 \text{ y} 1 = 0.6;
```

```
49 \quad y2=1-y1;
50 T = 318.15; //[K]
51 \text{ P1\_sat} = \operatorname{approx}(\exp(16.59158 - (3643.31/(T-33.424)))
       ,2);//[KPa]
52 \text{ P2\_sat} = \operatorname{approx}(\exp(14.25326 - (2665.54/(T-53.424)))
       ,2);//[KPa]
53 A = approx(2.771 - (0.00523*T), 3);
v1 = 0.1; //Assumed
v2=0.1; //Assumed
56 \text{ a1=v1};
57 \text{ a}2=v2;
58 i = -1;
59 \text{ while}(i==-1)
     P = approx(1/((y1/(a1*P1_sat))+(y2/(a2*P2_sat))),2);
60
     x1=approx(y1*P/(a1*P1_sat),4);
61
     x2=1-x1;
62
     b1=approx(exp(A*(x2^2)),4);
63
     b2=approx(exp(A*(x1^2)),4);
64
     dt = abs(b1-a1);
65
     if(dt==0)
66
67
        i=0;
68
        v1 = b1;
69
        v2=b2;
70
        break;
71
      end
72
     a1=b1;
73
      a2=b2;
74 end
75 x1_b=x1;
76 	 x2_b=1-x1_b;
77 P_b = P;
78 v1_b=v1;
79 \quad v2_b = v2;
80 disp('(b)P and [xi] for T=318.15K and y1=0.60')
81 disp('DEW P calculations')
82 disp('kPa',P_b,'P = ')
83 disp(x1_b, 'x1 = ')
84 disp(x2_b, 'x2 = ')
```

```
85
   //(c) Calculate T and (yi) for P = 101.33 KPa and x1
       =0.85
87
88 //BUBL T calculation
89 P = 101.33;
90 \times 1 = 0.85;
91 \times 2 = 1 - \times 1;
92 T1_sat = approx((3643.31/(16.59158 - log(P))) + 33.424, 2);
93 T2_sat=approx((2665.54/(14.25326-log(P)))+53.424,2);
94 T=(x1*T1_sat)+(x2*T2_sat);
95 a=T; // Initial
96 i = -1;
97 while (i == -1)
      A = approx(2.771 - (0.00523*a), 4);
98
      v1=approx(exp(A*(x2^2)),4);
99
      v2=approx(exp(A*(x1^2)),4);
100
101
      P1_sat = approx(exp(16.59158-(3643.31/(a-33.424)))
          ,2);//[KPa]
      P2_sat = approx(exp(14.25326-(2665.54/(a-53.424)))
102
          ,2);//[KPa]
      alpha=P1_sat/P2_sat;
103
      P1_sat=approx(P/((x1*v1)+(x2*v2/alpha)),2);
104
105
      b = approx((3643.31/(16.59158 - log(P1_sat)))
          +33.424,2);
106
      dt=abs(b-a);
107
      if(dt==0)
108
         i=0;
109
         T=b;
110
         break;
111
      end
112
      a=b;
113 end
114 T_c = T;
115  y1_c=approx(x1*v1*P1_sat/P,3);
116 y2_c=1-y1_c;
117 \operatorname{disp}('(c)T \text{ and } [yi] \text{ for } P=101.33 \text{ kPa} \text{ and } x1=0.')
118 disp('BUBL T calculations')
```

```
119 disp('K',T_c, 'Temperature = ')
120 \text{ disp}(y1_c, 'y1 = ')
121 \text{ disp}(y2_c, 'y2 = ')
122
123 //(d) Calculate T and (xi) for P = 101.3 KPa and y1
       =0.4
124 P = 101.3;
125 \text{ y} 1 = 0.4;
126 \text{ y} 2 = 1 - \text{y} 1;
127 T1_{\text{sat}} = \operatorname{approx}((3643.31/(16.59158 - \log(P))) + 33.424, 2);
128 T2_{sat} = approx((2665.54/(14.25326 - log(P))) + 53.424, 2);
129 T=(y1*T1_sat)+(y2*T2_sat);
130 v1=1;
           //Initially
           //Initially
131 v2=1;
132 a=T; // Initial
133 i = -1;
134 while (i == -1)
      A = approx(2.771 - (0.00523*a), 4);
135
136
      P1_sat = approx(exp(16.59158-(3643.31/(a-33.424)))
          ,2);//[KPa]
      P2_sat = approx(exp(14.25326-(2665.54/(a-53.424)))
137
          ,2);//[KPa]
138
      alpha=P1_sat/P2_sat;
      x1=approx((y1*P)/(v1*P1_sat),4);
139
140
      x2=1-x1;
141
      v1=approx(exp(A*(x2^2)),4);
142
      v2=approx(exp(A*(x1^2)),4);
      P1_sat = P*((y1/v1) + (y2*alpha/v2));
143
144
      b = approx((3643.31/(16.59158 - log(P1_sat)))
          +33.424,2);
      dt = abs(a-b);
145
      if(dt==0)
146
147
         T=a;
148
         i=0;
149
         break;
150
      end
151
      a=b;
152 end
```

```
153 T_d=T;
154 x1_d=x1;
155 x2_d=x2;
156 disp('(d)T \text{ and } [xi] \text{ for } P=101.33 \text{ kPa} \text{ and } y1=0.40')
157 disp('DEW T calculations')
158 \operatorname{disp}('K',T,'T=')
159 disp(x1_d, 'x1 = ')
160 disp(x2_d, 'x2 = ')
161
162 / (e) \text{ Taz}, (xi_az) and (yi_az) for T = 318.15K
163 T = 318.15;
164 // Relative Volatility
                                 alpha_12 = (y1/x1)/(y2/x2)
165 //At Azeotrope y1=x1 and y2=x2 and alpha_12=1
166 \text{ P1\_sat} = \operatorname{approx}(\exp(16.59158 - (3643.31/(T-33.424))))
        ,2);//[KPa]
167 \text{ P2\_sat} = \operatorname{approx}(\exp(14.25326 - (2665.54/(T-53.424))))
        ,2);//[KPa]
168 //From eqn (10.5) alpha_12 = (v1*P1_sat)/(v2*P2_sat)
169 \text{ A=approx}(2.771-(0.00523*T),4);
170
171 //When x1=0 v2=1 and v1=\exp(A)
172 alpha_12_x10=P1_sat*exp(A)/P2_sat;
173
174 //When x1=1 v1=1 and v2=\exp(A)
175 alpha_12_x11=P1_sat/(P2_sat*exp(A));
176
   //But this is not Azeotrope (at Azeotrope alpha_12
       =1)
178
    //v1_az/v2_az = (P2_sat/P1_sat) = K
179
180 K=P2_sat/P1_sat;
181
182 / \ln (v1/v2) = \ln (K) = A(1 - (2*x1))
183 x1_az=approx((A-log(K))/(2*A),3);
184 \text{ x2_az=1-x1_az};
185 y1_az=x1_az;
186 \quad y2_az=x2_az;
187 v1_az=approx(exp(A*(x2_az^2)),3);
```

Scilab code Exa 10.4 Find the Dewpoint and Bubblepoint Pressure

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8
  endfunction
10 //Example 10.4
11 //Caption : Program To Find the Dewpoint and
      Bubblepoint Pressure
12
13 T=283.15; //[K]
14 //(a) Dew Point Pressure
15 //Species=[" Methane ";" Ethane ";" Propane "];
16 y = [0.1, 0.2, 0.7];
17
18 P1=6.9; // [bar]
19 K1 = [20, 3.25, 0.92];
```

```
20 x1 = approx(y./K1,3);
21
22 P2=10.34; //[bar]
23 K2 = [13.2, 2.25, 0.65];
24 \text{ x2=approx}(y./K2,3);
25
26 P3=8.7; // [bar]
27 \text{ K3} = [16, 2.65, 0.762];
28 x3 = approx(y./K3,3);
29
30 i = 1;
31 \quad j=1;
32 P = [P1, P2, P3];
33 x = [x1; x2; x3];
34 \text{ E1=zeros}(1,3);
35 for(i=1:3)
      for(j=1:3)
36
37
        E1(i)=E1(i)+x(i,j);//Summation
38
        //j = j + 1;
39
      end
      //i = i + 1;
40
41 end
42 P_{dew} = 8.7;
43 Ans=[y',K1',x1',K2',x2',K3',x3';1,0,E1(1),0,E1(2),0,
      E1(3)];
                                  P=6.9 bar
44 disp(
                                                     P = 10.34 \text{ bar}
           P = 8.7 \, \text{bar}')
                                      yi/Ki
45 \text{ disp}(Ans,')
                   уi
                             Ki
                                                  Ki
                                                           yi/Ki
            Κi
                      yi/Ki')
46 disp('Last Row Represents the summation')
47 disp('KPa', P_dew, 'The dew Point Pressure')
48
49 T = 283.15; //[K]
50 //(b) Bubble Point Pressure
51 // Species = [" Methane ";" Ethane ";" Propane "];
52 x = [0.1, 0.2, 0.7];
53
54 \text{ P1} = 26.2; // [bar]
```

```
55 \text{ K1} = [5.6, 1.11, 0.335];
56 \text{ y1=approx}(x.*K1,3);
57
58 P2=27.6; //[bar]
59 \text{ K2} = [5.25, 1.07, 0.32];
60 y2=approx(x.*K2,3);
61
62 P3=26.54; //[bar]
63 K3 = [5.49, 1.1, 0.33];
64 y3 = approx(x.*K3,3);
65
66 i = 1;
67 j = 1;
68 P = [P1, P2, P3];
69 y = [y1; y2; y3];
70 E2=zeros(1,3);
71 for(i=1:3)
72
     for(j=1:3)
        E2(i)=E2(i)+y(i,j);//Summation
73
74
        //j = j + 1;
75
     end
76
      //i=i+1;
77 end
78 \text{ P_Bubble} = 26.54;
79 Ans=[x',K1',y1',K2',y2',K3',y3';1,0,E2(1),0,E2(2),0,
      E2(3)];
80 disp(
                                 P=26.2 bar
                                                    P=27.6 bar
           P = 26.54 \text{ bar}'
81 disp(Ans,
                  хi
                            Κi
                                     xiKi
                                               Κi
                                                        xiKi
                     xiKi')
           Κi
82 disp('Last Row Represents the summation')
83 disp('KPa', P_Bubble, 'The Bubble Point Pressure')
84
85 / End
```

Scilab code Exa 10.5 Find L V xi and yi for a System

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
9
10 //Example 10.5
11 //Caption : Program to Find L V {xi} and {yi} for a
      System
12
13 z1=0.45;
14 z2=0.35;
15 z3=0.2;
16 P=110; // [KPa]
17 T=353.15; //[K]
18 P1_sat=195.75; // [KPa]
19 P2_sat = 97.84; //[KPa]
20 P3_sat=50.32; // [KPa]
21
22 //BUBL Calculation
23 \times 1 = z1;
24 x2=z2;
25 x3=z3;
26 P_BUBL = (x1*P1_sat) + (x2*P2_sat) + (x3*P3_sat);
27
28 //DEW Calculation
29 y1=z1;
```

```
30 \text{ y}2=z2;
31 y3=z3;
32 P_Dew=1/((y1/P1_sat)+(y2/P2_sat)+(y3/P3_sat));
33
34 // Since P_Bubl < P < P_dew
35 //Flash Calculation
36 K1=P1_sat/P;
37 \text{ K2=P2\_sat/P};
38 K3=P3_sat/P;
39
40 // Finding V from Eqn (10.17)
41 //E((zi*Ki)/(1+(V*(Ki-1))))=1
42
43 x = 0;
44 F_x = (((z_1 * K_1) / (1 + ((K_1 - 1) * x))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * x)))
        ))+((z3*K3)/(1+((K3-1)*x)))-1);
45 \quad F_a=F_x;
46
47 x = 0.9;
48 F_x = (((z_1 * K_1) / (1 + ((K_1 - 1) * x))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * x)))
         ))+((z3*K3)/(1+((K3-1)*x)))-1);
49 \quad F_b = F_x;
50 A = 0;
51 B=0.9;
52 i = 1;
53 while(i==1)
54
       a=A;
55
       F_a = (((z_1 * K_1) / (1 + ((K_1 - 1) * a))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * a))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * a))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * a)))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * a)))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * a)))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * a)))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * a)))))
            a)))+((z3*K3)/(1+((K3-1)*a)))-1);
56
       b=B;
       F_b = (((z_1 * K_1) / (1 + ((K_1 - 1) * b))) + ((z_2 * K_2) / (1 + ((K_2 - 1) * b))))
57
            b)))+((z3*K3)/(1+((K3-1)*b)))-1);
       x1=((a*F_b)-(b*F_a))/(F_b-F_a);
58
       F_x1 = (((z1*K1)/(1+((K1-1)*x1)))+((z2*K2)/(1+((K2-1)*x1)))
59
            -1)*x1)))+((z3*K3)/(1+((K3-1)*x1)))-1);
60
        if((F_a*F_x1)<0) then
61
62
           flag=1;
```

```
63
        A=a;
64
        B=x1;
      else((F_x1*F_b)<0)
65
66
        flag=2;
67
        A = x1;
68
        B=b;
69
      end
      x1_a=approx(x1,4);
70
      b_a = approx(b,4);
71
      a_a = approx(a,4);
72
73
      if(x1_a==b_a)
74
        V = approx(x1,4);
75
        i=0;
76
        break;
77
      elseif(x1_a==a_a)
        root=approx(x1,4);
78
79
        i=0;
80
        break;
81
      end
82
83 end
84 disp(V, 'Hence By solving the polynomial V = ')
85 L=1-V;
86 //from eqn 10.16
87 //yi = (zi*Ki)/(1+(V*(Ki-1)))
88 y1=approx((z1*K1)/(1+((K1-1)*V)),4);
89 y2=approx((z2*K2)/(1+((K2-1)*V)),4);
90 y3=approx((z3*K3)/(1+((K3-1)*V)),4);
91 	 x1 = approx(y1/K1,4);
92 \text{ x2=approx}(y2/K2,4);
93 \times 3 = approx(y3/K3,4);
94 y = [y1 y2 y3];
95 x = [x1 x2 x3];
96 disp(L, 'Moles Of liquid')
97 disp(V, 'Moles Of vapor')
98 disp(x, 'Mole fraction Of liquid')
99 disp(y, 'Mole fraction Of vapor')
100
```

Scilab code Exa 10.6 Find the Composition of Vapor and Liquid Phases

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8
  endfunction
10 //Example 10.6
11 //Caption : Program To Find the Composition of Vapor
       and Liquid Phases
12
13 // Given Values
14 z = [0.1, 0.2, 0.7];
15 K = [10, 1.76, 0.52];
16
17 V_01 = [0.1:0.1:1]
18 for(i=1:10)
19
     for(j=1:3)
20
       y_01(i,:) = approx((z.*K)./(1+(V_01(i)*(K-1))),3);
21
22
     Sum(i) = sum(y_01(i,:));
23 end
24
25 for (i=1:10)
26
     if (Sum(i+1)<1)</pre>
27
       a1=V_01(i);
28
       i = -1;
```

```
29
        break;
30
     end
31 end
32
33 V_001 = [a1:0.01:a1+0.1]
34 for (i=1:10)
     for (j=1:3)
35
        y_001(i,:) = approx((z.*K)./(1+(V_001(i)*(K-1)))
36
           ,3);
37
     end
     Sum(i) = sum(y_001(i,:));
38
39 end
40
41 for(i=1:10)
42
     if (Sum(i+1)<1)</pre>
        a01=V_001(i);
43
        i = -1;
44
        break;
45
46
     end
47 \text{ end}
48
49 V_0001 = [a01:0.001:a01+0.01];
50
51 for(i=1:10)
52
      for(j=1:3)
        y_0001(i,:) = approx((z.*K)./(1+(V_0001(i)*(K-1)))
53
           ,3);
54
55
     Sum(i) = sum(y_0001(i,:));
56 end
57
58 for (i=1:10)
      if (Sum(i+1)<1)</pre>
59
        a001=V_0001(i);
60
        i = -1;
61
62
        break;
63
     end
64 end
```

```
65 \text{ V=a001};
66 y_02 = approx((z.*K)./(1+(a1*(K-1))),3);
67 y_03 = approx((z.*K)./(1+((a1+0.1)*(K-1))),3);
68 y_0273 = approx((z.*K)./(1+(V*(K-1))),3);
69 x_0273 = approx(y_0273./K,3);
70
71 Ans=[z',K',y_02',y_03',y_0273',x_0273';1,0,sum(y_02)]
      , sum(y_03), sum(y_0273), approx(sum(x_0273), 2)];
72 disp(Ans, ' z
                          K
                                   y, V=0.2 y, V=0.3 y, V
      =0.273 \text{ x}, V=0.273')
73 disp('NOTE: Last Row represents the summation')
74 disp('Hence for V=0.273~E(yi)=0~and~E(xi)=0')
75 \operatorname{disp}(V, \operatorname{Yaction} \text{ of } \operatorname{Vapor} (V) = ')
76
77 //End
```

Chapter 11

Solution Thermodynamics Theroy

Scilab code Exa 11.4 Find the Expression For Enthalpies

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
10 //Example 11.4
11 //Caption : Program To Find the Expression For
      Enthalpies
12
  //H=400x1 + 600x2 + x1x2(40x1 + 20x2)
                                            Given
13
14
15 // Substituting x2=1-x1
```

```
17 H=poly([600 -180 0 -20], 'x1', 'c')
                                                  //(A)
18
  //K = dH/dx1
19
20
21 K = poly([-180 \ 0 \ -60], 'x1', 'c')
22
  //Using Eqn 11.15
23
                          H1=H+x2*K
24
25
   //substituting x2=1-x1
26
27 H1 = poly([420 \ 0 \ -60 \ 40], 'x1', 'c') //(B)
28
29 // Similarly for H2
30
31 H2=poly([600 0 0 40], 'x1', 'c')
                                                //(C)
32
33 //Now to calculate H1_inf and H2_inf
34
35 / x1 = 0 in (B)
36 H1_inf=420; //[J/mol]
37
38 //x2=0 in (C) i.e. x1=1
39 H2_{inf} = 640; //[J/mol]
40
41 disp(H1, 'H1 = ');
42 \text{ disp}(H2, 'H2 = ');
43 \operatorname{disp}('J/\operatorname{mol}', \operatorname{H1\_inf}, 'H1\_\operatorname{inf} = ')
44 disp('J/mol', H2_inf, 'H2_inf = ')
45
46 / End
```

Scilab code Exa 11.5 Plot the Fugacity and Fugacity Coefficient Vs P

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8 endfunction
9
10 //Example 11.5
11 //Caption: Program to Plot the Fugacity and
      Fugacity Coefficient Vs P
12
13 // Using Eqn 11.30
14
15 //G = t(T) + RT \ln f
16 //G' = t(T) + rt ln f'
17
18 //Hence \ln(f/f') = (1/RT)*(G-G')
19
20 //G = H - TS
21 //G' = H - TS'
22
23 //\ln (f/f') = (n/R) * (((H-H')/T) - (S-S')) (A)
24
25 R=8.314;
26 n=18.015;
27 f_{=1}; //[kPa]
28 P_=f_;
29 H_=3076.8; //[J/g]
30 S_=10.3450; //[J/g/K]
31 T=573.15; //[K]
32 P=[10 50 100 200 500 1000 1500 2000 2500 3000 3500
      4000 4500 5000 5500 6000 6500 7000 7600 8000
      8400];
33 H=[3076.6 3075.7 3074.2 3072.1 3064.8 3052.1 3038.9
      3025 3010.4 2995.1 2979 2962 2944.2 2925.5 2905.8
       2885 2862.9 2839.4 2808.8 2786.8 2763.1];
```

```
34 S = [9.282 8.5380 8.2166 7.8937 7.4614 7.1251 6.9207]
      6.7696 6.6470 6.5422 6.4491 6.3642 6.2852 6.2105
      6.1388 6.0692 6.0008 5.9327 5.8503 5.7942
      5.7366];
35
36 \text{ K=approx}(\exp((n/R).*(((H-H_{-})/T)-(S-S_{-}))),0);
37
38 f = K * f_{;}
39 P(22) = 8592.7; // [kPa]
40 P_sat = P(22)
41 f(22)=6738.9;
42 f_sat=f(22)
43
44 si=approx(f./P,4);
45 si_sat=si(22)
46
47 Vl=approx (1.403*n,2) / [cm^3/mol]
48 // Using Eqn 11.41
49 P_new=linspace (8592.7,10000,10);
50 \text{ f_new=approx}(f_sat.*exp(Vl.*(P_new-P_sat)/(R*1000*T))
      ),1);
51 si_new=f_new./P_new;
52 subplot (1,2,1)
53 plot (P/1000, f/1000, 'b')
54 plot(P_new/1000, f_new/1000, 'g')
55 dotsx=[0 P_sat/1000];
56 dotsy=[f_sat/1000 f_sat/1000];
57 plot (dotsx, dotsy, 'b--')
58 dotsx=[0 f_sat/1000];
59 dotsy=[P_sat/1000 P_sat/1000];
60 plot (dotsy, dotsx, 'g--')
61 \text{ dotsx} = [11, 8];
62 \text{ dotsx} = [6, 6];
63 plot(dotsx, dotsy, 'w')
64 legend('f vs P(till P_sat)', 'f vs P(Beyond P_sat)', '
      f_sat', P_sat'
65 xtitle('f vs P', 'P X 10^-3 /kPa', 'f X 10^-3 /kPa')
66 subplot (1,2,2)
```

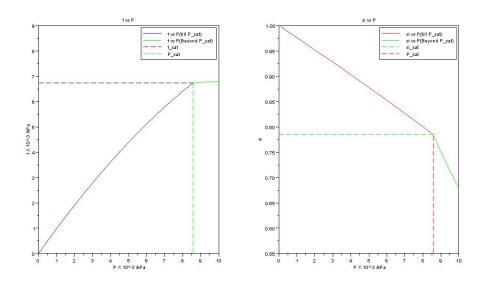


Figure 11.1: Plot the Fugacity and Fugacity Coefficient Vs P

```
67 plot(P/1000,si,'r')
68 plot(P_new/1000, si_new, 'g')
69 dotsx=[0 P_sat/1000];
70 dotsy=[si_sat si_sat];
71 plot(dotsx,dotsy,'g--')
72 dotsx=[0.55 si_sat];
73 dotsy=[P_sat/1000 P_sat/1000];
74 \text{ plot}(dotsy, dotsx, 'r--')
75
  legend('si vs P(till P_sat)', 'si vs P(Beyond P_sat)'
76
      , 'si_sat', 'P_sat')
  xtitle('si vs P', 'P X 10^-3 /kPa', 'si')
77
78
79 //End
```

Scilab code Exa 11.7 Find the Fugacity Coefficient for the mixture

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
9
10 //Example 11.7
11 //Caption : Program to Find the Fugacity Coefficient
       for the mixture
12
13 T=200; //[K]
14 P=30; // [bar]
15 R=83.14;
16 x1=0.4; //[N2]
17 x2=1-x1; // [CH4]
18
19 B11=-35.2; //[\text{cm}^3/\text{mol}]
20 B22=-105; //[\text{cm}^3/\text{mol}]
21 B12=-59.8; //[\text{cm}^3/\text{mol}]
22
23 delta_12=approx((2*B12)-B11-B22,1);
24 si_1=approx(exp((P/(R*T))*(B11+(x2^2*delta_12))),4);
25 \text{ si}_2 = \text{approx}(\exp((P/(R*T))*(B22+(x1^2*delta_12))),4);
26
27 B=approx((x1^2*B11)+(2*x1*x2*B12)+(x2^2*B22),2);
28 Z=approx(1+((B*P)/(R*T)),2);
29
```

```
30 disp(si_1,si_2, 'Fugacity Coefficients are ')
31 disp(B, 'Second Viral coefficient is ')
32 disp(Z, 'Compressibility Factor is ')
33
34 //End
```

Scilab code Exa 11.8 Find the Fugacity of 1 butene vapor

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
     funcprot(0)
8 endfunction
10 //Example 11.8
11 //Caption : Program to Find the Fugacity of 1-butene
       vapor
12
13 T=473.15; //[K]
14 P=70; // [bar]
15 Tc = 420; //[K]
16 Pc = 40.43; // [bar]
17 omega=0.191;
18
19 //By interpolation in Tables E.15 and E.16
20 \text{ si}_0=0.627;
21 \text{ si}_1=1.096;
22 // Using Eqn (11.64)
23 si=approx(si_0*(si_1^omega),3);
24 f=approx(si*P,1);
```

```
25 disp(si, 'Fugacity coefficient is ')
26 disp('bar',f,'fugacity is ')
27
28 //End
```

Scilab code Exa 11.9 Find the Fugacity Coefficients for mixture

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8 endfunction
10 //Example 11.9
11 //Caption : Program to Find the Fugacity
      Coefficients for mixture
12
13 P=25; // [KPa]
14 T=323.15; //[K]
15 R=83.14;
16 \times 1 = 0.5;
17 	 x2=1-x1;
18
19 ij = [11, 22, 12];
20 Tc_ij=[535.5,591.8,563.0];
21 Pc_ij=[41.5,41.1,41.3];
22 Vc_ij = [267,316,291];
23 Zc_ij=approx((Pc_ij.*Vc_ij)./(R*Tc_ij),3);
24 omega_ij=[0.323,0.262,0.293];
25
```

```
26 Tr_ij=approx(T./Tc_ij,3);
27 B0=approx(0.083-(0.422./(Tr_ij.^1.6)),3)
28 B1=approx(0.139-(0.172./(Tr_ij.^4.2)),3)
29 B_ij=round((R*Tc_ij./Pc_ij).*(B0+(omega_ij.*B1)));
30
31 delta_12 = (2*B_ij(3)) - B_ij(1) - B_ij(2);
32 R=8314;
33 si_1=approx(exp((P/(R*T))*(B_ij(1)+(x2^2*delta_12)))
34 \text{ si}_2 = \text{approx}(\exp((P/(R*T))*(B_ij(3)+(x1^2*delta_12)))
      ,3);
35
36 Ans=[ij',Tc_ij',Pc_ij',Vc_ij',Zc_ij',omega_ij',Tr_ij
      ',B0',B1',B_ij'];
37 disp(Ans,' ij
                         Tcij
                                   Pcij
                                        Vcij
                                                    Zcij
                    Trij
                               B0
                                                   Bij')
           Wij
                                         Β1
38
39 disp(si_1,si_2, 'Fugacity Coefficients are ')
40
41 / End
```

Scilab code Exa 11.10 Find the Excess Properties for a mixture

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
9
10 //Example 11.10
```

```
11 //Caption : Program to Find the Excess Properties
      for a mixture
12
13 T0 = 298.15; //[K]
14 T=323.15; //[K]
15 Cp_E = -2.86; //[J/mol/K]
16 Ho_E=897.9; //[J/mol]
17 Go_E=384.5; // [J/mol]
18
           Derivations
19 / (a)
20
21 //G_E = -a * (T ln T - T) + bT + c
\frac{22}{\sqrt{S_E}} = a \ln T - b
23 / H_E = aT + c
24
  //Where
25
26
27 / a = Cp_E
28 / c = Ho_E - aT0
29 //b = ((Go_E + a(T ln T0 - T0) - c)/T0)
30
31 //(b)
32 \quad a=Cp_E;
33 c=approx(Ho_E-(a*T0),1);
34 b=approx((Go_E+(a*((T0*log(T0))-T0)-c))/T0,4);
35 G_E = approx((-a*(T*log(T)-T))+(b*T)+c,1);
36 \quad S_E = \operatorname{approx}((a * \log(T)) - b, 3);
37 H_E=approx((a*T)+c,1);
38
39 disp('J/mol', G_E, 'G_E = ')
40 disp('J/mol/K',S_E,'S_E = ')
41 disp('J/mol', H_E, 'H_E = ')
42
43 / End
```

Chapter 12

Solution Thermodynamics Applications

Scilab code Exa 12.1 Reduce the set of VLE Data and Plot the Graphs

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
9
10 //Example 12.1
11 //Caption : Program to Reduce the set of VLE Data
and Plot the Graphs
12
13 P
=[90.15,91.78,88.01,81.67,78.89,76.82,73.39,66.45,62.95,57.70,50.
14 x1
```

```
=[0.000,0.063,0.248,0.372,0.443,0.508,0.561,0.640,0.702,0.763,0.8
15 y 1
      = [0.000, 0.049, 0.131, 0.182, 0.215, 0.248, 0.268, 0.316, 0.368, 0.412, 0.4
16 	 x2=1-x1;
17 y2=1-y1;
18 P1_sat=P(13);
19 P2_sat=P(1);
20 \text{ K=zeros}(1,13);
21 for(i=1:13)
22
     if(i ~= 1)
23
        ln_V1(i) = approx(log(y1(i)*P(i)/(x1(i)*P1_sat))
24
     end
25
      if(i ~= 13)
        ln_V2(i) = approx(log(y2(i)*P(i)/(x2(i)*P2_sat))
26
            ,3);
27
     end
28 end
29 \ln_V1(1) = \%nan;
30 \ln_V 2(13) = \% nan;
31 for(i=2:12)
     K(i) = approx(((x1(i)*ln_V1(i))+(x2(i)*ln_V2(i)))/(
32
         x1(i)*x2(i)),3); //K=G_E/(x1*x2*R*T)
33
     k(i) = approx(((x1(i)*ln_V1(i))+(x2(i)*ln_V2(i))),3)
         //K = G_E/(R*T)
34
35 end
36 \text{ K}(1) = \% \text{nan};
37 k(1) = %nan;
38 \text{ K}(13) = \% \text{nan};
39 k(13) = %nan;
40 \quad A21 = 0.70;
41 A12=1.35;
42 K_{new}=approx((A21.*x1)+(A12.*x2),3);
43 // Using Eqn (12.10(a) and 12.10(b))
44 \ln_V1_{\text{new}} = \operatorname{approx}((x2.*x2).*(A12+(2*(A21-A12).*x1))
```

```
,3);
45 V1_{new=approx(exp(ln_V1_{new}),3)};
46 \ln_{V2} = approx((x1.*x1).*(A21+(2*(A12-A21).*x2))
      ,3);
47 V2_{new}=approx(exp(ln_V2_{new}),3);
48 // \text{Using Eqn} (12.11)
49 P_{new} = (x1.*V1_{new}*P1_{sat}) + (x2.*V2_{new}*P2_{sat});
50
51 \quad A21_new=0.596;
52 \quad A12_new=1.153;
53
54 K_new1=approx((A21_new.*x1)+(A12_new.*x2),3);
55 //Using Eqn (12.10(a) and 12.10(b))
56 \ln_V1_{new1} = approx((x2.*x2).*(A12_{new}+(2*(A21_{new}-
      A12_new).*x1)),3);
57 V1_new1=approx(exp(ln_V1_new1),3);
58 ln_V2_new1=approx((x1.*x1).*(A21_new+(2*(A12_new-
      A21_new).*x2)),3);
59 V2_new1=approx(exp(ln_V2_new1),3);
60 // \text{Using Eqn} (12.11)
61 P_new1=(x1.*V1_new1*P1_sat)+(x2.*V2_new1*P2_sat);
62
63 subplot (1,2,1)
64 plot(x1,P,'bo')
65 plot(y1,P,'gs')
66
67 plot(x1,P_new, 'b-')
68 plot(y1,P_new, 'g-')
70 plot(x1,P_new1, 'b---')
71 plot(y1, P_new1, 'g---')
72
73 legend('Actual(P vs x1)', 'Actual(P vs y1)', 'By Gibbs
       Duhem (P vs x1)', 'By Gibbs Duhem (P vs y1)', 'By
      Barkers Method (Accurate)')
74
75 xtitle('(a)', 'x1, y1', 'P/kPa')
76
```

```
77 subplot(1,2,2)
78 plot(x1,ln_V1, 'bs')
79 plot(x1,ln_V2, 'gv')
80
81 plot(x1,K,'ro')
82
83 plot(x1, K_new, 'r-')
84 plot(x1,ln_V1_new,'b-')
85 plot(x1,ln_V2_new,'g-')
86
87 plot(x1,K_new1,'r--')
88 plot(x1,ln_V1_new1, 'b---')
89 plot(x1,ln_V2_new1, 'g---')
90
91 legend('Actual(ln V1 vs x1)', 'Actual(ln V2 vs x1)', '
      G_E/x1x2RT vs x1', 'By Gibbs Duhem(G_E/x1x2RT vs
      x1)', 'By Gibbs Duhem(ln V1 vs x1)', 'By Gibbs
      Duhem(In V2 vs x1)', 'By Barkers Method(Accurate)'
92 xtitle('(b)', 'x1')
93
94 / End
```

Scilab code Exa 12.2 Find the Excess Enthalpy as function of x1

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
6 A = round(V*10^n)/10^n; //V-Value n-To what place
```

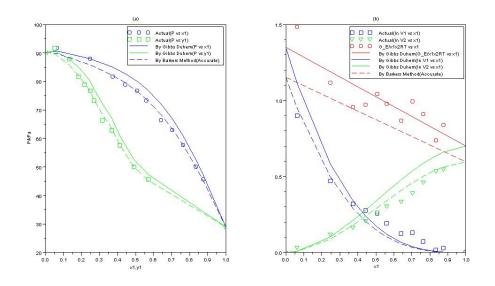


Figure 12.1: Reduce the set of VLE Data and Plot the Graphs

```
7
     funcprot(0)
8
   endfunction
9
  //Example 12.2
10
  //Caption : Program to Find the Excess Enthalpy as
      function of x1
12
13
   //H_E = x1x2(40x1+20x2)
                             (A)
   //Find H1_E and H2_E
14
15
  //H1_E=H_E+((1-x1)*(dH_E/dx1)) let d=dH_E/dx1
16
17
   //H2_E=H_E-(x1*(dH_E/dx1))
                                let d=dH_E/dx1
18
19
  //Replacing x2=1-x1 in (A)
20
21
22 H_E=poly([0 20 0 -20], 'x1', 'c');
23 d=poly([20 0 -60], 'x1', 'c');
24 H1_E=poly([20 0 -60 40], 'x1', 'c');
```

```
25 H2_E=poly([0 0 0 40], 'x1', 'c');
26
27 disp(H1_E, 'Expression For H1_E(x1) is ')
28 disp(H2_E, 'Expression For H2_E(x1) is ')
29
30
31 //End
```

Scilab code Exa 12.4 Find the Heat of Formation of LiCl

```
1 clear;
 2 clc;
 4 //To find Approx Value
 5 function[A] = approx(V,n)
      A=round(V*10^n)/10^n;//V-Value n-To what place
 7
      funcprot(0)
 8
   endfunction
10 //Example 12.4
11 //Caption : Program to Find the Heat of Formation of
        LiCl
12
13 //
                 Li + 0.5 Cl2 \longrightarrow LiCL(s)
                                                        (A)
14
         LiCl(s) + 12H2O(1) \longrightarrow LiCl(12H2O)
15 //
                                                        (B)
16
17 // Net Reaction
18 / \text{Li} + 0.5 \text{Cl} + 12 \text{H2O}(1) \longrightarrow \text{LiCl}(12 \text{H2O})
                                                        (Net)
19
20 //From Table C.4
21 Hf_A = -408610; //[J]
22 Hf_B=-33614; //[J]
```

Scilab code Exa 12.5 Calculate the Heat transfer rate in the evaporator

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
9
10 //Example 12.5
11 //Caption: Program to Calculate the Heat transfer
      rate in th evaporator
12
13 M_LiCl=42.39;
14 M_H20=18.015;
15 T1=298.15; //[K]
16 T2=405.15; // [K]
17 //Step a
18 m_LiCl=0.15*2;
19 \text{ m}_H20=2-\text{m}_LiC1;
20 n_LiCl = (m_LiCl * 1000) / M_LiCl
21 n_H20 = (m_H20 * 1000) / M_H20;
22 	 dH_LiCl = -33800;
23 dH_a=-n_LiCl*dH_LiCl//[J/s]
```

```
24
25 //Step b
26 m_LiCl=0.15*2;
27 \text{ m}_{H}20=0.45;
28 n_LiCl=(m_LiCl*1000)/M_LiCl;
29 n_H20 = (m_H20 * 1000) / M_H20;
30 \text{ dH_LiCl} = -23260;
31 dH_b=n_LiCl*dH_LiCl//[J/s]
32
33 //Step c
34 \text{ m_LiCl=0.75};
35 \text{ Cp} = 2.72;
36 \ dT = T2 - T1;
37 dH_c=m_LiCl*Cp*dT*1000 // [J/s]
38
39 / \text{step d}
40 \text{ m}_H20=2-\text{m}_LiC1;
41 dH_T2=2740.3; //[KJ/s/mol] form Steam Tables
42 dH_T1=104.8; //[KJ/s/mol] from Steam Tables
43 dH_d=m_H20*(dH_T2-dH_T1)*1000//[J/s]
44
45 dH = approx((dH_a + dH_b + dH_c + dH_d)/1000, 1);
46
47 disp('kW or KJ/s',dH,'The required Heat Transfer
       rate is ')
48
49 //End
```

Scilab code Exa 12.6 Calculate Heat Transfer Rate in a evaporator

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

```
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
10 //Example 12.6
11 //Caption : Program to Calculate Heat Transfer Rate
      in Single effect Evaporator
12
13 T0 = 298.15; //[K]
14 T=361.5; //[K]
15 mT=1.25; //[Kg/s]
                      10% NaOH
16 m_steam=1; //[Kg/s] at P=76 torr and 361.5K
17 m_50NaOH=mT-m_steam; //[Kg/s] at 361.5K
18
19 //From Steam tables
20 / at 76 torr and 361.15K
21 H_steam = 2666; //[KJ/kg]
22 //for 10% NaOH soln at 294.15K
23 H_10NaOH = 79; // [KJ/Kg]
24 // for 50% NaOH soln at 361.15K
25 H_50NaOH = 500; //[KJ/Kg]
26
27 	ext{ dH=(m\_steam*H\_steam)+(m\_50NaOH*H\_50NaOH)-(mT*)}
      H_10NaOH);
28 \quad Q = dH;
29 disp('kW or kJ/s',Q,'Heat Transfer rate')
30
31 / End
```

Scilab code Exa 12.9 Calculate the Heat Transformed per Kg of Solution

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
  endfunction
9
10 //Example 12.9
11 //Caption : Program to Calculate the Heat
      Transformed per Kg of Solution formed
12
13 T = 294.15; //[K]
14 m_NaOH_soln=1; //[kg]
15 m_NaOH_solid=0.45*m_NaOH_soln;//[Kg]
16 m_H20=0.55*m_NaOH_soln; //[Kg]
17
18 //From Steam Tables
19 H_NaOH_soln=216; //[kJ/Kg]
20 H_NaOH_solid=1113; //[kJ/Kg]
21 H_H20=88; //[kJ/Kg]
22
23 dH=m_NaOH_soln*H_NaOH_soln-(m_NaOH_solid*
      H_NaOH_solid) - (m_H2O*H_H2O);
24 \quad Q = dH;
25
  disp('kW or kJ/kg',Q,'Heat Transferred per Kg of
26
     NaOH Soln')
27
28 / End
```

Chapter 13

Chemical Reaction Equilibria

Scilab code Exa 13.1 Determine the Expressions for mole Fractions yi

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
   endfunction
10 //Example 13.1
11 //Caption : Program to determine the Expressions for
       mole Fractions yi
12
13 / CH4 + H2O \longrightarrow CO + 3H2
14
15 n_CH4=2; // Moles of CH4
16 n_H20=1; //Moles of H20
17 \text{ n_CO=1;} // \text{Moles of CO}
18 n_H2=4; // Moles of H2
```

```
19
20 v_CH4 = -1;
21 v_H20 = -1
22 v_C0=1;
23 \text{ v}_H2=3;
24
v = v CH4 + v H20 + v CO + v H2;
26 n=n_CH4+n_H20+n_C0+n_H2;
27
28 //y_CH4 = (n_CH4 + (v_CH4e)/n + (v*e))
29 //y_H2O = (n_H2O + (v_H2Oe) / n + (v*e))
30 //y_{CO} = (n_{CO} + (v_{CO} * e) / n + (v * e))
31 //y_H2 = (n_H2 + (v_H2 * e) / n + (v * e))
32
33 y_CH4 = '(n_CH4 + (v_CH4e)/n + (v*e))';
34 y_H20 = (n_H2O + (v_H2Oe) / n + (v*e));
35 y_CO = (n_CO + (v_CO * e) / n + (v * e));
36 y_H2 = (n_H2 + (v_H2 * e) / n + (v * e));
37
38
39
  //Hence
40
41
42 y_CH4 = (2-e/8+2e);
43 y_H20 = (1-e/8+2e);
44 y_CO = (1+e/8+2e);
45 y_H2 = (4+3e/8+2e);
46
47 disp(y_CH4, 'y_CH4 = ')
48
49 disp(y_H20, 'y_H20 = ')
50
51 \text{ disp}(y\_CO, 'y\_CO = ')
52
   disp(y_H2, 'y_H2 = ')
53
54
55 / End
```

Scilab code Exa 13.3 Determine the Expression for yi for two reactions

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
      funcprot(0)
8
   endfunction
9
10 //Example 13.3
11 //Caption: Program to Determine the Expression for
      yi for two reactions
12
13 / CH4 + H2O \longrightarrow CO + 3H2
                                   (A)
14
  //CH4 + 2H2O --> CO2 + 4H2
15
                                     (B)
16
17 Species=['CH4', 'H2O', 'CO', 'CO2', 'H2', 'sum'];
18 v_A = ['-1', '-1', '1', '0', '3', '2'];
19 v_B = ['-1', '-2', '0', '1', '4', '2'];
20 \text{ m}_CH4=2;
21 \text{ m}_H20=3;
22 \text{ mt} = \text{m}_{CH4} + \text{m}_{H20};
23 y = ['(m_CH4+vie1+vje2)/(mt+vie1+vje2)', '(m_H2O+vie1+vje2)']
      vje2)/(mt+vie1+vje2)','(vie1)/(mt+vie1+vje2)','(
      vje2)/(mt+vie1+vje2)', '(vie1+vje2)/(mt+vie1+vje2)
       ',''];
24
25
   //Hence
26
```

Scilab code Exa 13.4.a Alternate Program to 13 iv

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8 endfunction
10 //Example 13.4 Alternate
11 //Caption : Alternate Program to 13.4
12
13 T = [298.15, 418.15, 593.15];
14 t = approx(T/T(1), 4);
15 R=8.314;
16
17
18 / C2H4(g) + H2O(g) \longrightarrow C2H5OH(g)
19
20 // Values From Table C.1 At T=298.15K
```

```
21
22 A_ethanol=3.518;
23 \quad A_{ethene=1.424};
24 \text{ A_water=} 3.470;
25
26 B_ethanol=20.001*10^-3;
27 B_{ethene} = 14.394*10^{-3};
28 \text{ B_water=} 1.450*10^{-3};
29
30 C_{ethanol=-6.002*10^-6};
31 C_{ethene} = -4.392*10^{-6};
32 C_{water=0};
33
34 D_ethanol=0;
35 D_{ethene=0};
36 D_water=0.121*10^5;
37
38 dA=A_ethanol-A_ethene-A_water
39 dB=B_ethanol-B_ethene-B_water
40 dC=C_ethanol-C_ethene-C_water
41 dD=D_ethanol-D_ethene-D_water
42
43 // Values from Table C.4 at T=298.15K
44 H_ethanol = -235100; //[J/mol]
45 H_ethene=52510; //[J/mol]
46 H_water=-241572; //[J/mol]
47
48 G_ethanol = -168490; //[J/mol]
49 G_ethene=68460; //[J/mol]
50 G_{\text{water}} = -228572; //[J/mol]
51
52 dHo=H_ethanol-H_ethene-H_water
53 dGo=G_ethanol-G_ethene-G_water
54
55 // \text{Using Eqn} (13.21)
56 Ko=approx(exp(-dGo./(R*T(1))),3)
57 \text{ KO=Ko*ones}(1,3);
58 // Using Eqn(13.22)
```

```
59 K1 = exp((dHo/(R*T0))*(1-(T(1)./T)));
60 // Using Eqn (13.24)
61 K2=approx(exp((dA.*(log(t)-((t-1)./t)))+(0.5*dB*T(1)
      .*((t-1).^2)./t)+((1/6)*dC*T(1)*T(1).*((t-1).^2)
      .*(t+2)./t)+(0.5*dD.*((t-1).^2)./((T(1)^2).*(t)
      .^2))),4);
62
63 \text{ K=KO.*K1.*K2};
64
65 Ans=[T',t',K0',K1',K2',K'];
66 disp(Ans, ' T/K
                                        K0
                                                     K1
              K2
                          K')
67
68 //End
```

Scilab code Exa 13.4 Find the equillibrium constant for Vapor Phase

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8
   endfunction
9
10 function [Q] = IDCPH(TO, T, dA, dB, dC, dD)
11
     t=T/T0;
     Q = (dA + ((dB/2) * T0 * (t+1)) + ((dC/3) * T0 * T0 * ((t^2) + t+1))
12
        +(dD/(t*T0*T0)))*(T-T0)
13
     funcprot(0);
14 endfunction
15
```

```
16 function [Q] = IDCPS (TO, T, dA, dB, dC, dD)
17
                  t=T/T0;
                  Q = ((dA)*log(t)) + (((dB*T0)+(((dC*T0*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*t*T0)+(dD/(t*t*t*T0)+(dD/(t*t*t*t*T0)+(dD/(t*t*t*t*t*T0)+(dD/(t*t*t*t*t0)+(dD/(t*t*t*t*t0)+(dD/(t*t*t*t0)+(dD/(t*t*t*t0)+(dD/(t*t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(dD/(t*t0)+(d
18
                             *T0)))*(t+1)/2))*(t-1))
19
                  funcprot(0);
20 endfunction
21
22 //Example 13.4
23 //Caption: Program to Find the equillibrium
                     constant for Vapor Phase Hydration
24
25 T0 = 298.16; //[K]
26 \text{ T1} = 418.15; //[K]
27 T2=593.15; //[K]
28 R=8.314;
29
30 / C2H4(g) + H2O(g) \longrightarrow C2H5OH(g)
31 //Values From Table C.1 At T=298.15K
32
33 \quad A_{ethanol=3.518};
34 \quad A_{ethene} = 1.424;
35 \text{ A_water} = 3.470;
36
37 B_ethanol=20.001*10^-3;
38 B_ethene=14.394*10^-3;
39 \text{ B_water=} 1.450*10^-3;
40
41 C_{ethanol=-6.002*10^-6};
42 C_{ethene} = -4.392*10^-6;
43 C_water=0;
44
45 D_{ethanol=0};
46 D_{ethene=0};
47 D_water=0.121*10^5;
48
49 dA=A_ethanol-A_ethene-A_water
50 \, dB=B_{ethanol-B_{ethene-B_{water}}
51 dC=C_ethanol-C_ethene-C_water
```

```
52 dD=D_ethanol-D_ethene-D_water
53
54 // Values from Table C.4 at T=298.15K
55 H_ethanol = -235100; //[J/mol]
56 H_ethene=52510; //[J/mol]
57 H_water = -241572; //[J/mol]
58
59 G_ethanol = -168490; // [J/mol]
60 G_ethene=68460; //[J/mol]
61 G_{\text{water}} = -228572; // [J/\text{mol}]
62
63 dHo=H_ethanol-H_ethene-H_water
64 dGo=G_ethanol-G_ethene-G_water
65
66 \quad I1 = approx(IDCPH(T0,T1,dA,dB,dC,dD),3)
67 \quad I2=approx(IDCPS(T0,T1,dA,dB,dC,dD),5)
68
69 // Using Eqn 13.18
70 //dG_418/RT = ((dGo - dHo)/RTo) + (dHo/RT) + ((1/T)*I1) - I2
         c1 = dG_418 / RT
71
72 c1=approx(((dGo-dHo)/(R*TO))+(dHo/(R*T1))+((1/T1)*I1
      )-12,4)
73
74 \quad I3 = approx(IDCPH(T0, T2, dA, dB, dC, dD), 3)
75 I4=approx(IDCPS(T0,T2,dA,dB,dC,dD),5)
76
77 //Using Eqn 13.18
78 //dG_593/RT = ((dGo - dHo)/RTo) + (dHo/RT) + ((1/T)*I1) - I2
        c2 = dG_{593}/RT
79
80 c2=approx(((dGo-dHo)/(R*TO))+(dHo/(R*TO))+((1/TO)*IO)
      )-I4,4)
81
82 K_413 = approx(exp(-c1), 4);
83 K_593 = \exp(-c2);
84
85 disp('X 10^{-1}', K_413*10, 'Equilibrium Constant at T =
```

```
413.15K is ')

86 disp('X 10^-3',approx(K_593*1000,3),'Equilibrium

Constant at T = 593.15K is ')

87

88 //End
```

Scilab code Exa 13.5 Calculate the Fraction of Heat Reacted

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
     funcprot(0)
8 endfunction
10 //Example 13.5
11 //Caption : Program to Calculate the Fraction of
      Heat Reacted for Various Cases
12
13 //CO(g) + H2O(g) \longrightarrow CO2(g) + H2(g)
14
15 v_C0 = -1;
16 v_H20=-1;
17 v_C02=1;
18 v_H2=1;
19 v = v_C0 + v_H20 + v_C02 + v_H2;
20
21 // Calculate e (Fraction of Stream) in each case
22
23 //(a)
24 n_H20_a=1;/mol
```

```
25 \text{ n_CO_a=1;} // \text{mol}
26 T_a=1100; //[K]
27 P_a=1; // [bar]
28
29 x=10^4/T_a;
30 //at this x the value of ln K=0 form Graph
31 y = 0;
32 \text{ nt=n_H2O_a+n_CO_a};
33 K = \exp(y);
34
35 //y_H2O = (n_H2O + (v_H2O * e)) / nt
36 //y_{CO} = (n_{CO} + (v_{CO} * e)) / nt
37 / y_H2 = (v_H2 * e) / nt
\frac{1}{38} / \frac{y_{CO2}}{v_{CO2}} = \frac{v_{CO2}}{v_{DO2}} / nt
39
40
41 y_H20 = (1-e)/2
42 y_C0 = (1 - e)/2
43 y_H2 = 'e/2'
44 y_C02 = 'e/2'
45
46
   //K = (y_H2*y_CO2)/(y_CO*y_H2O)
47
48
49 K='e^2/((1-e)^2)=1';
50
51
52 //Solving
53 e_a=0.5;
54
55 //(b) same as in (a) P<sub>b</sub>=10bar
56
57 // Pressure has no effect on fraction of stream
58 e_b=e_a;
59
60 //(c) same as in (a) N2=2mols included
61
62 //Since N2 just act as diluent
```

```
63 //It only changes the total moles fraction remains
       the same
64 \text{ e_c=e_a};
65
66 // (d)
67 \text{ n_H20_d=2;}//\text{mol}
68 \text{ n_CO_d=1; //mol}
69 T_d=1100; //[K]
70 P_d=1; //[bar]
71
72 x=10^4/T_d;
73 //at this x the value of ln K=0 form Graph
74 y = 0;
75 nt=n_H20_d+n_C0_d;
76 K = \exp(y);
77
78 //y_H2O = (n_H2O + (v_H2O * e)) / nt
79 //y_{CO} = (n_{CO} + (v_{CO} * e)) / nt
80 //y_H2 = (v_H2 * e) / nt
81 //y_{CO2}=(v_{CO2}*e)/nt
82
83 y_H20 = (1-e)/3
84 y_CO = (2 - e)/3
85 \text{ y_H2} = 'e/3'
86 y_CO2 = 'e/3'
87
88 //K=(y_H2*y_CO2)/(y_CO*y_H2O)
89
90 K='e^2/((1-e)(2-e))=1';
91
92 // Solving
93 = approx(2/3,3);
94 \text{ e_d=approx}(e/2,3);
95
96 // (e)
97 //Here the y_CO and y_H2O are interchanged
98
99 //No change in Fraction of stream
```

```
100 e_e=e_d;
101
102 //(f)
103 n_H2O_f = 1; //mol
104 n_CO_f = 1; //mol
105 n_CO2_f = 1;; // [mol]
106 T_f = 1100; //[K]
107 P_f=1; // [bar]
108
109 x = 10^4/T_f;
110 //at this x the value of ln K=0 form Graph
111 y = 0;
112 nt=n_H20_f+n_C0_f+n_C02_f;
113 K = \exp(y);
114
115 //y_H2O = (n_H2O + (v_H2O * e)) / nt
116 //y_{CO} = (n_{CO} + (v_{CO} * e)) / nt
117 //y_{CO2} = (n_{CO2} + (v_{CO2} * e)) / nt
118 //y_H2 = (v_H2 * e) / nt
119
120
121 y_H20 = (1-e)/3
122 y_CO = (1 - e)/3
123 y_H2 = (1+e)/3
124 y_C02 = 'e/2'
125
126
   //K = (y_H2*y_CO2)/(y_CO*y_H2O)
127
128
129 K='(e*(e+1))/((1-e)^2)=1';
130
131 // Solving
132 \text{ e_f=approx}(1/3,3);
133
134 / (g)
135 n_H2O_g=1; //mol
136 n_CO_g=1; //mol
137 T_g = 1650; //[K]
```

```
138 P_g=1; // [bar]
139
140 x = 10^4/T_g;
141 //at this x the value of ln K=0 form Graph
142 y = -1.15;
143 nt=n_H20_g+n_C0_g;
144 K = \exp(y);
145
146 //y_H2O = (n_H2O + (v_H2O * e)) / nt
147 //y_{CO} = (n_{CO} + (v_{CO} * e)) / nt
148 //y_H2 = (v_H2 * e) / nt
149 //y_{CO2} = (v_{CO2} * e) / nt
150
151
152 y_H20 = (1-e)/2
153 y_CO = (1 - e)/2
154 y_H2 = 'e/2'
155 y_C02 = 'e/2'
156
157
158
   //K = (y_H2 * y_CO2) / (y_CO * y_H2O)
159
160 Exp='e^2/((1-e)^2)=0.316';
161
162 //Solving
163 p=poly([K -2*K K-1], 'e', 'c');
164
165 root=roots(p);
166 e_g=approx(root(1),2);
167
   //Other Root is negative and the Fraction of steam
168
       cannot be negative
169
170
171 disp('(a)1mol H20 and 1 mol CO T=1100K P=1bar')
172 disp('(b)1mol H20 and 1 mol CO T=1100K P=10bar')
173 disp('(c)1mol H20 and 1 mol CO 2mol N2 T=1100K P=1
       bar')
```

Scilab code Exa 13.6 Find the Maximum Conversion of Ethylene to ethanol

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A] = approx(V,n)
6
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8 endfunction
9
10 function [Q] = IDCPH(TO, T, dA, dB, dC, dD)
     t=T/T0;
11
12
     Q = (dA + ((dB/2) * T0 * (t+1)) + ((dC/3) * T0 * T0 * ((t^2) + t+1))
        +(dD/(t*T0*T0)))*(T-T0)
13
     funcprot(0);
14 endfunction
15
16 function [Q] = IDCPS (TO, T, dA, dB, dC, dD)
     t=T/T0;
17
18
     Q = ((dA)*log(t)) + (((dB*T0)+(((dC*T0*T0)+(dD/(t*t*T0)
        *T0)))*(t+1)/2))*(t-1))
19
     funcprot(0);
```

```
20 endfunction
21
22 function[si]=PHIB(Tr,Pr,omega)
23
     B0=0.083-(0.422/(Tr^1.6));
24
     B1=0.139-(0.172/(Tr^4.2));
25
     si = exp((Pr/Tr)*(B0+(omega*B1)));
     funcprot(0);
26
27
28 endfunction
29
30
31 //Example 13.6
32 //Caption: Program to find the Maximum Conversion
      of Ethylene to ethanol
33
34 \text{ T0} = 298.16; //[K]
35 T1 = 523.15; //[K]
36 P=35; // [bar]
37 R=8.314;
38
39 / C2H4(g) + H2O(g) \longrightarrow C2H5OH(g)
40 // Values From Table C.1 At T=298.15K
41
42 A_ethanol=3.518;
43 \quad A_{ethene} = 1.424;
44 \text{ A_water=} 3.470;
45
46 B_ethanol=20.001*10^-3;
47 B_ethene=14.394*10^-3;
48 B_water=1.450*10^-3;
49
50 C_{ethanol=-6.002*10^-6};
51 C_{ethene} = -4.392*10^-6;
52 C_water=0;
53
54 D_ethanol=0;
55 D_{ethene=0};
56 D_water=0.121*10^5;
```

```
57
58 dA = A_{ethanol} - A_{ethene} - A_{water}
59 dB=B_ethanol-B_ethene-B_water
60 dC=C_ethanol-C_ethene-C_water
61 dD=D_ethanol-D_ethene-D_water
62
63 // Values from Table C.4 at T=298.15K
64 H_ethanol=-235100; //[J/mol]
65 H_ethene=52510; //[J/mol]
66 H_water=-241572; //[J/mol]
67
68 G_ethanol = -168490; //[J/mol]
69 G_ethene=68460; //[J/mol]
70 G_{water} = -228572; //[J/mol]
71
72 dHo=H_ethanol-H_ethene-H_water
73 dGo=G_ethanol-G_ethene-G_water
74
75 I1=approx(IDCPH(T0,T1,dA,dB,dC,dD),3)
76 I2=approx(IDCPS(T0,T1,dA,dB,dC,dD),5)
77
78 //Using Eqn 13.18
79 //dG_418/RT = ((dGo - dHo)/RTo) + (dHo/RT) + ((1/T)*I1) - I2
        c1 = dG_418 / RT
80
81 c1=approx(((dGo-dHo)/(R*TO))+(dHo/(R*T1))+((1/T1)*I1
      )-12,4)
82 K_523 = approx(exp(-c1), 4);
83 disp('X 10^-3', approx(K_523*1000,3), 'Equilibrium')
      Constant at T = 523.15K is ')
84
85 // Values Frm App B
86 Tc = [282.3, 647.1, 513.9];
87 Pc = [50.4, 220.55, 61.48];
88 omega=[0.087, 0.345, 0.645];
89
90 Tr=approx(T1./Tc,3);
91 Pr = approx(P./Pc,3);
```

```
92 si=approx(PHIB(Tr,Pr,omega),3);
93
94 // Using eqn
95 //(y_ETOH*si_ETOH)/(y_C2H4*si_C2H4*y_H20*si_H2O) = (P/
      Po)K
   //y_ETOH/(y_C2H4*y_H20)=c=((si_C2H4*si_H2O)/si_ETOH)
96
      (P/Po)K
97 c=approx(((si(1)*si(2))/si(3))*(P*K_523),3)
98
99 //y_C2H4 = (1-e)/(6-e)
100 //y ETOH = (5-e)/(6-e)
101 //y_H2O = (e)/(6-e)
102
103 //Solving we get a Eqn
104 poly([1.342 -6 1], 'e', 'c')
105 root=approx(roots(poly([1.342 -6 1], 'e', 'c')),3)
106
107 \text{ r=root}(1)*100;
108 //Since e > 1 not possible so e=0.233
109
110 disp('%',r,'The Maximum Conversion of ethylene to
       ethanol by Vapor-Phase Hydration is ')
111
112 //End
```

Scilab code Exa 13.7 Find the Composition of Product Steam

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
```

```
funcprot(0)
8
  endfunction
9
10 //Example 13.7
11 //Caption : Program to Find the Composition of
      Product Steam at Equillibrium
12
13 T=1393.15; //K
14 P=1; //[bar]
15 x = 10^4/T;
16 //C2H2 \longrightarrow 2C + H2 (I)
17 //2C + 2H2 \longrightarrow C2H4 (II)
18
19 // Values Of In K (at 1000/T) for Reactions I and II
       from Graph
20 K_I = exp(12.9);
21 K_{II} = \exp(-12.9);
22 \quad K = K_I * K_I ;
23
24 // Application in Eqn (13.5)
25
26 //y_C2H4/(y_C2H2*y_H2)=c=(P/Po)K
27 c = P * K;
28 / y_H2=y_C2H2=(1-e)/(2-e)
29 //y_C2H4 = e/(2-e)
30
31
32 //The Eqn comes out to be
33 poly([1 -4 2], 'e', 'c')
34
35 root=approx(roots(poly([1 -4 2], 'e', 'c')),3)
36 e=root(1);
37 / \text{Since e} > 1 \text{ not possible so e} = 0.293
38 \text{ y_C2H2=approx}((1-e)/(2-e),3);
39 y_H2 = y_C2H2;
40 y_C2H4 = approx(e/(2-e), 3);
41
42 disp(y_H2,y_C2H2,y_C2H4, 'Equilibrium Composition of
```

```
H2 C2H2 and C2H4 Respectively ')
43
44 //End
```

Scilab code Exa 13.8 Find the Mole fraction of Ethyl Acetate

```
1 clear;
2 clc;
3
4 //To find Approx Value
  function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
6
     funcprot(0)
8
   endfunction
9
10 //Example 13.8
11 //Caption : Program to Find the Mole fraction of
      Ethyl Acetate
12
13 \quad T0 = 298.15;
14 T=373.15; //[K]
15 R=8.314;
16 / \text{CH3COOH}(1) + \text{C2H5OH}(1) \longrightarrow \text{CH3COOC2H5}(1) + \text{H2O}(1)
17
18 //From Table C.4
19 dHo_EtAc = -480000; //[J]
20 dHo_H2O=-285830; //[J]
21 dHo_EtOH=-277690; //[J]
22 dHo_AcH=-484500; //[J]
23
24 dGo_EtAc = -332200; //[J]
25 dGo_H2O=-237130; //[J]
26 dGo_EtOH=-174780; //[J]
```

```
27 dGo_AcH=-389900; //[J]
28
29 dHo_298=dHo_EtAc+dHo_H2O-dHo_EtOH-dHo_AcH;
30 dGo_298=dGo_EtAc+dGo_H2O-dGo_EtOH-dGo_AcH;
31
32 \text{ K}_298 = \text{approx}(\exp(-dGo_298/(R*T0)), 4);
33
34 // \text{Using Eqn} (13.15)
35 //\ln (K_373/K_298) = c = -(dHo_298/R) * ((1/373.15)
       -(1/298.15)
36 c = approx(-(dHo_298/R)*((1/373.15)-(1/298.15)),4);
37 \text{ K}_373 = \text{approx}(\text{K}_298 * \text{exp}(\text{c}), 4);
38
39 //x_AcH=x_EtOH=(1-e)/2 and x_EtAc=x_H2O=e/2
40 //K = (x_E t A c * x_H 2O) / (x_A c H * x_E t O H)
41
42 //Hence The Eqn is
43 q=poly([K_373 -2*K_373 K_373-1], 'e', 'c')
44 root=approx(roots(q),4)
45 e=root(1);
46 //Since Other Root is > 1 hence e = 0.6879
47 x_EtAc=approx(e/2,3);
48
49 disp(x_EtAc, 'Composition of Ethyl Acetate in the
       Reacting Mixture')
50
51 / End
```

Scilab code Exa 13.9 Determine Composition and Temperature of Steam

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

```
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8 endfunction
10 function [Q] = MCPH (TO, T, A, B, C, D)
11
     t=T/T0;
12
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
         /(t*T0*T0)))
13
      funcprot(0);
14 endfunction
15
16 function [Q] = IDCPH(TO, T, dA, dB, dC, dD)
17
     t=T/T0;
     Q = (dA + ((dB/2) * T0 * (t+1)) + ((dC/3) * T0 * T0 * ((t^2) + t+1))
18
         +(dD/(t*T0*T0)))*(T-T0)
      funcprot(0);
19
20 endfunction
21
22 function [Q] = IDCPS (TO, T, dA, dB, dC, dD)
23
     t=T/T0;
24
     Q = ((dA) * log(t)) + (((dB*T0) + (((dC*T0*T0) + (dD/(t*t*T0)))))
         *T0)))*(t+1)/2))*(t-1))
25
      funcprot(0);
26 endfunction
27
28 //Example 13.9
29 //Caption : Program to Determine Composition and
      Temperature of Product Steam
30
31 P=1; // [bar]
32 \text{ T0} = 298.15; //[K]
33 R=8.314;
34
35 //SO2 + 0.5O2 \longrightarrow SO3
36 dHo_298=-98890; //[J/mol]
37 \text{ dGo}_298 = -70866; // [J/mol]
```

```
38
39 n_02_i=0.5*1.2; // Moles O2 Entering
40 n_N2_i = n_02_i * (79/21); //Moles N2 Entering
41
42 / n_SO2 = 1 - e
43 // n_O 2 = 0.6 - (0.5 * e)
44 / n_SO3 = e
45 / n_N 2 = 2.257
46
   //By Energy Balance
47
   //(dHo_298*e)+dHo_P = dH = 0
                                                   (A)
49
   //dHo_P=Cp*(T-298.15)
                                 Cp=E nCp
                                               (B)
51
   //\text{Cp\_SO2} = \text{R*MCPH}(\text{T0}, \text{T}, 5.699, 0.801E - 3, 0, -1.015E + 5)
52
   //\text{Cp-O2}=\text{R*MCPH}(\text{T0},\text{T},3.639,0.506\text{E}-3,0,-0.227\text{E}+5)
54 / Cp_SO3 = R*MCPH(T0, T, 8.06, 1.056E - 3, 0, -2.028E + 5)
   //\text{Cp_N2}=\text{R*MCPH}(\text{T0},\text{T},3.28,0.593E-3,0,0.04E+5)
56
   //T = (-(dHo_298*e)/Cp)+T0
57
                                                        (C)
58
   //K = (e/(1-e))*((3.857-(0.5*e))/(0.6-(0.5*e)))^0.5
                        (D)
60
   //\ln K = ((dHo_298-dGo_298)/(R*T0))-(dHo_298/(R*T))+
61
       I1 - (I2/T)
                    (E)
62
   //I1 = IDCPS(T0, T, 0.5415, 0.002E - 3, 0, -0.8995E + 5)
64
   //I2 = IDCPH(T0, T, 0.5415, 0.002E - 3, 0, -0.8995E + 5)
65
66 //Iteration
67 A1=300; // Initial
68 i = -1;
69
70 while (i==-1)
```

```
71
72
        I1 = IDCPS(T0, A1, 0.5415, 0.002E-3, 0, -0.8995E+5);
        I2=IDCPH(T0,A1,0.5415,0.002E-3,0,-0.8995E+5);
73
        //Applying in Eqn (E)
74
75
        K = \exp(((dHo_298 - dGo_298)/(R*T0)) - (dHo_298/(R*T0))
           A1))+I1-(I2/A1));
        //Applying in Eqn (D)
76
        if(isreal(K))
77
          x = 0:
78
          // p=poly([-0.6*(K^2) 1.7*(K^2) 3.857-(1.6*(K
79
              (2) 0.5*((K^2)-1), 'e', 'c')
          // (0.5*((K^2)-1)*(x^3)) + ((3.857-(1.6*(K^2)))
80
             *(x^2) + (1.7*(K^2)*x) + (-0.6*(K^2))
          F_x = (0.5*((K^2)-1)*(x^3))+((3.857-(1.6*(K^2)))
81
             *(x^2) + (1.7*(K^2)*x) + (-0.6*(K^2));
82
          F_a=F_x;
83
84
          x = 1;
          F_x = (0.5*((K^2)-1)*(x^3))+((3.857-(1.6*(K^2)))
85
             *(x^2) + (1.7*(K^2)*x) + (-0.6*(K^2));
          //F_x = (x^3) - (4*x) + 1;
86
          F_b=F_x;
87
          root = -100;
88
          A = 0;
89
90
          B=1:
91
          i=1;
          while (i==1)
92
93
           a=A;
           F_a = (0.5*((K^2)-1)*(a^3))+((3.857-(1.6*(K^2))
94
              )*(a^2))+(1.7*(K^2)*a)+(-0.6*(K^2));
            //F_a = (a^3) - (4*a) + 1;
95
96
           b=B:
97
            F_b = (0.5*((K^2)-1)*(b^3))+((3.857-(1.6*(K^2))
              )*(b^2)+(1.7*(K^2)*b)+(-0.6*(K^2));
            //F_b = (b^3) - (4*b) + 1:
98
            x1=((a*F_b)-(b*F_a))/(F_b-F_a);
99
            F_x1 = (0.5*((K^2)-1)*(x1^3))+((3.857-(1.6*(K
100
               ^2)))*(x1^2))+(1.7*(K^2)*x1)+(-0.6*(K^2));
```

```
//F_x1=(x1^3)-(4*x1)+1;
101
102
103
            if((F_a*F_x1)<0) then
104
              flag=1;
105
              A = a;
106
              B=x1;
            else((F_x1*F_b)<0)
107
108
             flag=2;
109
             A = x1;
110
             B=b;
111
           end
112
           x1_a=approx(x1,4);
113
           b_a = approx(b,4);
           a_a = approx(a, 4);
114
           if(x1_a==b_a)
115
             root=approx(x1,5);
116
117
             i=0;
118
             break;
119
           elseif(x1_a==a_a)
             root=approx(x1,5);
120
121
             i=0;
122
             break;
123
           end
124
        end
125
126
        e=root;
        Cp_SO2=R*MCPH(T0,A1,5.699,0.801E-3,0,-1.015E+5);
127
        Cp_02=R*MCPH(T0,A1,3.639,0.506E-3,0,-0.227E+5);
128
        Cp_SO3=R*MCPH(T0,A1,8.06,1.056E-3,0,-2.028E+5);
129
130
        Cp_N2=R*MCPH(T0,A1,3.28,0.593E-3,0,0.04E+5);
131
132
        n_S02=1-e;
133
        n_02=0.6-(0.5*e);
        n_S03=e;
134
135
        n_N2=2.257;
        if(n_S02<0 | n_02<0 | n_S03<0)</pre>
136
137
           e=0;
138
        end
```

```
139
                                Cp = (n_S02*Cp_S02) + (n_02*Cp_02) + (n_S03*Cp_S03) + (n_02*Cp_02) + (n_02*Cp_0
                                           n_N2*Cp_N2);
                                //Applying in Eqn (C)
140
                                B = (-(dHo_298*e)/Cp)+T0;
141
142
                                m = (A1+B)/2;
143
                                dT = approx(abs(m-A1), 2);
                                if (dT < 0.1)</pre>
144
                                        i=0;
145
146
                                        T = approx(A1,1);
                                        e=approx(e,2);
147
148
                                        break;
149
                           end
150
                                A1 = m;
151
                                i = -1;
152
                        else
153
                                i = -1;
154
                                A1 = A1 + 1;
155
                        end
156 end
157 disp(e, 'Fraction')
158
159 n_S02=1-e
160 \quad n_02=0.6-(0.5*e)
161 n_S03 = e
162 \quad n_N2 = 2.257
163
164 \text{ nt}=n_S02+n_02+n_S03+n_N2;
165
166 y_SO2=approx(n_SO2/nt,4);
167 \text{ y}_02=approx(n_02/nt,4);
168 y_S03=approx(n_S03/nt,4);
169 y_N2=approx(n_N2/nt,4);
170
171 disp(T, 'Final Temperature')
172 disp(y_SO2, 'Composition of SO2')
173 disp(y_02, 'Composition of O2')
174 disp(y_SO3, 'Composition of SO3')
175 disp(y_N2, 'Composition of N2')
```

```
176
177 //End
```

Scilab code Exa 13.12 Find the Product Composition for Two Reactions

```
1 clear;
2 clc;
3
5 //To find Approx Value
6 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
8
     funcprot(0)
9
  endfunction
10
11 function [Q] = IDCPH(TO, T, dA, dB, dC, dD)
12
     t=T/T0;
13
     Q = (dA + ((dB/2) * T0 * (t+1)) + ((dC/3) * T0 * T0 * ((t^2) + t+1))
        +(dD/(t*T0*T0)))*(T-T0)
     funcprot(0);
14
15 endfunction
16
17 function [Q] = IDCPS (TO, T, dA, dB, dC, dD)
18
     t=T/T0;
19
     Q = ((dA)*log(t)) + (((dB*T0)+(((dC*T0*T0)+(dD/(t*t*T0)
        *T0)))*(t+1)/2))*(t-1))
20
     funcprot(0);
21 endfunction
22
23
24 //Example 13.12
25 // Caption: Program to Find the Product Composition
      for Two Reactions
```

```
26
27 T0 = 298.16; //[K]
28 T1=750; //[K]
29 R=8.314;
30 P=1.2; // [bar]
31
32 / C4H10 \longrightarrow C2H4 + C2H6
                               (I)
33 //C4H10 \longrightarrow C3H6 + CH4
                                (II)
34
35 //Values From Table C.1 At T=298.15K
36
37 A_butane=1.935;
38 \quad A_ethene=1.424;
39 A_ethane=1.131;
40 \quad A_propene=1.637;
41 A_methane=1.702;
42
43 B_butane=36.915*10^-3;
44 B_ethene=14.394*10^-3;
45 B_ethane=19.225*10^-3;
46 B_propene=22.706*10^-3;
47 B_methane=9.081*10^-3;
48
49 C_butane = -11.402*10^-6;
50 \text{ C_ethene} = -4.392*10^-6;
51 C_{ethane=-5.561*10^-6};
52 C_propene = -6.915*10^-6;
53 C_methane = -2.164*10^-6;
54
55 D_butane=0;
56 D_{ethene=0};
57 D_{ethane=0};
58 D_propene=0;
59 D_methane=0;
60
61 dA_I=A_ethene+A_ethane-A_butane;
62 dA_II=A_methane+A_propene-A_butane;
63
```

```
64 dB_I=B_ethene+B_ethane-B_butane;
65 dB_II=B_methane+B_propene-B_butane;
66
67 dC_I=C_ethene+C_ethane-C_butane;
68 dC_II=C_methane+C_propene-C_butane;
69
70 dD_I=D_ethene+D_ethane-D_butane;
71 dD_II=D_methane+D_propene-D_butane;
72
73 // Values from Table C.4 at T=298.15K
74 H_butane = -125790; //[J/mol]
75 H_ethene=52510; //[J/mol]
76 H_ethane = -83820; //[J/mol]
77 H_propene=19710; //[J/mol]
78 H_methane = -74520; //[J/mol]
79
80 G_butane=-16570; //[J/mol]
81 G_ethene=68460; //[J/mol]
82 G_ethane=-31855; //[J/mol]
83 G_propene=62205; // [J/mol]
84 G_{methane} = -50460; // [J/mol]
85
86 dHo_I=H_ethene+H_ethane-H_butane
87 dHo_II=H_methane+H_propene-H_butane
88
89 	ext{dGo_I=G_ethene+G_ethane-G_butane}
90 dGo_II=G_methane+G_propene-G_butane
91
92 I1_I = approx(IDCPH(T0,T1,dA_I,dB_I,dC_I,dD_I),3)
93 I1_II=approx(IDCPH(T0,T1,dA_II,dB_II,dC_II,dD_II),3)
94 I2_I=approx(IDCPS(T0,T1,dA_I,dB_I,dC_I,dD_I),5)
95 I2_II=approx(IDCPS(T0,T1,dA_II,dB_II,dC_II,dD_II),5)
96
97 //Using Eqn 13.18
98 //dG_418/RT = ((dGo - dHo)/RTo) + (dHo/RT) + ((1/T)*I1) - I2
         c1 = dG_{4}18 / RT
99
100 c1_{I=approx}(((dGo_{I}-dHo_{I})/(R*T0))+(dHo_{I}/(R*T1))
```

```
+((1/T1)*I1_I)-I2_I,4)
101 c1_{II}=approx(((dGo_{II}-dHo_{II})/(R*T0))+(dHo_{II}/(R*T1))
       )+((1/T1)*I1_II)-I2_II,4)
102
103 \text{ K_I=approx}(exp(-c1_I),4)
104 \text{ K_II=approx}(exp(-c1_II),4)
105
106 k = (K_II/K_I)^0.5;
107 e_I = approx(((K_I/P)/(1+(K_I*(1/P)*(1+k)*(1+k))))
       ^0.5,4);
108
109 e_II=approx(k*e_I,4);
110
111 n_C4H10=1-e_I-e_II;
112 n_C2H4=e_I;
113 n_C2H6=e_I;
114 \quad n_C3H6=e_{II};
115 n_CH4=e_{II};
nt = n_C4H10 + n_C2H4 + n_C2H6 + n_C3H6 + n_CH4;
117
118 y_C4H10=approx(n_C4H10/nt,4);
119 y_C2H4=approx(n_C2H4/nt,4);
120 y_C2H6=approx(n_C2H6/nt,4);
121 y_C3H6=approx(n_C3H6/nt,4);
122 y_CH4=approx(n_CH4/nt,4);
123
124 y = [y_C4H10 y_C2H4 y_C2H6 y_C3H6 y_CH4];
125 disp(y,' Y_C4H10 Y_C2H4
                                     Y_{-}C2H6
                                                 Y_C3H6
       Y_CH4')
126
127 / End
```

Scilab code Exa 13.13 Find the Composition at different Temperatures

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8 endfunction
9
10 //Example 13.13
11 //Caption : Program to Find the Composition at
      different Temperatures
12
13 n_{air} = 2.381 / [mol]
14 n_02=0.21*n_air;
15 \text{ n_N2=0.79*n_air};
16 R=8.314;
17
18 P=20; // [bar]
19 T=[1000 1100 1200 1300 1400 1500];
20 dG_H2O=[-192420 -187000 -181380 -175720 -170020
      -164310];
21 dG_CO=[-200240 -209110 -217830 -226530 -235130
      -243740];
22 dG_CO2=[-395790 -395960 -396020 -396080 -396130
      -396160];
23
24 KI='y_H2O/((y_O2)^0.5*y_H2)(P/Po)^-0.5'
25 KII='y_CO/((y_O2)^0.5)(P/Po)^0.5'
26 KIII='y_CO2/y_O2'
27
28 n='3.38+((e2-e1)/2)'
29 y_H2 = -e1/n
30 y_CO = 'e2/n'
31 y_02 = ((0.5(1-e1-e2))-e3)/n
32 \text{ y_H20} = (1+e1)/n
33 y_CO2 = 'e3/n'
34 \text{ y}_{N2} = 1.88 / n
```

```
35
36 KI= (1+e1)(2n) 0.5*(P/Po) -0.5
37 KII='(e3*(P/Po)^0.5)/(1-e1-e2-2e3)^0.5*(n/2)^0.5'
38 KIII='2e3/(1-e1-e2-2e3)'
39
40 K_I = approx(exp(-dG_H20./(R.*T)), 1)
41 K_{II}=approx(exp(-dG_CO./(R.*T)),1)
42 K_III=approx(exp(-dG_CO2./(R.*T)),1)
43
44 //Now since the values of KI KII KIII valyes are so
      High the mole fraction of O2 must be very small
   //Hence We eleminate O2, Hence 2 Eqns are,
45
46
47 //C + CO2 \longrightarrow 2CO
                              (a)
48 / H2O + C \longrightarrow H2 + CO
                             (b)
49
50 Ka='(y_CO^2/y_CO^2)*(P/P_0)'
51 Kb='((y_H2*y_CO)/y_H2O)*(P/Po)'
52
n = 3.38 + (e_a + e_b)
54 \text{ y}_H2 = 'e_b/n'
55 \text{ y_CO} = (2 e_a + e_b) / n
56 \text{ y}_H20 = (1 - e_b)/n
57 y_C02 = (0.5 - e_a)/n
58 \text{ y}_{N2} = 1.88/n
59
60 Ka='(2e_a+e_b)^2/((0.5-e_a)*n)*(P/Po)'
61 Kb='e_b(2e_a+e_b)/((1-e_b)*n)*(P/Po)'
62
63 dG_new_a = (2*dG_CO) - dG_CO2;
64 \quad dG_new_b = dG_CO - dG_H2O;
65
66 Ka=approx(exp((-dG_new_a./(R.*T))),3);
67 Kb=approx(exp((-dG_new_b./(R.*T))),3);
68
69 // Calculation of e_a and e_b
70
71 a=0.1; // Initial Value
```

```
72
73 b=0.7; // Initial Value
74
75 C1=Ka/20;
76 \text{ C2=Kb/20};
77
78 for(i=1:6)
79 c = -1;
80 while (c==-1)
      fa=approx((((a^2)*(4+C1(i)))+(b^2)+((4+C1(i))*(a*b))
         ))+(2.88*C1(i)*a)-(0.5*C1(i)*b)-(1.69*C1(i)))
82
      dfax = approx(((2*a*(4+C1(i)))+((4+C1(i))*b)+(2.88*
         C1(i)),4);
      dfay = approx((2*b) + ((4+C1(i))*a) - (0.5*C1(i)),4);
83
84
85
      fb=approx(((b^2*(1+C2(i)))+((2+C2(i))*a*b)-(C2(i)*a*b))
         a)+(2.38*C2(i)*b)-(3.38*C2(i))),4);
86
      dfbx=approx((((2+C2(i))*b)-C2(i)),4);
      dfby = approx(((2*b*(1+C2(i)))+((2+C2(i))*a)+(2.38*
87
         C2(i))),4);
88
      A=[dfax dfay;dfbx dfby];
89
      B=[-fa;-fb];
90
      Ans=approx(A\setminus B,4);
91
92
      da=Ans(1);
93
      db = Ans(2);
94
      if (da == 0 & db == 0)
95
96
        c = 0;
97
        e_a(i)=a;
        e_b(i)=b;
98
99
        break;
100
      end
      a=a+da;
101
      b=b+db;
102
103 end
104 end
```

```
105
106 \text{ n=3.38+(e_a+e_b)};
107 y_H2=approx(e_b./n,3);
108 y_CO = approx(((2*e_a)+e_b)./n,3);
109 y_H20=approx((1-e_b)./n,3);
110 y_CO2=approx((0.5-e_a)./n,3);
111 y_N2 = approx(1.88./n,3);
112
113 Ans=[T', Ka', Kb', e_a, e_b];
114 Ans1=[T',y_H2,y_C0,y_H20,y_C02,y_N2];
115
116 plot(T', y_H2, 'r-')
117 plot(T',y_CO,'b-')
118 plot(T',y_H20,'g-')
119 plot (T', y_CO2, 'm-')
120 plot(T',y_N2,'y-')
121
122 legend('H2', 'CO', 'H2O', 'CO2', 'N2',)
123 xtitle ('Equllibrium Compositions', 'T/K', 'yi')
124
125
126
127 disp(Ans, ' T/K
                                            Kb
                               Ka
                                                         e_a
              e_b ')
128
129 \tt disp(Ans1, {}^{\prime}) - T/K
                               y_H2
                                         y_{-}CO
                                                   y_H2O
       y_{-}CO2 y_{-}N2,
130
131 / End
```

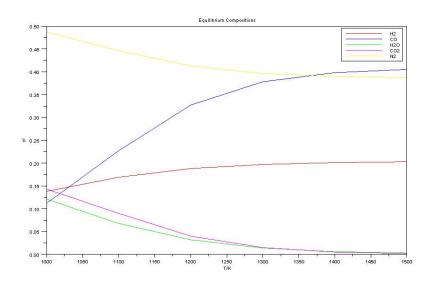


Figure 13.1: Find the Composition at different Temperatures

Chapter 14

Topics In Phase Equilibria

Scilab code Exa 14.1 Find the Fugacity Coefficients of N2 and CH4

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
   endfunction
10 //Example 14.1
11 //Caption : Program to Find the Fugacity
      Coefficients of Nitrogen and Methane
12
13 Tc = [126.2 190.6];
14 T = 200; //[K]
15 Tr=T./Tc;
16 \text{ Pc} = [34 \ 45.99];
17 P=30; // [Bar]
18 Pr=P./Pc;
```

```
19 R=83.14;
20 bi=approx(0.08664.*R.*Tc./Pc,3);
21 ai=approx(((0.42748.*(R^2).*(Tc.^2).*(Tr.^(-0.5))./
      Pc)/(10<sup>5</sup>)),3); //10^{-5}ai
y = [0.4 \ 0.6];
23 a = approx(((y(1)^2)*ai(1))+(2*y(1)*y(2)*sqrt((ai(1)*))
      ai(2)))+((y(2)^2)*ai(2)),2); //10^-5a
24 b=approx((y(1)*bi(1))+(y(2)*bi(2)),3);
25
26 q=(a*10^5)/(b*R*T);
27 Beta=0.051612;
28 //Z=1+Beta-(q*(Z-Beta)/(Z*(Z+Beta)))
29
30 Z=1; // initial
31 A=Z;
32 \text{ for } i=0:10
     B=1+Beta-((q*Beta)*(A-Beta)/(A*(A+Beta)));
33
      if((B-A) == 0.0001)
34
35
         break;
36
      end
37
      A = B;
38
      i=i+1;
39 end
40 Z=approx(B,5);
41
42 I = log((Z+Beta)/Z)
43 a1=approx((2*y(1)*ai(1))+(2*y(2)*<mark>sqrt</mark>((ai(1)*ai(2)))
      -a),2);
                 //10^{-5}a1
44 a2=approx((2*y(2)*ai(2))+(2*y(1)*sqrt((ai(2)*ai(1)))
      -a),2);
                //10^{-5}a2
45 \text{ b1=bi(1)};
46 b2=bi(2);
47 q1=approx(q*(((a1+a)/a)-(b1/b)),5);
48 q2=approx(q*(((a2+a)/a)-(b2/b)),5);
49 \ln_{\text{si1}} = \operatorname{approx}((((b1/b)*(Z-1))-(\log(Z-Beta))-(q1*I))
             //ln si1
      ,5);
50 \ln_{\text{si2}}=\text{approx}((((b2/b)*(Z-1))-(\log(Z-Beta))-(q2*I))
      ,5); //ln si2
```

```
51 si1=approx(exp(ln_si1),5);
52 si2=approx(exp(ln_si2),5);
53 q = [q1 q2];
54 ln_si=[ln_si1 ln_si2];
55 si=[si1 si2];
56 \ a_=[a1 \ a2];
57 b_{=}[b1 b2];
58 q_{=}[q1 q2];
59
60 disp('bar cm^6 mol^-2',a,'a = ')
61 disp('cm^3 mol6-1',b,'b = ')
62 \text{ disp}(q, q = ')
63
64 Ans=[Tc',Tr',Pc',bi',ai',a_',b_',q_',ln_si',si'];
                                              Pc
65 \text{ disp}(Ans,')
                        \mathrm{Tc}
                                  \operatorname{Tr}
                                       b
                                                               ln
                аi
                           a
                                                    q
                 si')
       s i
66
67 / End
```

Scilab code Exa 14.5 Derive the equations from LLE data

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
9
10 //Example 14.5
11 //Caption : Program to derive the equations from LLE
```

```
data
12
13 function [Root] = RF(A,B,K)
14
        //By Regula Falsi Method
15
16
        i=1;
       while(i==1)
17
18
        a=A;
19
        F_a = \log((1-a)/a) + (2*a*K) - K;
20
21
        F_b = log((1-b)/b) + (2*b*K) - K;
22
        x1=((a*F_b)-(b*F_a))/(F_b-F_a);
23
        F_x1 = log((1-x1)/x1) + (2*x1*K) - K;
24
25
        if((F_a*F_x1)<0) then
26
          flag=1;
27
          A = a;
28
          B=x1;
29
        else((F_x1*F_b)<0)
30
          flag=2;
31
          A = x1;
32
          B=b;
33
        end
34
        x1_a=approx(x1,4);
        b_a = approx(b,4);
35
36
        a_a = approx(a, 4);
37
        if(x1_a==b_a)
38
39
          Root=approx(x1,4);
40
          i=0;
          break;
41
        elseif(x1_a==a_a)
42
43
          Root=approx(x1,4);
          i=0;
44
          break;
45
46
        end
47
     end
48 endfunction
```

```
49
50 //Example 14.5
51
52 //G_E/RT = Ax1x2
                                                            (A)
53
54 / \ln V1 = A * x2^2 = A(1-x1)^2
55 / \ln V2 = A * x1^2
56
57 /A[(1-x1_a)^2 - (1-x1_b)^2] = ln(x1_b/x1_a)
                                                            (B)
58
59 //A[(x1_a)^2-(x1_b)^2] = \ln((1-x1_b)/(1-x1_a))
                                                            (C)
60
61 / x1_b = 1 - x1_a
                                                            (D)
62
63 //A(1 - 2*x1) = ln((1-x1)/x1)
                                                            (E)
64
65 / A = a/T + b - clnT
                                                            (F)
66
67 / H_E = R(a + cT) x 1 x 2
                                                            (\mathbf{G})
68
69 //Cp_E = (dH_E/dT) = Rcx1x2
                                                            (H)
70
71
72 T=linspace (250.1,450,20);
73 A = (-975.*(T.^-1)) + 22.4 - (3.*log(T));
74
75 subplot (3,2,1)
76 plot(T, A)
77 x = [250.001 450];
78 y = [2 2];
79 plot(x,y,'b--')
80
81 x = [272.9 \ 272.9];
82 y = [1.9001 2.01];
83 plot(x,y,'r--')
84
85 \quad x = [391.2 \quad 391.2];
86 y = [1.9001 2.01];
```

```
87 plot(x,y,'g--')
88
89 legend('A vs T(K)', 'T=272.9, A=2', 'T=391.2, A=2')
90
91 xtitle('(a)A vs T', 'T(K)', 'A')
92
93 subplot (3,2,2)
94
95 clear;
96
97 T=linspace(272.9,391.2,100);
98 K=approx((-975*(T.^-1))+22.4+(-3.*log(T)),4);
99
100 root=zeros(100,1);
101 \text{ for}(z=1:13)
     root(z) = RF(0.4, 0.49, K(z));
102
103 end
104
105 \text{ for}(z=14:80)
      root(z) = RF(0.01, 0.49, K(z));
106
107 end
108
109 \text{ for}(z=81:100)
      root(z) = RF(0.4, 0.49, K(z));
110
111 end
112 x1=root;
113 plot2d(x1,T,rect=[0,250,1,450])
114
115 x = [0 \ 0.55];
116 y = [272.9 \ 272.9];
117 \text{ plot2d}(x,y,style=3)
118
119 x = [0 \ 0.55];
120 y = [391.2 391.2];
121 plot2d(x,y,style=4)
122
legend('T vs x1', 'T=272.9K(LCST)', 'T=391.2K(UCST)')
124 xtitle('(b)T vs x1', 'x1', 'T(K)')
```

```
125
126 \text{ root}=1-x1;
127 \text{ x1=root};
128 plot2d(x1,T,rect=[0,250,1,450])
129
130 x = [0.5 0.51];
131 y = [272.9 \ 272.9];
132 \text{ plot2d}(x,y)
133
134 \quad x = [0.5 \quad 0.51];
135 y = [391.2 391.2];
136 \text{ plot2d}(x,y)
137
138 clear;
139 // xset ('window', 1)
140
141
142 T=linspace (250.1,450,20);
143 A = (-540.*(T.^-1)) + 21.1 - (3.*log(T));
144
145 subplot (3,2,3)
146 plot(T, A)
147 x = [250.001 450];
148 y = [2 2];
149 plot(x,y,'b---')
150
151 x = [346 346];
152 y = [1.51 2.2];
153 plot(x,y,'r--')
154
155 legend('A vs T(K)', 'A=2', 'T=346K(UCST)')
156 xtitle('(a)A vs T', 'T(K)', 'A')
157 subplot (3,2,4)
158 clear;
159 T=linspace(250,346,100);
160 K = approx((-540*(T.^-1))+21.1+(-3.*log(T)),4);
161
162 root=zeros(100,1);
```

```
163 \quad for(z=1:100)
164
      root(z) = RF(0.1, 0.49, K(z));
165 end
166 x1=root';
167 \text{ plot2d}(x1,T,rect=[0,250,1,450])
168 x = [0 0.55];
169 y = [346 346];
170 \text{ plot2d}(x,y,style=3)
171 legend('T vs x1', 'T=346K(UCST)')
172 xtitle('(b)T vs x1', 'x1', 'T(K)')
173 root=1-x1;
174 \text{ x1=root};
175
176 \text{ plot2d}(x1,T,rect=[0,250,1,450])
177 x = [0.49 0.51];
178 y = [345.4 345.4];
179 \text{ plot2d}(x,y)
180
181 clear;
182 //xset ('window', 2)
183
184
185 T=linspace(250.1,450,20);
186 A = (-1500.*(T.^-1)) + 23.9 - (3.*log(T));
187
188 subplot (3,2,5)
189 plot(T,A)
190 x = [250.001 450];
191 y = [2 \ 2];
192 plot(x,y,'b--')
193
194 x = [339.7 \ 339.7];
195 y = [1.35 \ 2.2];
196 plot(x,y,'r--')
197
198 legend ('A vs T(K)', 'A=2', 'T=339.7K(LCST)')
199 xtitle('(a)A vs T', 'T(K)', 'A')
200 subplot (3,2,6)
```

```
201 clear;
202 T=linspace (339.7,450,100);
203 K=approx((-1500*(T.^-1))+23.9+(-3.*log(T)),4);
204
205 root=zeros(100,1);
206 \text{ for}(z=1:100)
207
      root(z) = RF(0.1, 0.49, K(z));
208 end
209 \text{ x1=root};
210 plot2d(x1,T,rect=[0,300,1,480])
211 x = [0 0.55];
212 y = [339.7 339.7];
213 \text{ plot2d}(x,y,style=3)
214 legend('T vs x1', 'T=339.7K(LCST)')
215 xtitle('(b)T vs x1', 'x1', 'T(K)')
216 \quad root=1-x1;
217 x1=root;
218
219 plot2d(x1,T,rect=[0,300,1,480])
220 x = [0.49 0.51];
221 y = [339.7 339.7];
222 plot2d(x,y)
223
224 //End
```

Scilab code Exa 14.8 Determine the Phase equlibrium data for the System

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

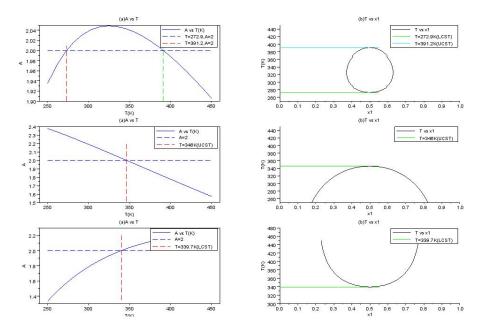


Figure 14.1: Derive the equations from LLE data

```
4 //To find Approx Value
   function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8
   endfunction
10 // \text{Exampl}_14.8
11 // Solution : Program to Determine the Phase
      equlibrium data for the System
12
13 \quad A12=4.62424;
14 \quad A21 = 3.35629;
   alpha12=3.78608;
15
16 alpha21=1.81775;
17 B11=-996;
18 B22=-1245;
   B12 = -567;
19
20
21 P1_sat=103.264; //[kPa]
```

```
22 P2_sat=5.633; //[kPa]
23
24 T = 308.15; //[K]
25 R=8314;
26
27
           //G_E/RT = T1 = A21*x1 + A12*x2 - Q
28
            //V1=\exp[(x2^2)*[A12 + (2*(A21-A12)*x1) - Q - (x1*(
29
                        dQ/dx1))]]
30
            //V2=exp[(x1^2)*[A21 + (2*(A12-A21)*x2) - Q + (x2*(
31
                        dQ/dx1))]]
32
            //Q = (alpha12 * x1 * alpha21 * x2) / ((alpha12 * x1) + (alpha21 * x2)) / ((alpha12 * x1) + (alpha21 * x1) + (alpha21 * x1) / 
                        *x2))
34
            //dQ/dx_1=dQ_x_1=(alpha_1_2*alpha_2_1*(alpha_2_1*x_2^2 -
                         alpha12*x1^2))/((alpha12*x1 + alpha21*x2)^2)
36
37
           //P = (x1*V1*P1_sat)/si1 + (x2*V2*P2_sat)/si2
38
39
           //d12=2B12-B11-B22
40
           //\sin 1 = \exp \left[ \left( \left( B11 * (P - P1_sat) \right) + \left( P * y2^2 * d12 \right) \right) \right) / RT \right]
41
42
43
           //\sin 2 = \exp \left[ \left( \left( B22 * (P - P2 \cdot sat) \right) + \left( P * y1^2 * d12 \right) \right) \right) / RT \right]
44
            //y1 = (x1*V1*P1_sat)/(si1*P)
45
46
            //y2 = (x2*V2*P2_sat)/(si2*P)
47
48
49
50
          //BUBL P
51
52 	 x1 = [0.01:0.01:0.99];
53 \times 2 = 1 - \times 1;
54
55 for(i=1:99)
```

```
56
57
     si1=1; //Assumed
     si2=1; //Assumed
58
59
60
     dP = 100;
61
     while (dP > 0.0001)
62
63
       Q=approx(((alpha12*x1(i)*alpha21*x2(i))/((
          alpha12*x1(i)) + (alpha21*x2(i))),4);
       dQ_x1=approx((alpha12*alpha21*((alpha21*((x2(i))
64
          ^2)) - (alpha12*((x1(i))^2))))/(((alpha12*x1(
          i)) + (alpha21*x2(i)))^2),4);
65
       V1 = approx(exp((x2(i)^2)*(A12 + (2*(A21-A12)*x1(i)))))
          )) - Q - (x1(i)*dQ_x1)),4);
       V2=approx(exp((x1(i)^2)*(A21 + (2*(A12-A21)*x2(i
66
          )) - Q + (x2(i)*dQ_x1)),4);
67
68
       Pi=approx((((x1(i)*V1*P1_sat)/si1) + ((x2(i)*V2*
          P2_sat)/si2)),4);
69
70
       y1=approx((x1(i)*V1*P1_sat)/(si1*Pi),4);
       y2=approx((x2(i)*V2*P2_sat)/(si2*Pi),4);
71
72
73
       d12 = (2*B12) - B11 - B22;
74
75
       si1=approx(exp(((B11*(Pi-P1_sat))+(Pi*(y2^2)*d12)))
          ))/(R*T)),4);
       si2=approx(exp(((B22*(Pi-P2_sat))+(Pi*(y1^2)*d12)))
76
          ))/(R*T)),4);
77
       Pf = approx(((x1(i)*V1*P1_sat)/si1) + ((x2(i)*V2*)
78
          P2_sat)/si2),4);
79
80
       dP=abs(Pf-Pi);
81
     end
     P(i)=Pf;
82
     y(i) = y1;
83
84 end
```

```
85
86 for (i=1:99)
      if(P(i)>104.61)
87
        P(i) = %nan;
88
89
      end
90 end
91 \times 1(100) = 1;
92 y(100)=1;
93 P(100)=P1_sat;
94
95 subplot (1,2,1)
96 P_{=}[5.633 104.6];
97 x = [0 0.0117];
98 plot2d(x,P_,rect=[0,0,0.02,104.6])
99
100 P_{=}[104.6 104.6];
101 x = [0 \ 0.02];
102 plot(x,P_,'r')
103
104 P_{=}[5.633 5.633];
105 y1 = [0 0.02];
106 plot(y1,P_,'b')
107
108 P_{=}[104.6 120];
109 \text{ xa} = [0.0117 \ 0.0117];
110 plot(xa,P_, 'g--')
111
legend('P vs x1', 'P* = 104.6 \,\mathrm{kPa}', 'P vs y1', 'x1_a
       =0.0117')
113 xtitle('P-x-y', 'x1, y1', 'P/kPa')
114
115 P_{=}[100 \ 120];
116 y1 = [0.02 \ 0.02];
117 plot(y1,P_,'w')
118
119 subplot (1,2,2)
120
121 P_{=}[104.6 104.6];
```

```
122 x = [0.943 0.96];
123 plot(x,P_,'r')
124
125 P_{=}[104.3 104.6];
126 \text{ y1} = [0.946 \ 0.946];
127 plot(y1,P_,'b--')
128
129 P_{=}[104.6 104.8];
130 \text{ xb} = [0.95 \ 0.95];
131 plot(xb,P_, 'g—')
132
133 plot2d(x1,P,rect=[0.943,103,1,105])
134 plot2d(y,P,style=3,rect=[0.943,103,1,105])
135
   legend('P*=104.6 \,\mathrm{kPa}', 'y1*=0.946', 'x1_b=0.95', 'P vs
136
       x1', 'P vs y1')
137 xtitle ('P-x-y(Ether Rich Region)', 'x1, y1', 'P/kPa')
138
139 //End
```

Scilab code Exa 14.9 Prepare a Table of Temperature and Compostion Data

```
1 clear;
2 clc;
3
4 //To find Approx Value
5 function[A]=approx(V,n)
6 A=round(V*10^n)/10^n;//V-Value n-To what place
7 funcprot(0)
8 endfunction
```

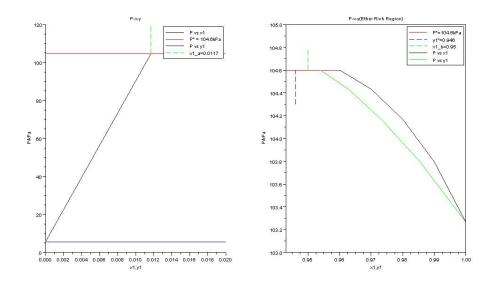


Figure 14.2: Determine the Phase equlibrium data for the System

```
9
10 //Example 14.9
  //Caption : Program to Prepare a Table of
      Temperature/Compostion Data
12 subplot (1,2,1)
13 P=101.33; //[kPa]
14 T=[333.15 343.15 348.15 353.15 353.25 363.15
      373.15];
15 P1_sat=[52.22 73.47 86.40 101.05 101.33 136.14
      180.04];
16 P2_sat=[19.92 31.16 38.55 47.36 47.56 70.11 101.33];
17  P_=P1_sat+P2_sat;
18 plot(P_,T,'b');
19
20 Ans=[T',P1_sat',P2_sat',P_'];
  disp(Ans,'
                   Τ
                            P1\_sat
                                      P2_sat
                                                P1_sat+
      P2_sat')
\frac{1}{2} //Hence P lies between T=333.15 and 343.15
P = [101.33 \ 101.33];
```

```
24 Tp=[330.15 343.15];
25 xgrid();
26 plot(P,Tp,'r--')
27
28 //Thus by interpolation
29 P = [50.14 104.63];
30 \quad T_{=}[342.15 \quad 342.15];
31
32 plot(P,T_, 'g--');
33
34 legend('P* vs T', 'P=101.33\,\mathrm{kPa}', 'T=342.15\mathrm{K}')
35 xtitle('T vs P1_sat + P2_sat', 'P1_sat + P2_sat(kPa)'
      , 'T(K)')
36
37 T_{=}342.15; //[K]
38
39 subplot (1,2,2)
40
41 plot(P1_sat,T,'b')
42
43 //Hence P1_sat @ T=T_{-}=342.15 by interpolation
44 P = [41 70];
45 Tp = [342.15 \ 342.15];
46 xgrid();
47 plot(P,Tp,'r---')
48
49 //Thus by interpolation P1_sat = 71.3kPa
50 P = [71.3 71.3];
51 T_{=}[330.15 342.15];
52
53 plot(P,T_, 'g--');
54
55
56 legend('P1_sat vs T','T=342.15K','P=71.3kPa')
57 xtitle('T vs P1_sat', 'P1_sat(kPa)', 'T(K)')
58
59 P_sat=71.3;
60 T(1) = 342.15;
```

```
61 P=101.33; //[kPa]
62 P1_sat(1)=P_sat;
63 P2_sat(1)=P-P_sat;
64
65 y_I=approx(P1_sat/P,3);
66 y_II=approx(1-(P2_sat/P),3);
67 for(i=1:7)
    if (y_I(i)>1)
68
      y_I(i)=%nan;
69
    elseif(y_II(i)>1)
70
       y_II(i)=%nan;
71
72
    end
73 end
74
75 Ans=[T',y_I',y_II'];
76 disp(Ans, ' T
                          77
78 / End
```

Scilab code Exa 14.10 Illustrate the Concepts of Pure Gas Adsorption

```
1 clear;
2 clc;
3
4 //Example 14.10
5 //Caption : Program to illustrate the Concepts of
    Pue Gas Adsorption
6
7 subplot(2,1,1)
8 m=4.7087;
9 b=2.1941;
```

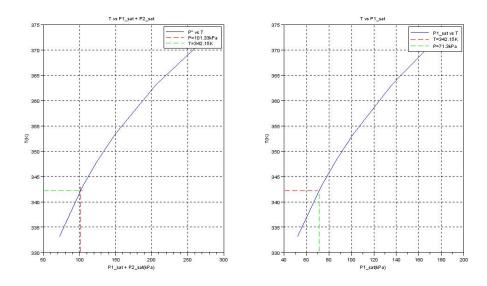


Figure 14.3: Prepare a Table of Temperature and Compostion Data

```
10 t=0.3984;
11 P=linspace(0,40,10);
12 N=(m.*P)./((b+(P.^t)).^(1/t));
13 plot(P,N)
14 m = 0.6206;
15 b=1.5454;
16 t=1;
17 n=(m.*P)./((b+(P.^t)).^(1/t));
18 plot(P,n,'b--')
19 legend('Toth Equation', 'Langmuir Equation')
20 xtitle('Adsorption Isotherm(n vs P)', 'P(kPa)', 'n(mol
      /kg)')
21
22 subplot(2,1,2)
23 \quad C0 = 0.4016;
24 \quad C1 = -0.6471;
25 \quad C2 = 0.4567;
26 \quad C3 = -0.12;
27 n=linspace(0,1.6,20);
```

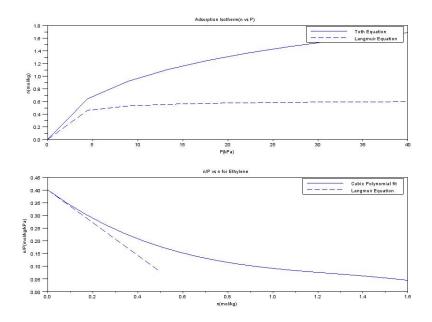


Figure 14.4: Illustrate the Concepts of Pure Gas Adsorption

```
28 K=CO+(C1*n)+(C2*(n^2))+(C3*(n^3));
29 plot(n,K)
30 n=linspace(0,0.5,20);
31 K=CO+(C1*n);
32 plot(n,K,'b--')
33 legend('Cubic Polynomial fit','Langmuir Equation')
34 xtitle('n/P vs n for Ethylene','n(mol/kg)','n/P(mol/kg/kPa)')
35
36 //End
```

Chapter 15

Thermodynamic Analysis Of Process

Scilab code Exa 15.1 Do a Thermodynamic Analysis of Steam Power Plant

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
     funcprot(0)
8 endfunction
10 function [Q] = MCPS (TO, T, A, B, C, D)
11
     t=T/T0;
     Q = (A) + (((B*T0) + (((C*T0*T0) + (D/(t*t*T0*T0)))*(t+1)
12
        /2))*((t-1)/log(t)))
13
     funcprot(0);
14 endfunction
15
16 function[Q]=MCPH(TO,T,A,B,C,D)
```

```
17
     t=T/T0;
18
     Q = (A + ((B/2) * T0 * (t+1)) + ((C/3) * T0 * T0 * ((t^2) + t+1)) + (D
         /(t*T0*T0)))
19
     funcprot(0);
20 endfunction
21
22 //Example 15.1
23 //Caption : Program to do a Thermodynamic Analysis
      of Steam Power Plant
24
25 State=['Supercooled Liquid', 'Superheated Vapor', 'Wet
        Vapor, x=0.9378', 'Saturated Liquid'];
26 T=[318.98 773.15 318.98 318.98];
27 P = [8600 8600 10 10];
28 H=[203.4 3391.6 2436 191.8];
29 S = [0.6580 6.6858 7.6846 0.6493];
30 \quad T0 = 298.15;
31 T1 = 460; //[K]
32 R=8.314;
33 T_sigma=T0;
34 / CH4 + 2O2 \longrightarrow CO2 + 2H2O
35 \text{ dH}_{CO2} = -393509;
36 \text{ dH}_H20 = -241818;
37 \text{ dH}_CH4 = -74520;
38
39 \quad dG_CO2 = -394359;
40 \text{ dG}_H20 = -228572;
41 dG_CH4 = -50460;
42
43 dH_298=dH_CO2+(2*dH_H2O)-dH_CH4
44 dG_298 = dG_C02 + (2*dG_H20) - dG_CH4
45
46 \, dS_{298} = approx((dH_{298} - dG_{298})/T0,3);
47
48 // Moles Entering
49 ni_02=2*1.25;
50 ni_N2=approx(ni_02*(79/21),3);
51 ni=ni_02+ni_N2;
```

```
52
53 // Moles After Combustion
54 n_C02=1;
55 n_H20=2;
56 n_02=0.5;
57 \quad n_N2=ni_N2;
58 n=n_CO2+n_H2O+n_O2+n_N2;
59 m = [n_C02 n_H20 n_N2 n_02];
60
61 y_C02 = approx(n_C02/n, 4);
62 y_H20 = approx(n_H20/n, 4);
63 y_02 = approx(n_02/n, 4);
64 y_N2 = approx(n_N2/n,4);
65
66 y = [y_C02 y_H20 y_02 y_N2];
67 yT = sum(y);
68
69 //Step(a)
70 dH_a=0
71 dS_a = approx(ni*R*((0.21*log(0.21))+(0.79*log(0.79)))
      ,3)//[J/K]
72
73 //Step(b)
74 dH_b=dH_298
75 dS_b = dS_298 / [J/K]
76
77 //Step(c)
78 	 dH_c=0
79 dS_c = approx(-n*R*sum(y.*log(y)),3)//[J/K]
80
81 / \operatorname{Step}(d)
82 //For CO2
83 CpH_CO2 = approx(R*MCPH(T0,T1,5.457,1.045*(10^-3)
      ,0,-1.157*(10^5)),3);
84 //For H2O
85 CpH_H20 = approx(R*MCPH(T0,T1,3.470,1.450*(10^-3))
      ,0,0.121*(10^5)),3);
86 //For O2
```

```
87 CpH_02 = approx(R*MCPH(T0,T1,3.639,0.506*(10^-3)
       ,0,-0.227*(10^5)),3);
88 //For N2
89 CpH_N2=approx(R*MCPH(T0,T1,3.280,0.593*(10^-3))
       ,0,0.040*(10^5)),3);
90
91 / For CO2
92 CpS_C02 = approx(R*MCPS(T0,T1,5.457,1.045*(10^-3))
       ,0,-1.157*(10^5)),3);
93 //For H2O
94 CpS_H20 = approx(R*MCPS(T0,T1,3.470,1.450*(10^-3))
       ,0,0.121*(10^5)),3);
95 //For O2
96 \text{ CpS}_02 = \text{approx}(R*MCPS(T0,T1,3.639,0.506*(10^-3))
       ,0,-0.227*(10^5)),3);
97 //For N2
98 CpS_N2 = approx(R*MCPS(T0,T1,3.280,0.593*(10^-3))
       ,0,0.040*(10^5)),3);
99
100 CpH=[CpH_CO2 CpH_H2O CpH_N2 CpH_O2];
101 CpS=[CpS_C02 CpS_H20 CpS_N2 CpS_02];
102
103 Comp = [ 'CO2' 'H2O' 'N2' 'O2'];
104
105 Ans=[CpH', CpS'];
106 disp(Ans, 'CpH
                            \mathrm{CpS}', \mathtt{Comp}')
107
108 CpHt=approx(sum(m.*CpH),3)//[J/K]
109 CpSt=approx(sum(m.*CpS),3)//[J/K]
110
111 dH_d = approx(CpHt*(T1-T0),0)//[J]
112 dS_d = approx((CpSt*log(T1/T0)),3)//[J/K]
113
114 dH=dH_a+dH_b+dH_c+dH_d/[J]
dS=dS_a+dS_b+dS_c+dS_d//[J/K]
116
117 rm = 84.75; //[kg/s]
118
```

```
119 rn_CH4=approx((rm*(H(1)-H(2))*1000)/dH,2)//[mol/s]
120
121 rW_ideal = approx(rn_CH4*((dH/1000)-(T0*dS/1000))
       /1000,2) *1000 // [KW]
122
123 //(a) Furnace/Boiler
124 rS_a=approx((rn_CH4*dS/1000)+(rm*(S(2)-S(1))),2)//
      kJ/s/K
125
126 \text{ rW}_a = \operatorname{approx} (T_sigma*rS_a/1000, 2)*1000 // [kW]
127
128 //(b) Turbine
129 rS_b=approx(rm*(S(3)-S(2)),2)//[kW/K]
130
131 rW_b = approx(T_sigma*rS_b/1000, 2)*1000//[kW]
132
133 //(c) Condenser
134 Q_c=H(4)-H(3); //[kJ/kg]
135 rQ_c=approx(rm*Q_c/1000,1)*1000//[kJ/s]
136 rS_c=approx((rm*(S(4)-S(3)))-(rQ_c/T_sigma),2)//[kW/
      K
137 rW_c=approx(T_sigma*rS_c/1000,2)*1000//[kW]
138
139 //(d) Pump
140 rS_d=approx(rm*(S(1)-S(4)),2)//[kW/K]
141 rW_d = approx(T_sigma*rS_d/1000, 2)*1000//[kW]
142
143 rS=[rS_a rS_b rS_c rS_d];
144 pS=approx(rS/sum(rS)*100,1);
145 T = [sum(rS) sum(pS)];
146 Process=['Furnace/boiler' 'Turbine' 'Condenser' '
      Pump'];
147 Ans=[rS',pS'];
148 disp(Ans,' S(kW/K) %', Process')
149 disp(T)
150 rW_ideal = 80000;
151 rW=[rW\_ideal rW\_a rW\_b rW\_c rW\_d]/1000;
152 pW=approx(rW/sum(rW)*100,1);
```

Scilab code Exa 15.2 Prepare a Thermodynamic Analysis of Linde System

```
1 clear;
2 clc;
4 //To find Approx Value
5 function[A] = approx(V,n)
     A=round(V*10^n)/10^n;//V-Value n-To what place
7
     funcprot(0)
8 endfunction
9
10 //Example 15.2
11 //Caption : Program to Prepare a Thermodynamic
      Analysis of Linde System
12
13
14 State=['Superheated Vapor', 'Superheated Vapor','
      Superheated Vapor', 'Saturated Liqiud', 'Saturated
      Vapor', 'Superheated Vapor'];
```

```
15 T=[300 300 207.1 111.5 111.5 295];
16 P=[1 60 60 1 1 1];
17 H=[1199.8 1140 772 285.4 796.9 1188.9];
18 S = [11.629 9.359 7.798 4.962 9.523 11.589];
19 Given=[T',P',H',S'];
20 disp(Given, 'T/K
                           P/kPa
                                     H/kJ/Kg
                                                  S/kJ/kg/K
      ,State')
21 T_sigma=300; //[K]
22 \text{ rQ=5}; //[KJ]
23 rW=1000; //[KJ/s]
24 z=approx((H(6)-H(2)-rQ)/(H(6)-H(4)),4);
25
26 / rW_{ideal} = (dH*rm) - (T_{sigma}(dS*rm))
27 \text{ rW\_ideal=approx}(((z*H(4))+((1-z)*H(6))-H(1))-((
      T_sigma)*((z*S(4))+((1-z)*S(6))-S(1))),1);
28
29 //(a) Compression/cooling
30 rQ_a=(H(2)-H(1))-rW; //[kJ]
31 rS_a=approx((S(2)-S(1))-(rQ_a/T_sigma),4); //[kJ/Kg/K]
32
33 \text{ rW}_a=T_sigma*rS_a; // [KJ/Kg]
34
35 //(b) Exchanger
36 \text{ rS_b=approx}(((S(6)-S(5))*(1-z))+(S(3)-S(2))-(rQ/s)
      T_{sigma}, 4); //[kJ/Kg/K]
37 \text{ rW_b=T_sigma*rS_b;}//[\text{KJ/Kg}]
38
39 //(c) Throttle
40 rS_c=approx(((S(4)*z)+(S(5)*(1-z))-S(3)),4); //[KJ/Kg]
      /K]
41 rW_c=T_sigma*rS_c; //[KJ/kg]
42
43 S=[rS_a rS_b rS_c];
44 pS=approx((S/sum(S))*100,1);
45 \quad ES = [sum(S) \quad sum(pS)];
46
47 W=approx([rW_ideal rW_a rW_b rW_c],1);
```

```
48 pW=approx((W/sum(W))*100,1);
49 EW = [sum(W) sum(pW)];
50 Ans=[S',pS'];
51 Process=['Compression/Cooling'; 'Exchanger'; 'Throttle
      <sup>'</sup>];
52
                             \%', Process)
53 disp(Ans,'
                     Si
54 disp(ES, 'Sum')
55 Ans=[W',pW'];
56
57 Process=['Ideal'; 'Compression/Cooling'; 'Exchanger'; '
      Throttle '];
58 \text{ disp}(Ans,')
                             \%', Process)
                     Wi
59 disp(EW, 'Sum')
```