

Scilab Textbook Companion for  
Chemical Engineering Thermodynamics  
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# Book Description

**Title:** Chemical Engineering Thermodynamics

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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=106 //pa
6  a=4.19
7  b=0.0373
8  R=8314.3
9  Tc=405.5
10 Pc=11.28*106
11 //calculations
12 disp(" part b")
13 an=27*R2*Tc2 /(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 m3/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 m3/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 respectivey",dss,
        dg)
11 printf("\n change in entropy and gibbs energy of
        universe are %.3f kJ/kg K and %d kJ/kg
        respectivey",-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")
```

---