

Scilab Textbook Companion for
Chemical Engineering Thermodynamics
by T. E. Daubert¹

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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

Purpose Usefulness and Definitions of Thermodynamics

Scilab code Exa 1.1 Example 1

```
1  clc
2  clear
3  // Initialization of variables
4  P=2050 //kPa
5  T=700 //K
6  E=10 //J
7  // calculations
8  Pe=P*10^3 *0.3048^2 /4.4482 /144
9  Te=T*1.8-460
10 Ee=E*10^8 /(1055.1)
11 // results
12 printf(" Temperature = %d F" ,Te)
13 printf("\n Pressure = %d lbf/in^2 " ,Pe)
14 printf("\n Energy = %.3e Btu" ,Ee)
```

Chapter 2

PVT Properties of Fluids Equations of State

Scilab code Exa 2.1 Example 1

```
1  clc
2  clear
3  //Initialization of variables
4  basis = 1 //kmol n butane
5  P=1.013*10^5 //N/m^2
6  R=8.3143*10^3 //J/kmol K
7  T=272.6 //K
8  //calculations
9  V=basis*R*T/P
10 Ts=373.1 //K
11 Vs=basis*R*Ts/P
12 //results
13 printf("Volume in case 1 = %.2 f m^3",V)
14 printf("\n Volume in case 2 = %.2 f m^3",Vs)
```

Scilab code Exa 2.2 Example 2

```

1  clc
2  clear
3  // Initialization of variables
4  Vb=30 //m^3/kmol
5  P=1.013*10^5 //Pa
6  R=8.3143*10^3 //J/kmol K
7  T=373.1 //K
8  // calculations
9  Z=P*Vb/(R*T)
10 // results
11 printf(" Compressibility factor = %.3f",Z)

```

Scilab code Exa 2.3 Example 3

```

1  clc
2  clear
3  // Initialization of variables
4  Pc=22.12*10^6 //Pa
5  Tc=647.3 //K
6  Vc=0.05697 //m^3/Kmol
7  R=8.3143*10^3
8  Tr=0.7
9  // calculations
10 Zc=Pc*Vc/(R*Tc)
11 T=Tr*Tc
12 Ps=10^6 //Pa
13 w=-log10(Ps/Pc) -1
14 // results
15 printf(" critical compressibility factor = %.3f",Zc)
16 printf(" \n Accentric factor = %.4f",w)

```

Scilab code Exa 2.4.b Example 4b

```

1  clc
2  clear
3  //Initialization of variables
4  basis= 1 //kmol ammonia
5  P=10^6 //pa
6  a=4.19
7  b=0.0373
8  R=8314.3
9  Tc=405.5
10 Pc=11.28*10^6
11 //calculations
12 disp(" part b")
13 an=27*R^2*Tc^2 /(64*Pc)
14 bn=R*Tc/(8*Pc)
15 V=3
16 //results
17 printf(" Since an and bn are same as a and b, V is
    the same = %d m^3/kmol",V)

```

Scilab code Exa 2.4.c Example 4c

```

1  clc
2  clear
3  //Initialization of variables
4  disp(" part c")
5  disp(" USing SRK equation , P= RT/(V-b) -alph*a/(V*(V+
    b))")
6  disp(" By trail and error method ,")
7  //calculations
8  v2=2.98
9  //results
10 printf(" volume = %.2 f m^3/kmol" ,v2)

```

Scilab code Exa 2.4 Example 4

```
1 clc
2 clear
3 //Initialization of variables
4 basis= 1 //kmol ammonia
5 P=10^6 //pa
6 a=4.19
7 b=0.0373
8 R=8314.3
9 Tc=405.5
10 Pc=11.28*10^6
11 //calculations
12 disp("case a")
13 disp("Using vandwerwaals equation, ")
14 disp("(P+a/v^2)*(V-b) = R*T, on solving by trail and
      error method,")
15 V=3
16 printf("Volume = %d m^3/kmol",V)
```

Scilab code Exa 2.5 Example 5

```
1 clc
2 clear
3 //Initialization of variables
4 Pc=22.12*10^6 //Pa
5 Tc=647.3 //K
6 Zc=0.234
7 T=973.1 //K
8 P=25*10^6 //Pa
9 //calculations
10 Tr=T/Tc
11 Pr=P/Pc
12 Z=0.916
13 Zn=Z+0.05*(Zc-0.27)
```

```
14 //results
15 printf("Compression factor = %.3f ",Zn)
```

Scilab code Exa 2.6 Example 6

```
1 clc
2 clear
3 //Initialization of variables
4 w=0.3448
5 Z0=0.898
6 Z1=0.08
7 //calculations
8 Z=Z0 + Z1*w
9 //results
10 printf("Compression factor = %.3f ",Z)
```

Chapter 3

Conservation of Energy First law of Thermodynamics

Scilab code Exa 3.1 Example 1

```
1  clc
2  // Initialization of variables
3  clear
4  mass=4000 //kg/m^2
5  Patm=1.013*10^5 //pa
6  g=9.807
7  M=28
8  R=8.3143*10^3
9  T=303 //K
10 P1=800*10^3 //pa
11 // calculations
12 Ps=Patm+mass*g
13 n=1/M
14 V1=n*R*T/P1
15 W=Ps*(2*V1)
16 // results
17 printf("Work done on the surroundings = %d J",W)
```

Scilab code Exa 3.2.b Example 2b

```
1  clc
2  clear
3  // Initialization of variables
4  t1=1000 //K
5  p1=20 //Mpa
6  p2=10 //Mpa
7  ti=600 //K
8  t2=700 //K
9  v1=0.02188
10 vi=0.02008
11 v2=0.02825
12 Ei=2617.5
13 E2=2893.1
14 E1=3441.8
15 x=0.22
16 m=1 //kg
17 cp=4.186
18 t3=639 //K
19 H3=2409.5
20 H1=3879.3
21 // calculations
22 Tf= ti+ (v1-vi)/(v2-vi) *(t2-ti)
23 Hf=H3 - m*cp*(t3-Tf)
24 Q2=Hf-H1
25 // results
26 disp(" part b")
27 printf("Heat transfer = %.1f kJ/kg",Q2)
```

Scilab code Exa 3.2 Example 2

```

1  clc
2  clear
3  // Initialization of variables
4  t1=1000 //K
5  p1=20 //Mpa
6  p2=10 //Mpa
7  ti=600 //K
8  t2=700 //K
9  v1=0.02188
10 vi=0.02008
11 v2=0.02825
12 Ei=2617.5
13 E2=2893.1
14 E1=3441.8
15 x=0.22
16 m=1 //kg
17 cp=4.186
18 t3=639 //K
19 H3=2409.5
20 H1=3879.3
21 // calculations
22 Tf= ti+ (v1-vi)/(v2-vi) *(t2-ti)
23 Ef= Ei+ x*(E2-Ei)
24 Q1=Ef-E1
25 // results
26 disp(" part a")
27 printf("Heat transfer = %.1f kJ/kg",Q1)

```

Scilab code Exa 3.3 Example 3

```

1  clc
2  clear
3  // Initialization of variables
4  p1=2.181
5  p2=2.637

```



```

6 p3=3.163
7 vg1=0.09150
8 vg2=0.07585
9 vg3=0.06323
10 vl1=0.00118
11 vl2=0.00120
12 vl3=0.00122
13 M=18
14 t1=490 //K
15 t2=500 //K
16 t3=510 //K
17 R=8.3143
18 //calculations
19 lam1= (p2-p1)*10^3 *M*(vg2-vl2) *2.154/ log(t3/t1)
20 lam2 = log(p3/p1) *R/(1/t1 -1/t3)
21 err=(lam2-lam1)/lam1
22 //results
23 printf("latent heat using calyperon equation = %d kJ
    /kmol",lam1)
24 printf("\n latent heat using the clasius calyperon
    equation = %d kJ/kmol",lam2)
25 printf("\n Error = %d percent",err*100)

```

Scilab code Exa 3.4 Example 4

```

1 clc
2 clear
3 //Initialization of variables
4 h1=147360
5 h2=29790
6 //calculations
7 Hr=h1-h2
8 //results
9 printf("heat of reaction = %d kJ/kmol",Hr)

```

Scilab code Exa 3.5 Example 5

```
1  clc
2  clear
3  // Initialization of variables
4  R=8314.3
5  T=700 //K
6  T2=437.5 //K
7  T3=350 //K
8  T4=T3
9  p2=0.552 //Mpa
10 p1=2.758 //Mpa
11 cp=29.3
12 R0=8.3
13 k=1.4
14 // calculations
15 cv=cp-R0
16 Q1=-R*T*log(p2/p1)
17 Q2=cv*(T2-T)
18 dH2= cp*(T2-T)
19 p3=p2*T3/T2
20 p3=0.345
21 Q3=cp*(T3-T2)
22 dE3=cv*(T3-T2)
23 W3=Q3-dE3
24 T5=T4*(p1/p3)^((k-1)/k)
25 dH4= cp*(T5-T4)
26 W4=-cv*(T5-T4)
27 Q5= cp*(T-T5)
28 dE5=cv*(T-T5)
29 W5=Q5-dE5
30 // results
31 disp(" part a isothermal")
32 printf("dH = 0, dE=0, Q= W = %d kJ/kmol",Q1/10^3)
```

```

33 disp("part 2 isometric")
34 printf("dH = %d kJ/kmol, W=0, Q= dE = %d kJ/kmol",
        dH2, Q2)
35 disp("part 3 isobaric")
36 printf("dE = %d kJ/kmol, W= %d kJ/kmol, Q= dH = %d
        kJ/kmol", dE3, W3, Q3)
37 disp("part 4 adiabatic")
38 printf("dH = %d kJ/kmol, W= -dE = %d kJ/kmol, Q= 0
        kJ/kmol", dH4, W4)
39 disp("part 5 isobaric")
40 printf("dE = %d kJ/kmol, W= %d kJ/kmol, Q= dH = %d
        kJ/kmol", dE5, W5, Q5)
41 disp("The graph cannot be plotted since volume axis
        values are not known. In the textbook it is
        randomly drawn to be of that shape.")

```

Scilab code Exa 3.6 Example 6

```

1  clc
2  clear
3  // Initialization of variables
4  p=[2.75 0.5 0.31 0.31 2.75]
5  v=[116.17 654.8 654.8 597 110.65]
6  t=[440 440 170 140 410]
7  h=[3325 3356 2802.6 2738.5 3257.7]
8  e=[3005.6 3028.6 2602.6 2553.6 2953.4]
9  // calculations
10 dh1=h(2) - h(1)
11 de1=e(2) - e(1)
12 q2=e(3) - e(2)
13 dh2=h(3) - h(2)
14 dh3=h(4) - h(3)
15 de3=e(4) - e(3)
16 W3= p(3) *(v(4) - v(3))
17 Q3= de3+W3

```

```

18 dh4=h(5) -h(4)
19 de4=e(5) -e(4)
20 dh5=h(1) - h(5)
21 de5= e(1) - e(5)
22 W5= p(5) *(v(1) - v(5))
23 q5 = de5+W5
24 //results
25 printf("In case 1 , dH = %.1f kJ/kg dE = %.1f kJ/kg
      W= pDv kJ/kg Q= %.1f + W kJ/kg",dh1,de1,de1)
26 printf("\n In case 2, W =0 kJ/kg Q = dE = %d kJ/kg
      dH = %.1f kJ/kg",q2,dh2)
27 printf("\n In case 3, dH= %.1f kJ/kg dE = %.1f kJ/kg
      W= %.1f kJ/kg Q = %.1f kJ/kg",dh3,de3,W3,Q3)
28 printf("\n In case 4, Q= 0 kJ/kg dH = %.1f kJ/kg dE
      = -W = %.1f kJ/kg",dh4,de4)
29 printf("\n In case 5, dH = %.1f kJ/kg dE = %.1f kJ/
      kg W = %.1f kJ/kg Q = %.1f kJ/kg",dh5,de5,W5,q5)
30 xlabel("Volume (m^3/kg)")
31 ylabel("Pressure (Mpa)")
32 plot(v,p)

```

Scilab code Exa 3.7 Example 7

```

1 clc
2 clear
3 //Initialization of variables
4 P=0.1*10^6 //Pa
5 P2=0.55*10^6 //Pa
6 M=28.84
7 R=8314.4
8 T1=303.1 //K
9 T2=316.1 //K
10 d1=0.154 //m
11 d2=0.028 //m
12 mass=0.25 //m^3/s

```

```

13 Q=2.764*10^8 //J/h
14 cp=29.3*10^3
15 //calculations
16 rho1= P*M/(T1*R)
17 u1=mass/(%pi/4 *d1^2)
18 rho2= P2*M/(R*T2)
19 u2=u1*d1^2 *rho1/(d2^2 *rho2)
20 Wsd= (u2^2 - u1^2 )/2 + cp/M *(T2-T1) + Q/(mass*rho1
      *3600)
21 mdot= u1*%pi/4 *d1^2 *rho1
22 Ws=Wsd*mdot/745.7
23 //results
24 printf("Power input to the compressor = %d hp",Ws)

```

Scilab code Exa 3.8 Example 8

```

1 clc
2 clear
3 //Initialization of variables
4 u1=1.1 //m/s
5 rho1=1.21*10^3 //kg/m^3
6 d1=0.078
7 z1=4
8 h2=18 //m
9 g=9.806
10 //calculations
11 mdot= u1*rho1*%pi/4 *d1^2
12 Wsd= z1+h2
13 Ws=Wsd*mdot*g
14 dP= Ws*rho1/mdot
15 //results
16 printf("Power input = %d W",Ws)
17 printf("Pressure drop = %.3 f Mpa",dP/10^6)

```

Scilab code Exa 3.9 Example 9

```
1  clc
2  clear
3  // Initialization of variables
4  eff=0.75
5  Hf=[-110600 -241980 -393770 0]
6  Hc=[30.35 36 45.64 29.30]
7  T2=540 //C
8  T1=25 //C
9  mass=500 //kmol H2 produced
10 // calculations
11 dHr= Hf(3) + Hf(4) - Hf(1) -Hf(2)
12 dHpr= (eff*(Hc(3) +Hc(4)) + (1-eff)*(Hc(2)+Hc(1)))*(
      T2-T1)
13 q= dHr*eff +dHpr
14 heat = q*mass/eff
15 // results
16 printf("Heat produced = %.3e kJ",heat)
```

Scilab code Exa 3.10 Example 10

```
1  clc
2  clear
3  // Initialization of variables
4  eff=0.75
5  Hf=[-110600 -241980 -393770 0]
6  Hc=[30.35 36 45.64 29.30]
7  T2=540 //C
8  T1=25 //C
9  mass=500 //kmol H2 produced
10 work=10^6 //kJ
```

```

11 // calculations
12 dHr= Hf(3) + Hf(4) - Hf(1) -Hf(2)
13 dHpr= (eff*(Hc(3) +Hc(4)) + (1-eff)*(Hc(2)+Hc(1)))*(
      T2-T1)
14 q= dHr*eff +dHpr
15 heat = q*mass/eff
16 qe=heat-work
17 // results
18 printf("Heat produced = %.3e kJ",qe)

```

Scilab code Exa 3.11 Example 11

```

1 clc
2 clear
3 // Initialization of variables
4 so3=6
5 h2=-296840 //kJ/kmol
6 h3=-395720 //kJ/kmol
7 t2=400 //C
8 t1=25 //C
9 // calculations
10 Hr=so3*(h3-h2)
11 cp=[1.059 0.967 0.714]
12 n=[82.76 11 8]
13 M=[28 32 64]
14 Ht= sum(cp.*n.*M)
15 Hre=Ht*(t2-t1)
16 Hpr=Hre-Hr
17 Tf=t1 + Hpr/3261.6
18 // results
19 printf("temperature of exit gases = %d C",Tf)

```

Scilab code Exa 3.12 Example 12

```
1 clc
2 clear
3 // Initialization of variables
4 x=0.25
5 Hr=1.4278*10^6 //kJ/kmol
6 ti=25 //C
7 cp=[1.24 2.39 1.11]
8 M=[44 18 32]
9 z=[12 3 0.5]
10 r=4.186
11 // calculations
12 v=cp.*M.*z
13 v2=sum(v)
14 T=ti+ Hr/(v2)
15 // results
16 printf(" Theoretical temperature = %d C",T)
```

Chapter 4

The Second Law of Thermodynamics and its Applications

Scilab code Exa 4.1 Example 1

```
1  clc
2  clear
3  // Initialization of variables
4  T=500 //K
5  Qr=5*10^6 //kJ
6  T2=600 //K
7  // calculations
8  dSS=Qr/T
9  dSS2=-Qr/T2
10 Ds=dSS+dSS2
11 // results
12 printf("Entropy change of the system = %d kJ/K",dSS)
13 printf("\n Entropy change of the surroundings = %d
    kJ/K",dSS2)
14 printf("\n Entropy change if the universe = %d kJ/K"
    ,Ds)
```

Scilab code Exa 4.2 Example 2

```
1  clc
2  clear
3  // Initialization of variables
4  p1=2.758 //Mpa
5  p2=0.552 //Mpa
6  T1=700 //K
7  T2=700 //K
8  n=1
9  R=8.3143
10 Cv=21
11 Cp=29.3
12 // calculations
13 dsa=n*R*log(p1/p2)
14 T3=437.5 //K
15 dsb=Cv*log(T3/T2)
16 T4=350 //K
17 dsc=Cp*log(T4/T3)
18 T5=634 //K
19 dsd=0
20 T6=700 //K
21 dse=Cp*log(T6/T5)
22 dstotal=dsa+dsb+dsc+dsd+dse
23 // results
24 printf("Entropy change in case a = %.3f kJ/kmol K",
        dsa)
25 printf("\n Entropy change in case b = %.3f kJ/kmol K
        ",dsb)
26 printf("\n Entropy change in case c = %.3f kJ/kmol K
        ",dsc)
27 printf("\n Entropy change in case d = %.3f kJ/kmol K
        ",dsd)
28 printf("\n Entropy change in case e = %.3f kJ/kmol K
```

```

    ",dse)
29 printf("\n Entropy change in total process = %.3f kJ
    /kmol K",dstotal)

```

Scilab code Exa 4.3 Example 3

```

1
2 clc
3 clear
4 //Initialization of variables
5 ratio=1/2
6 R=8.314
7 p1=0.5 //kPa
8 p2=0.1 //kPa
9 //calculations
10 ya=ratio/(1+ratio)
11 ds=-ya*R*log(ya) - (1-ya)*R*log(1-ya)
12 dss=R*log(p1/p2)
13 //results
14 printf("Entropy of mixing = %.3f kJ/kmol K",ds)
15 printf("\n Total entropy change of the universe = %
    .2f kJ/kmol K",dss)

```

Scilab code Exa 4.4 Example 4

```

1 clc
2 clear
3 //Initialization of variables
4 s1=7.096 //kJ/kg K
5 s2=7.915 //kJ/kg K
6 s3=7.16 //kJ/kg K
7 s4=7.014 //kJ/kg K
8 s5=6.999 //kJ/kg K

```

```

 9 //calculations
10 dsa=s2-s1
11 dsb=s3-s2
12 dsc=s4-s3
13 dsd=s5-s4
14 dse=s1-s5
15 dstotal=dsa+dsb+dsc+dsd+dse
16 //results
17 printf("Change in entropy in process a =%.3f kJ/kg
    K",dsa)
18 printf("\n Change in entropy in process b =%.3f kJ/
    kg K",dsb)
19 printf("\n Change in entropy in process c =%.3f kJ/
    kg K",dsc)
20 printf("\n Change in entropy in process d =%.3f kJ/
    kg K",dsd)
21 printf("\n Change in entropy in process e =%.3f kJ/
    kg K",dse)
22 printf("\n Change in entropy in total process =%.3f
    kJ/kg K",dstotal)

```

Scilab code Exa 4.5 Example 5

```

1 clc
2 clear
3 //Initialization of variables
4 m1=5000 //kg/h
5 cp1=3.2 //kJ/kg K
6 cp2=4.186 //kJ/kg K
7 t1=220 //C
8 t2=30 //C
9 T1=210 //C
10 T2=20 //C
11 //calculations
12 m2=m1*cp1*(t1-t2)/(cp2*(T1-T2))

```

```
13 ds=m1*cp1*log((t2+273.1)/(t1+273.1)) + m2*cp2*log((
    T1+273.1)/(T2+273.1))
14 //results
15 printf("Change in entropy = %d kJ/h K",ds)
```

Scilab code Exa 4.6 Example 6

```
1
2 clc
3 clear
4 //Initialization of variables
5 s1=218.8 //kJ/kmol K
6 s2=188.85 //kJ/kmol K
7 s3=237.8 //kJ/kmol K
8 s4=205.2 //kJ/kmol K
9 //calculations
10 ds=s1+s2-s3-0.5*s4
11 //results
12 printf("Entropy change = %.2f kJ/kmol K",ds)
```

Scilab code Exa 4.7 Example 7

```
1 clc
2 clear
3 //Initialization of variables
4 Q=6 //kJ/kg
5 p1=1.5 //Mpa
6 p2=0.1 //Mpa
7 t1=500 //C
8 t2=140.8 //C
9 h1=3473.1 //kJ
10 h2=2758.1 //kJ
11 s1=7.5698 //kJ/K
```

```

12 s2=7.5698 //kJ/K
13 eff=0.85
14 Ts=293.1 //K
15 //calculations
16 Wideal=h2-h1
17 Ws=eff*Wideal
18 dH=-Q-Ws
19 H2=h1+dH
20 S2=7.8005
21 ds=S2-s1
22 Wlost=Ts*ds+Q
23 //results
24 printf("lost work = %.1f kJ",Wlost)

```

Scilab code Exa 4.8 Example 8

```

1 clc
2 clear
3 //Initialization of variables
4 m=5000 ///kg/h
5 cp=3.2 //kJ/kg K
6 Ts=30+273.1 //K
7 t1=220 //C
8 t2=40 //C
9 Q=2.88*10^6 //kJ
10 //calculations
11 Q=m*cp*(t2-t1)
12 dss=m*cp*log((t2+273.1)/(t1+273.1))
13 Wlost=Ts*dss-Q
14 eff=Ts*dss/Q
15 //results
16 printf("Lost work = %d kJ",Wlost)
17 printf("\n Efficiency = %.3f",eff)

```

Scilab code Exa 4.9 Example 9

```
1  clc
2  clear
3  // Initialization of variables
4  R=8.314
5  cp=35.58
6  n=100/16
7  T1=300 //K
8  T2=500 //K
9  k=1.305
10 P2=3 //Mpa
11 P1=0.5 //Mpa
12 Ts=290 //K
13 // calculations
14 cv=cp-R
15 Wi=n*R*T1/(k-1) * ((P2/P1) ^ ((k-1)/k) -1)
16 Hi=Wi
17 Ha=n*cp*(T2-T1)
18 eta=abs(Hi/Ha)
19 dss1=cp*log(T2/T1) - R*log(P2/P1)
20 Wl1=Ts*dss1
21 dss2=n*cp*log(T2/T1)
22 dss3=abs(Ha/Ts)
23 dsst=dss2+dss3
24 Wl2=-Ts*dss2 +Ha
25 Wlost=Wl1+Wl2
26 // results
27 printf("Thermodynamic efficiency = %.3f",eta)
28 printf("\n Net work lost = %d kJ",Wlost)
```

Scilab code Exa 4.10 Example 10

```

1  clc
2  clear
3  // Initialization of variables
4  T1=673 //K
5  T2=293 //K
6  // calculations
7  eta=(T1-T2)/T1
8  // results
9  if eta>=0.5 then
10     printf("Max efficiency = %.3f and an efficiency
              of 0.5 is possible",eta)
11 else
12     printf("Max efficiency = %.3f and an efficiency
              of 0.5 is not possible",eta)
13 end

```

Scilab code Exa 4.11 Example 11

```

1  clc
2  clear
3  // Initialization of variables
4  T1=280 //K
5  T2=300 //K
6  // calculations
7  cop=T1/(T2-T1)
8  // results
9  printf("coefficient of performance = %.1f",cop)

```

Scilab code Exa 4.12 Example 12

```

1  clc
2  clear
3  // Initialization of variables

```



```

4 P=2 //Mpa
5 T1=212.4+273.1 //K
6 T2=25+273.1 //K
7 h1=2799.5
8 h2=104.89
9 s1=6.3409
10 s2=0.3674
11 //calculations
12 dh=h1-h2
13 ds=s1-s2
14 exergy=dh-T2*ds
15 //results
16 printf("exergy = %.1f kJ/kg",exergy)

```

Scilab code Exa 4.13 Example 13

```

1 clc
2 clear
3 //Initialization of variables
4 R=8314.3
5 T=700 //K
6 T2=437.5 //K
7 T3=350 //K
8 T4=T3
9 p2=0.552 //Mpa
10 p1=2.758 //Mpa
11 p3=0.345 //Mpa
12 cp=29.3
13 R0=8.3143
14 k=1.4
15 n=1
16 P0=0.103 //Mpa
17 //calculations
18 cv=cp-R0
19 p3=p2*T3/T2

```

```

20 p3=0.345
21 T5=T4*(p1/p3)^((k-1)/k)
22 G1=n*R*T*log(p2/p1)
23 V700=R*10^3 *T/(p2*10^9)
24 Sa= 209
25 Sb=199.2
26 Sc=204.7
27 S2=(T2-T)/6 *(Sa+4*Sc+Sb      )
28 G2=V700*(p3-p2)*10^3 -S2
29 saa=199.2
30 sbb=192.6
31 savg=(saa+sbb)*0.5
32 G3=-savg*(T3-T2)
33 pmid=(p3+p2)/2
34 vmid=2.88
35 sav=192.7
36 v4=8.435 //m^3
37 v5=1.911 //m^3
38 integ=(p1-p3)*10^3 /6 *(v4+4*vmid+v5)
39 G4=integ - sav*(T5-T3)
40 Sav=194.25
41 G5= -Sav*(T-T5)
42 Gt=G1/10^3 +G2+G3+G4+G5
43 //results
44 printf("in case 1, Change in gibbs free energy = %d
      kJ",G1/10^3)
45 printf("\n in case 2, Change in gibbs free energy =
      %d kJ",G2)
46 printf("\n in case 3, Change in gibbs free energy =
      %d kJ",G3)
47 printf("\n in case 4, Change in gibbs free energy =
      %d kJ",G4)
48 printf("\n in case 5, Change in gibbs free energy =
      %d kJ",G5)
49 printf("\n Net change in gibbs energy = %d kJ",Gt)

```

Scilab code Exa 4.14 Example 14

```
1
2 clc
3 clear
4 // Initialization of variables
5 v=1/430
6 pi=4.08 //Mpa
7 pf=10 //Mpa
8 pf2=1 //Mpa
9 pii=0.1 //Mpa
10 R=8314.3
11 n=1/28
12 T=273.1
13 // calculations
14 logpr=v*(pf-pii)*10^6 /(R*T*n)
15 pr=exp(logpr)
16 p=pr*pi
17 logpr=v*(pf2-pii)*10^6 /(R*T*n)
18 pr=exp(logpr)
19 p2=pr*pi
20 // results
21 printf("Final pressure = %.2f Mpa",p)
22 printf("\\n Final pressure in case 2 = %.2f Mpa",p2)
```

Scilab code Exa 4.15 Example 15

```
1 clc
2 clear
3 // Initialization of variables
4 Hvap=338.14 //kJ/kg
5 T=409.3 //K
```

```

6 //calculations
7 dss=Hvap/T
8 dg=0
9 //results
10 printf("change in entropy and gibbs energy of system
        are %.3f kJ/kg K and %d kJ/kg respectively",dss,
        dg)
11 printf("\n change in entropy and gibbs energy of
        universe are %.3f kJ/kg K and %d kJ/kg
        respectively",-dss,-dg)

```

Scilab code Exa 4.16 Example 16

```

1 clc
2 clear
3 //Initialization of variables
4 T=373.1 //K
5 R=8314.3
6 Pd=0.1013*10^6 //Pa
7 P=10 //Mpa
8 p3=5*10^6 //Pa
9 vf=0.0373
10 a=424.447
11 //calculations
12 Vd=R*T/Pd
13 V=0.5
14 dss=-R*(log(p3/Pd) + log((V-vf)/(Vd-vf)))
15 dhh=R*T/10^3 - p3/10^3 *V+ a/V^2
16 //results
17 printf("Change in entropy = %.4f kJ/kmol K",dss
        /10^3)
18 printf("\n change in enthalpy= %d kJ/kmol",dhh)

```

Scilab code Exa 4.18 Example 18

```
1  clc
2  clear
3  // Initialization of variables
4  Tc=647.3 //K
5  dh=1.1
6  Db=-2
7  v2=0.234
8  v1=0.27
9  // calculations
10 dh2=dh+Db*(v2-v1)
11 dhh=dh2*Tc
12 dhbar=dhh*4.18/18
13 disp("From steam tables ,")
14 h1=3777.5 //kJ/kg
15 h2=3928.2 //kJ/kg
16 dhs=h2-h1
17 err=abs(dhs-dhbar)/dhs
18 // results
19 printf("Enthalpy departure = %d kJ/kg",dhbar)
20 printf("\\n Percentage error = %.1f ",err*100)
```

Scilab code Exa 4.19 Example 19

```
1  clc
2  clear
3  // Initialization of variables
4  w=0.3448
5  R=8.3143
6  Tc=647.3
7  // calculations
8  disp("From charts of entropy")
9  h0=0.57
10 h1=0.05
```

```

11 h2=h0+w*h1
12 h3=h2*R*Tc
13 dh=-h3
14 //results
15 printf("Enthalpy departure = %d kJ/kmol",dh)
16 disp("The answer is a bit different due to rounding
      off error in the textbook")

```

Scilab code Exa 4.20 Example 20

```

1  clc
2  clear
3  //Initialization of variables
4  ta=310 //K
5  pa=80 //kPa
6  r=10
7  k=1.4
8  R=8.3143
9  n=5/29
10 cv=20.93
11 //calculations
12 Qab=0
13 tb=ta*r^(k-1)
14 va=R*ta/pa
15 vb=va/r
16 pb=R*tb/vb
17 Wab= -n*R*ta/(k-1) *((pb/pa)^((k-1)/k) -1)
18 vc=vb
19 Qbc=500 //kJ
20 Wbc=0
21 tc=tb+ Qbc/(n*cv)
22 pc=R*tc/vc
23 Qcd=0
24 td=tc/r^(k-1)
25 vd=va

```

```

26 pd=td/tc*(vc/vd)*pc
27 Wcd=-n*R*tc/(k-1) *((pd/pc)^((k-1)/k)-1)
28 Wda=0
29 Qda=n*cv*(ta-td)
30 eta0=1-1/r^(k-1)
31 //results
32 printf("Efficiency of cycle = %.3f",eta0)
33 p=[pa pb pc pd]
34 t=[ta tb tc td]
35 Q=[Qab Qbc Qcd Qda]
36 W=[Wab Wbc Wcd Wda]
37 disp('Pressure (kPa) = ')
38 format('v',6);p
39 disp(p)
40 disp("Temperature (K)= ")
41 format('v',6);t
42 disp(t)
43 disp("Heat (kJ)= ")
44 format('v',6);Q
45 disp(Q)
46 disp("Work done (kJ) = ")
47 format('v',6);W
48 disp(W)

```

Scilab code Exa 4.21 Example 21

```

1 clc
2 clear
3 //Initialization of variables
4 ta=310 //K
5 tc=917.3 //K
6 td=365.2 //K
7 n=0.602
8 k=1.4
9 //calculations

```

```

10 lntb= 1/(1-n)/k
11 tb=tc- lntb*(td-ta)
12 rc=(tb/ta)^(1/(k-1))
13 //results
14 printf("Temperature at B = %.1f K",tb)
15 printf("\n Compression ratio = %d ",rc)
16 disp("The answer given in textbook for rc is wrong.
      please check using a calculator")

```

Scilab code Exa 4.22 Example 22

```

1  clc
2  clear
3  //Initialization of variables
4  pr=4
5  k=1.4
6  ta=298 //K
7  pa=0.1 //Mpa
8  pdr=0.01
9  tc=900 //K
10 pri=0.005 //Mpa
11 //calculations
12 pb=pr*pa
13 nji=1- (pr)^((1-k)/k)
14 tb=ta*(pb/pa)^((k-1)/k)
15 pc=pb-pdr
16 pd=pa+pri
17 td=tc*(pd/pc)^((k-1)/k)
18 //results
19 p=[pa pb pc pd]
20 t=[ta tb tc td]
21 printf("ideal thermal efficiency = %.3f ",nji)
22 disp(" pressure (Mpa) = ")
23 format('v',6);p
24 disp(p)

```



```
25 disp("temperature (K) = ")
26 format('v',6);t
27 disp(t)
```

Scilab code Exa 4.23.a Example 23a

```
1 clc
2 clear
3 // Initialization of variables
4 sd=4.9269//kJ/kg/K
5 sf=1.1453//kJ/kg/K
6 sg=7.5320//kJ/kg/K
7 hf=359.86//kJ/kg
8 hg=2653.5//kJ/kg
9 hd=2409.7//kJ/kg
10 // calculations
11 x=(sd-sg)/(sf-sg)
12 he=x*hf+(1-x)*hg
13 etar=(hd-he)/(hd-hf)
14 // results
15 printf("Thermal efficiency = %.4f",etar)
```

Scilab code Exa 4.23.b Example 23b

```
1 clc
2 clear
3 // Initialization of variables
4 sd=6.7039//kJ/kg/K
5 sf=1.1453//kJ/kg/K
6 sg=7.5320//kJ/kg/K
7 hf=359.86//kJ/kg
8 hg=2653.5//kJ/kg
9 hd=3717.9//kJ/kg
```

```

10 // calculations
11 x=(sd-sg)/(sf-sg)
12 he=x*hf+(1-x)*hg
13 etar=(hd-he)/(hd-hf)
14 // results
15 printf("Thermal efficiency = %.4f",etar)

```

Scilab code Exa 4.24 Example 24

```

1 clc
2 clear
3 // Initialization of variables
4 ha=2510.6 //kJ/kg
5 hd=125.78 //kJ/kg
6 // calculations
7 kg=(10^6)/(ha-hd)
8 // results
9 printf("circulation rate = %d kg steam/h",kg)

```

Scilab code Exa 4.25 Example 25

```

1 clc
2 clear
3 // Initialization of variables
4 tin=298 //K
5 tout=273 //K
6 tout2=308 //K
7 tin2=294 //K
8 // calculations
9 eta1=(tin-tout)/tin
10 eta2=abs((tin2-tout2)/tin2)
11 // results
12 printf("Efficiency in case 1 = %.3f",eta1)

```

```
13 printf("\n efficiency in case 2 = %.3f", eta2)
```

Scilab code Exa 4.26 Example 26

```
1 clc
2 clear
3 // Initialization of variables
4 ma=500 //kg/h
5 cp1=3.2 //kJ/kg K
6 ta=20 //C
7 mb=200
8 mc=300 //kg/h
9 cp2=2.8 //kJ/kg K
10 tc=80 //C
11 tb=80 //C
12 me=50 //kg/h
13 te=120 //C
14 td=120 //C
15 hg=503.7
16 he=2706.3
17 // calculations
18 Ws=(mb+me)*hg + mc*cp2*(tc) - me*he -ma*cp1*(ta)
19 // results
20 printf("Net work done = %d kJ/h", Ws)
```

Scilab code Exa 4.27 Example 27

```
1 clc
2 clear
3 // Initialization of variables
4 hc=150 //Btu/lb
5 he=-115 //Btu/lb
6 hg=168 //Btu/lb
```

```
7 // calculations
8 frac=(hg-hc)/(hg-he)
9 // results
10 printf("Fraction of solid = %.3f",frac)
```

Scilab code Exa 4.28 Example 28

```
1 clc
2 clear
3 // Initialization of variables
4 H=2696.5 //kJ/kg
5 hg=2706.7 //kJ/kg
6 hf=504.7 //kJ/kg
7 // calculations
8 x= (H-hf)/(hg-hf)
9 x2=1
10 // results
11 printf("In case 1, fraction of vapor = %.3f",x)
12 printf("\n In case 2, fraction of vapor = %.3f",x2)
```

Chapter 5

Relationships among Thermodynamic Properties Graphical Representation of properties and processes

Scilab code Exa 5.5 Example 5

```
1
2 clc
3 clear
4 // Initialization of variables
5 R=8314.3
6 b=0.0306 //m^3/kmol
7 a=0.548*10^6 //pa m^6/kmol^6
8 T=973.1
9 P=25*10^6 //Pa
10 // calculations
11 Vi= R*T/P
12 x=poly(0, 'x')
13 vec=roots(P*x^2 *(x-b) +a*(x-b) - R*T*(x^2))
14 volume= vec(1)
15 dH=8.0906*10^6 -P*volume +0.548*10^6 /volume
```

```
16 //results
17 printf("Change in enthalpy = %.2e J/kmol",dH)
```

Chapter 7

Solution Properties and Physical Equilibria

Scilab code Exa 7.2 Example 2

```
1  clc
2  clear
3  //Initialization of variables
4  T=154.5 //C
5  P=8620*10^3 //Pa
6  Tc=135 //C
7  T0=273.1 //C
8  Pc=3648*10^3 //Pa
9  w=0.1756
10 V=0.154
11 R=8.3143*10^3
12 //calculations
13 Tr=(T+T0)/(T0+Tc)
14 Pr= P/Pc
15 Z=P*V/(R*(T+T0))
16 a= 0.42747*R^2 *(Tc+T0)^2 /Pc *(1+ (0.48508 +
    1.55171*w - 0.15613*w^2)*(1-sqrt(Tr)))^2
17 b=0.08664*R*(Tc+T0)/Pc
18 A= a*P/(R^2 *(T+T0)^2)
```

```

19 B=b*P/(R*(T+T0))
20 lnphi= (Z-1) - log(Z-B) - A/B *log((Z+B)/Z)
21 phi=exp(lnphi)
22 f=phi*P
23 //results
24 printf("fugacity = %d kPa",f/10^3)
25 //The answer is a bit different due to rounding off
    error in textbook

```

Scilab code Exa 7.3 Example 3

```

1  clc
2  clear
3  //Initialization of variables
4  T=154.5 //C
5  P=8620*10^3 //Pa
6  Tc=135 //C
7  T0=273.1 //C
8  Pc=3648*10^3 //Pa
9  w=0.1756
10 V=0.154
11 R=8.3143*10^3
12 D=0.35
13 Vc=0.263 //m^3/kmol
14 //calculations
15 Tr=(T+T0)/(T0+Tc)
16 Pr= P/Pc
17 Zc=Pc*Vc/(R*(Tc+T0))
18 phi1=0.44
19 phi2=phi1*10^(D*(Zc-0.27))
20 f=phi2*P
21 //results
22 printf("fugacity = %d kPa",f/10^3)

```

Scilab code Exa 7.4 Example 4

```
1  clc
2  clear
3  // Initialization of variables
4  f0=0.7
5
6  V=5.1e-2
7  P1=0.77 //Mpa
8  P2=10 //Mpa
9  R=8.3143*10^3
10 T=298 //K
11 // calculations
12 lnr= V/(R*T) *(P2-P1)*10^6
13 f=exp(lnr) *f0
14 // results
15 printf("Fugacity = %.3f Mpa",f)
```

Scilab code Exa 7.5 Example 5

```
1  clc
2  clear
3  // Initialization of variables
4  Pt=0.1013
5  ya=0.605
6  P1=0.1373
7  P2=0.06
8  xa=0.4
9  // calculations
10 if ya*Pt == xa*Pt & (1-ya)*Pt == (1-xa)*Pt then
11     printf("The system is ideal")
12 else
```

```
13     printf("The system is not ideal")
14 end
```

Scilab code Exa 7.6 Example 6

```
1  clc
2  clear
3  // Initialization of variables
4  Y=0.06
5  X=0.0012
6  P=2.53 //Mpa
7  // calculations
8  y=Y/(1+Y)
9  x=X/(1+X)
10 H=y*P/x
11 // results
12 printf("Henrys law constant = %.2 f Mpa" ,H)
```

Scilab code Exa 7.7 Example 7

```
1  clc
2  clear
3  // Initialization of variables
4  Hi=55
5  Pi=11.8
6  xi=0.514
7  H2=18.1
8  H3=26.9
9  Pi2=17.4
10 // calculations
11 ai=Pi/Hi
12 gam=ai/xi
13 a2=Pi/H2
```

```
14 gam2=a2/xi
15 a3=Pi2/H3
16 gam3=a3/(1-xi)
17 //results
18 disp("part a")
19 printf("Activity of acetic acid = %.4f ",a1)
20 printf("\n Activity coefficient = %.4f ",gam)
21
22 disp("part b")
23 printf("Activity of acetic acid = %.4f ",a2)
24 printf("\n Activity coefficient = %.4f ",gam2)
25
26 disp("part c")
27 printf("Activity of toluene = %.4f ",a3)
28 printf("\n Activity coefficient = %.4f ",gam3)
```

Chapter 8

Physical Equilibria among Phases

Scilab code Exa 8.1 Example 1

```
1 clc
2 clear
3 //Initialization of variables
4 function V = func(C,phi)
5     V=C+2-phi
6 endfunction
7 //calculations and results
8 disp("part a")
9 printf("degrees of freedom = %d ",func(2,2))
10 disp("part b")
11 printf("degrees of freedom = %d ",func(3,2))
12 disp("part c")
13 printf("degrees of freedom = %d ",func(3,3))
```

Scilab code Exa 8.2 Example 2

```

1  clc
2  clear
3  // Initialization of variables
4  T=95 //C
5  P=1013 //kPa
6  Tc=135 //C
7  Pc=3648 //kPa
8  T0=273.1 //C
9  D=0.3
10 P0=1800 //kPa
11 D2=0.42
12 // calculations
13 Zc=0.283
14 Tr=(T+T0)/(Tc+T0)
15 Pr=P/Pc
16 phic=0.88
17 phi2=phic*10^(D*0.013)
18 Prd= P0/Pc
19 phi3=0.78
20 phi4= phi3*10^(D2*0.013)
21 g1= phi2*P/(phi3*P0)
22 // results
23 printf("equation is g1 = %.3f *(y/x)",g1)

```

Scilab code Exa 8.3 Example 3

```

1  clc
2  clear
3  // Initialization of variables
4  ye=0.434
5  Pt=40.25 //kPa
6  xe=0.616
7  Pe1=22.9 //kPa
8  Pe2=29.6 //kPa
9  // calculations

```

```

10 ge= ye*Pt/(xe*Pe1)
11 gb=(1-ye)*Pt/((1-xe)*Pe2)
12 E= log10(ge) *(1+ (1-xe)*log(gb) /(xe*log(ge)))^2
13 B= log10(gb) *(1+ xe/(1-xe) *log(ge) /log(gb))^2
14 xe2=0.4
15 xb2=0.6
16 lnge2=E/(1+ E*xe2/(B*xb2))^2
17 lngb2=B/(1+ B*xb2/(E*xe2))^2
18 ge2=10^(lnge2)
19 gb2=10^(lngb2)
20 Pt1=ge2*Pe1
21 Pt2=gb2*Pe2
22 //results
23 printf("Total pressure in case 1 = %.2f kPa and in
        case 2 = %.2f kPa",Pt1, Pt2 )

```

Scilab code Exa 8.4 Example 4

```

1  clc
2  clear
3  //Initialization of variables
4  k4=1.8
5  k5=0.8
6  //calculations
7  A=[k4 k5;1 1]
8  b=[1; 1]
9  C=A\b
10 x4=C(1)
11 x5=C(2)
12 y4=k4*x4
13 y5=k5*x5
14 //results
15 printf("Vapor and liquid mole fractions of component
        1 = %.2f and %.2f respectively",y4,x4)
16 printf("\n Vapor and liquid mole fractions of

```

component 2 = %.2f and %.2f respectively",y5,x5)

Scilab code Exa 8.5 Example 5

```
1  clc
2  clear
3  // Initialization of variables
4  v1=81 //cm^3/gmol
5  v2=97 //cm^3/gmol
6  d1=9.2 //(cal/cm^3)^0.5
7  d2=8.6 //(cal/cm^3)^0.5
8  R=1.987
9  T=373.1 //K
10 // calculations
11 d=0.5*(d1+d2)
12 lng1=v1*(d1-d)^2 /(R*T)
13 lng2=v2*(d2-d)^2 /(R*T)
14 g1=exp(lng1)
15 g2=exp(lng2)
16 // results
17 printf("Activity coefficients of components are %.3f
    and %.3f respectively",g1,g2)
```

Scilab code Exa 8.6 Example 6

```
1  clc
2  clear
3  // Initialization of variables
4  xe=0.3
5  xe2=0.9
6  Pe0=810
7  Pa0=470
8  ge=1.85
```

```

9 ge2=1.05
10 ga=1.15
11 ga2=3
12 Pt=820 //mm
13 Pt2=900 //mm
14 //calculations
15 ye=ge*xe*Pe0/Pt
16 ya=ga*(1-xe)*Pa0/Pt
17 yt=ye+ya
18 ye2=ye/yt
19 ya2=ya/yt
20 ye3=ge2*xe2*Pe0/Pt2
21 ya3=ga2*(1-xe2)*Pa0/Pt2
22 yt2=ye+ya
23 ye4=ye3/yt2
24 ya4=ya3/yt2
25 //results
26 printf("In case 1, ye = %.3f and ya = %.3f",ye2,ya2)
27 printf("\n In case 1, ye = %.3f and ya = %.3f",ye4,
ya4)
28 disp('The calculations of ya in case 1 in textbook
is wrong. please use a calculator')

```

Scilab code Exa 8.7 Example 7

```

1 clc
2 clear
3 //Initialization of variables
4 m1=121
5 m2=18
6 p1=0.0042
7 p2=0.0858
8 //calculations
9 massfrac= (p1*m1)/(p1*m1+p2*m2)
10 //results

```



```
11 printf("mass fractions of DMA and water are %.3f and  
    %.3f respectively",massfrac,1-massfrac)
```

Scilab code Exa 8.9 Example 9

```
1 clc  
2 clear  
3 // Initialization of variables  
4 FR=25  
5 FE=19  
6 bf=130 //kg  
7 af=85 //kg  
8 // calculations  
9 law=FR/FE  
10 x1=45/150  
11 x2=65/150  
12 ER=18.5/6  
13 e=[0.5 0.1 0.9]  
14 r=[0.28 0.96 0.04]  
15 et=sum(e)  
16 rt=sum(r)  
17 ett=e/et  
18 rtt=r/rt  
19 // results  
20 disp("the compositions of raffinate are ")  
21 disp(rtt)  
22 disp("the compositions of extract are")  
23 disp(ett)
```

Scilab code Exa 8.10.a Example 10a

```
1 clc  
2 clear
```

```

3 //Initialization of variables
4 v1=0.1316
5 v2=0.2941
6 x1=0.5
7 x2=0.2
8 x3=0.8
9 d1=14.87
10 d2=16.34
11 //calculations and results
12 vm=x1*(v1+v2)
13 phi1=x1*v1/vm
14 phi2=(1-x1)*v2/vm
15 H11=vm*phi1*phi2*(d1-d2)^2 *10^3
16 disp(" case 1")
17 printf("enthalpy = %.1f kJ/mol",H11)

```

Scilab code Exa 8.10.b Example 10b

```

1 clc
2 clear
3 //Initialization of variables
4 v1=0.1316
5 v2=0.2941
6 x1=0.5
7 x2=0.2
8 x3=0.8
9 d1=14.87
10 d2=16.34
11 //calculations and results
12 vm=(1-x2)*v1+x2*v2
13 phi1=(1-x2)*v1/vm
14 phi2=(x2)*v2/vm
15 H12=vm*phi1*phi2*(d1-d2)^2 *10^3
16 disp(" case 2")
17 printf("enthalpy = %.1f kJ/mol",H12)

```

Scilab code Exa 8.10.c Example 10c

```
1  clc
2  clear
3  // Initialization of variables
4  v1=0.1316
5  v2=0.2941
6  x1=0.5
7  x2=0.2
8  x3=0.8
9  d1=14.87
10 d2=16.34
11 // calculations and results
12 vm=(1-x3)*v1+x3*v2
13 phi1=(1-x3)*v1/vm
14 phi2=(x3)*v2/vm
15 H13=vm*phi1*phi2*(d1-d2)^2 *10^3
16 disp(" case 3")
17 printf(" enthalpy = %.1f kJ/mol",H13)
```

Chapter 9

Chemical Equilibria

Scilab code Exa 9.1.a Example 1a

```
1 clc
2 clear
3 //Initialization of variables
4 g11=178900 //kJ/kmol
5 g12=207037 //kJ/kmol
6 g21=211852 //kJ/kmol
7 g22=228097 //kJ/kmol
8 //calculations
9 dG=g21-g11
10 //results
11 printf("Standard free energy change = %d kJ/kmol" ,dG
    )
```

Scilab code Exa 9.1.b Example 1b

```
1 clc
2 clear
3 //Initialization of variables
```

```

4 m1=54.1
5 m2=56.1
6 m3=2
7 cp1=2.122 //kJ/kmol K
8 cp2=2.213 //kJ/kmol K
9 cp3=14.499 //kJ/kmol K
10 hf1=110200 //kJ/kmol
11 hf2=-126 //kJ/kmol
12 T=700 //K
13 Ts=298 //K
14 // calculations
15 hf=hf1-hf2
16 cpn=cp1*m1-cp2*m2+cp3*m3
17 h700=hf+ cpn*(T-Ts)
18 s298=103.7
19 s700 = s298 + cpn*log(T/Ts)
20 G700=h700-T*s700
21 // results
22 printf("Change in gibbs energy = %d kJ/kmol",G700)
23 disp("The answer is a bit different due to rounding
      off error in textbook")

```

Scilab code Exa 9.2 Example 2

```

1 clc
2 clear
3 // Initialization of variables
4 g1=150670 //kJ/kmol
5 g2=71500 //kJ/kmol
6 R=8.314
7 Ts=298 //K
8 T=700 //K
9 // calculationd
10 G=g1-g2
11 G2=33875 //kJ/kmol

```

```

12 K1=exp(-G/R/Ts)
13 K2=exp(-G2/R/T)
14 //results
15 printf("In case 1, equilibrium constant = %.2e",K1)
16 printf("\n In case 2, equilibrium constant = %.5f",
    K2)

```

Scilab code Exa 9.3 Example 3

```

1  clc
2  clear
3  //Initialization of variables
4  R=8.3143
5  T1=1273 //K
6  T2=2273 //K
7  k2=0.0018
8  A=123.94
9  B=7.554
10 C=8.552*10^-3
11 D=-13.25e-6
12 E=7.002e-9
13 F=13.494e-13
14 //calculations
15 function y= cp(T)
16     y=A/T^2 +B/T +C +D*T +E*T^2 -F*T^3
17 endfunction
18 lnk=1/R *intg(T1,T2,cp)
19 k1=k2/ exp(lnk)
20 //results
21 printf("Equilibrium constant = %.5f ",k1)

```

Scilab code Exa 9.4.a Example 4a

```

1  clc
2  clear
3  // Initialization of variables
4  G=-30050 //kJ/kmol
5  R=8.314
6  T=573 //K
7  // calculations
8  lnk=G/(R*T)
9  k=exp(lnk)
10 x=poly(0,"x")
11 vec=roots(4*x^2 - k*(1-x)^2)
12 x2=vec(2)
13 // results
14 printf("Mole fraction of HCN = %.4f",x2)

```

Scilab code Exa 9.4.b Example 4b

```

1  clc
2  clear
3  // Initialization of variables
4  G=-30050 //kJ/kmol
5  R=8.314
6  T=573 //K
7  phi1=0.980
8  phi2=0.915
9  phi3=0.555
10 // calculations
11 lnk=G/(R*T)
12 k=exp(lnk)
13 kexp= k*phi1*phi2/phi3^2 /4
14 x=poly(0,"x")
15 vec=roots(x^2 - kexp*(1-x)^2)
16 x2=vec(2)
17 // results
18 printf("Mole fraction of HCN = %.4f",x2)

```

Scilab code Exa 9.5 Example 5

```
1 clc
2 clear
3 // Initialization of variables
4 kp=74
5 // calculations
6 f=poly(0,"f")
7 vec=roots(f^2 *(100-6*f) - kp^2 *(1-f)^2 *(9-6*f))
8 fn=vec(3)
9 // results
10 printf("Fractional conversion = %.3f",fn)
```

Scilab code Exa 9.6.a Example 6a

```
1 clc
2 clear
3 // Initialization of variables
4 C=3
5 phi=3
6 R=1
7 Sc=0
8 function V=fun(C,phi,R,Sc)
9     V=2+C-phi-R-Sc
10 endfunction
11 // calculations
12 V=fun(C,phi,R,Sc)
13 // results
14 printf("Degrees of freedom = %d ",V)
```

Scilab code Exa 9.6.b Example 6b

```
1 clc
2 clear
3 // Initialization of variables
4 C=3
5 phi=1
6 R=1
7 Sc=1
8 function V=fun(C,phi,R,Sc)
9     V=2+C-phi-R-Sc
10 endfunction
11 // calculations
12 V=fun(C,phi,R,Sc)
13 // results
14 printf("Degrees of freedom = %d ",V)
```

Scilab code Exa 9.6.c Example 6c

```
1 clc
2 clear
3 // Initialization of variables
4 C=6
5 phi=1
6 R=3
7 Sc=0
8 function V=fun(C,phi,R,Sc)
9     V=2+C-phi-R-Sc
10 endfunction
11 // calculations
12 V=fun(C,phi,R,Sc)
13 // results
14 printf("Degrees of freedom = %d ",V)
```

Scilab code Exa 9.7 Example 7

```
1 clc
2 clear
3 // Initialization of variables
4 a1=0.956
5 y=0.014
6 x=0.956
7 M=18
8 z=0.475
9 P=8.37 //Mpa
10 // calculations
11 m=y/(x*M) *10^3
12 w=0.0856
13 phi1=-0.04
14 phi2=0.06
15 phi=10^(phi1+ w*phi2)
16 f=z*phi*P
17 K=m/(f*a1)
18 // results
19 printf("Equilibrium constant = %.3f",K)
```

Scilab code Exa 9.9 Example 9

```
1 clc
2 clear
3 // Initialization of variables
4 y=0.18
5 z=0.6
6 // calculations
7 mole=[1-y-z 5-y-2*z y 3*y+4*z z]
8 s=sum( mole)
```

```

9 molef=mole/s
10 //results
11 disp("Product composition moles = ")
12 format('v',6);mole
13 disp(mole)
14 disp("Mole fraction = ")
15 format('v',6);molef
16 disp(molef)

```

Scilab code Exa 9.10.a Example 10a

```

1 clc
2 clear
3 //Initialization of variables
4 kp=1.09
5 feed=[ 1 5 0 0 0 ]
6 //calculations
7 x=poly(0,"x")
8 vec=roots(kp/4^4 /4 *(1-x)*(5-2*x)^2 *(6+2*x)^2 -x
          ^5)
9 x=vec(5)
10 pro=[1-x 5-2*x x 4*x 0]
11 //results
12 disp("Equilibrium composition (moles)= ")
13 format('v',6);pro
14 disp(pro)

```

Scilab code Exa 9.10.b Example 10b

```

1 clc
2 clear
3 //Initialization of variables
4 kp=1.09

```

```

5 kp2=0.154
6 feed=[ 1 5 0 0 0 ]
7 //calculations
8 x=poly(0,"x")
9 vec=roots(kp/4^4 /4 *(1-x)*(5-2*x)^2 *(6+2*x)^2 -x
           ^5)
10 x=vec(5)
11 pro=feed-[x 2*x -x -4*x 0]
12 y=poly(0,"y")
13 vec2=roots(kp2*(0.273-y)*(0.727-y)*(7.454+2*y)^2 -
            4*y^2 *(2.908+2*y)^2 *4)
14 y=vec2(4)
15 pro2=pro-[ y 0 y -2*y -2*y]
16 z=poly(0,"z")
17 vec3= roots(kp*(0.189-z)*(3.546-2*z)^2 *(7.622+2*z)
            ^2 -(0.643+z)*(3.076+4*z)^4 *4)
18 z=vec3(5)
19 pro3=pro2 - [z 2*z -z -4*z 0]
20 w=poly(0,"w")
21 vec4=roots(kp2*(0.229-w)*(0.603-w)*(7.542+2*w) -
            (2.916+2*w)^2 *(0.168+2*w)^2 *4)
22 w=vec4(4)
23 w=0.01
24 pro4=pro3-[w 0 w -2*w -2*w]
25 //results
26 disp("feed = ")
27 format('v',6);feed
28 disp(feed)
29 disp("After reactor 1,")
30 format('v',6);pro
31 disp(pro)
32 disp("After reactor 2,")
33 format('v',6);pro2
34 disp(pro2)
35 disp("After reactor 3,")
36 format('v',6);pro3
37 disp(pro3)
38 disp("After reactor 4")

```

```
39 format('v',6);pro4
40 disp(pro4)
41 disp("The answers are a bit different due to
    rounding off error in textbook")
```
