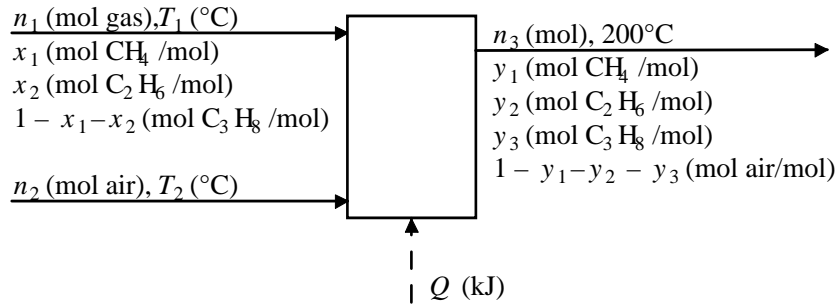


## CHAPTER TEN

### 10.1 b. Assume no combustion



11 variables  $(n_1, n_2, n_3, x_1, x_2, y_1, y_2, y_3, T_1, T_2, Q)$   
 -5 relations (4 material balances and 1 energy balance)  
 6 degrees of freedom

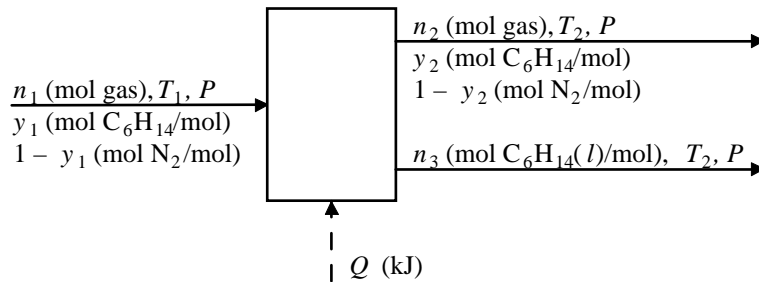
A feasible set of design variables:  $\{n_1, n_2, x_1, x_2, T_1, T_2\}$

Calculate  $n_3$  from total mole balance,  $y_1, y_2$ , and  $y_3$  from component balances,  $Q$  from energy balance.

An infeasible set:  $\{n_1, n_2, n_3, x_1, x_2, T_1\}$

Specifying  $n_1$  and  $n_2$  determines  $n_3$  (from a total mole balance)

c.



9 variables  $(n_1, n_2, n_3, y_1, y_2, T_1, T_2, Q, P)$   
 -4 relations (2 material, 1 energy, and 1 equilibrium:  $y_2 P = P_{C_6H_{14}}^*(T_2)$ )  
 5 degrees of freedom

A feasible set:  $\{n, y_1, T_1, P, n_3\}$

Calculate  $n_2$  from total balance,  $y_2$  from  $C_6H_{14}$  balance,  $T_2$  from Raoult's law:  
 $[y_2 P = P_{C_6H_{14}}^*(T_2)]$ ,  $Q$  from energy balance

An infeasible set:  $\{n_2, y_2, n_3, P, T_2\}$

Once  $y_2$  and  $P$  are specified,  $T_2$  is determined from Raoult's law

**10.2** 10 variables  $(n_1, n_2, n_3, n_4, x_1, x_2, x_3, x_4, T, P)$

–2 material balances

–2 equilibrium relations:  $[x_3 P = x_4 P_B^*(T), (1 - x_3)P = (1 - x_4)P_C^*(T)]$

6 degrees of freedom

**a.** A straightforward set:  $\{n_1, n_3, n_4, x_1, x_4, T\}$

Calculate  $n_2$  from total material balance,  $P$  from sum of Raoult's laws:

$$P = x_4 P_B^*(T) + (1 - x_4)P_C^*(T)$$

$x_3$  from Raoult's law,  $x_2$  from  $B$  balance

**b.** An iterative set:  $\{n_1, n_2, n_3, x_1, x_2, x_3\}$

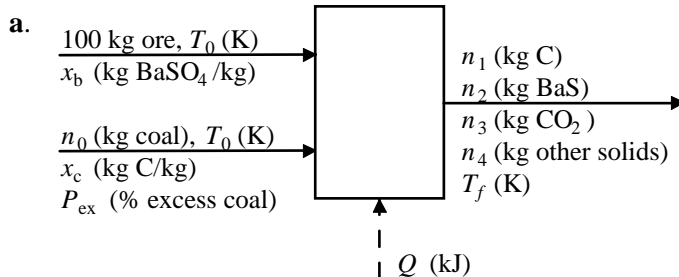
Calculate  $n_4$  from total mole balance,  $x_4$  from  $B$  balance.

Guess  $P$ , calculate  $T$  from Raoult's law for  $B$ ,  $P$  from Raoult's law for  $C$ , iterate until pressure checks.

**c.** An impossible set:  $\{n_1, n_2, n_3, n_4, T, P\}$

Once  $n_1, n_2$ , and  $n_3$  are specified, a total mole balance determines  $n_4$ .

**10.3**  $2\text{BaSO}_4(\text{s}) + 4\text{C}(\text{s}) \rightarrow 2\text{BaS}(\text{s}) + 4\text{CO}_2(\text{g})$



11 variables  $(n_0, n_1, n_2, n_3, n_4, x_b, x_c, T_0, T_f, Q, P_{\text{ex}})$

–5 material balances (C, BaS,  $\text{CO}_2$ ,  $\text{BaSO}_4$ , other solids)

–1 energy balance

+1 reaction

–1 relation defining  $P_{\text{ex}}$  in terms of  $n_0, x_b$ , and  $x_c$

5 degrees of freedom

**b.** Design set:  $\{x_b, x_c, T_0, T_f, P_{\text{ex}}\}$

Calculate  $n_0$  from  $x_b, x_c$ , and  $P_{\text{ex}}$ ;  $n_1$  through  $n_4$  from material balances,  $Q$  from energy balance

### 10.3 (cont'd)

c. Design set:  $\{x_B, x_c, T_0, n_2, Q\}$

Specifying  $x_B$  determines  $n_2 \Rightarrow$  impossible design set.

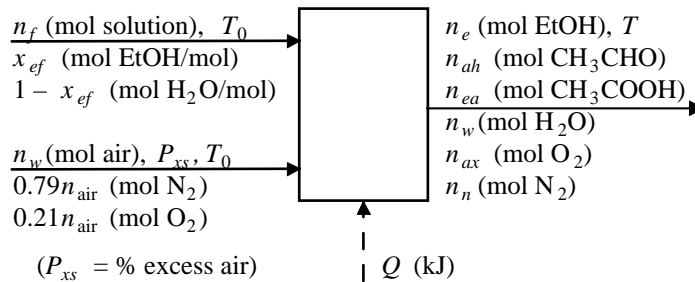
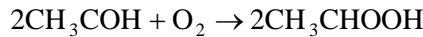
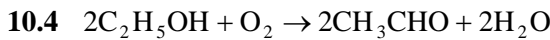
d. Design set:  $\{x_B, x_c, T_0, P_{ex}, Q\}$

Calculate  $n_2$  from  $x_B$ ,  $n_3$  from  $x_B$

$n_0$  from  $x_B, x_c$  and  $P_{ex}$

$n_1$  from C material balance,  $n_4$  from total material balance

$T_f$  from energy balance (trial-and-error probably required)



a. 13 variables  $(n_f, n_{aw}, n_e, n_{eh}, n_{ea}, n_w, n_{ex}, n_0, x_{ef}, T_0, T, Q, P_{xs})$

–6 material balances

–1 energy balance

–1 relation between  $P_{xs}, n_f, x_{ef}$ , and  $n_{air}$

+2 reactions

---

7 degrees of freedom

b. Design set:  $\{n_f, x_{ef}, P_{xs}, n_e, n_{ah}, T_0, T\}$

Calculate  $n_{air}$  from  $n_f, x_{ef}$  and  $P_{xs}$ ;  $n_n$  from  $N_2$  balance;

$n_{aa}$  and  $n_w$  from  $n_f, x_{ef}, n_e, n_{ah}$  and material balances;

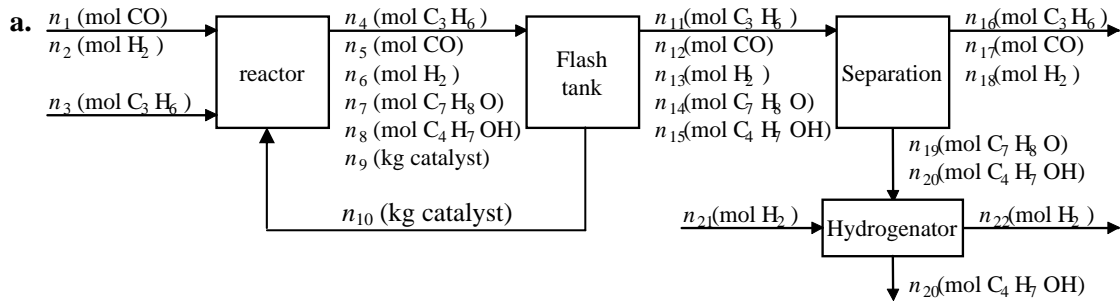
$n_{ex}$  from O atomic balance;  $Q$  from energy balance

c. Design set:  $\{n_f, x_{ef}, T_0, n_{air}, Q, n_e, n_w\}$

Calculate  $P_{xs}$  from  $n_f, x_{ef}$  and  $n_{air}$ ;  $n$ 's from material balances;  $T$  from energy balance (generally nonlinear in  $T$ )

d. Design set:  $\{n_{air}, n_n, \dots\}$ . Once  $n_{air}$  is specified, an  $N_2$  balance fixes  $n_n$

### 10.5



Reactor:      10 variables ( $n_1 - n_{16}$ )  
                   -6 material balances  
                   +2 reactions  


---

                   6 degrees of freedom  
                                     

Flash Tank:    12 variables ( $n_4 - n_{15}$ )  
                   -6 material balances  


---

                   6 degrees of freedom  
                                     

Separation:    10 variables ( $n_{11} - n_{20}$ )  
                   -5 material balances  


---

                   5 degrees of freedom  
                                     

Hydrogenator:   5 variables ( $n_{19} - n_{23}$ )  
                   -3 material balances  
                   +1 reaction  


---

                   3 degrees of freedom  
                                     

Process:        20 Local degrees of freedom  
                   -14 ties  

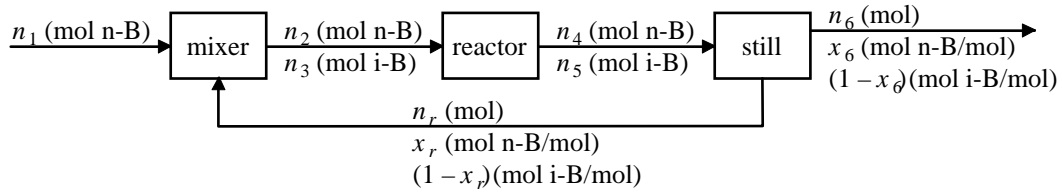

---

                   6 overall degrees of freedom  
                                     

The last answer is what one gets by observing that 14 variables were counted two times each in summing the local degrees of freedom. However, one relation also was counted twice: the catalyst material balances on the reactor and flash tank are each  $n_9 = n_{10}$ . We must therefore add one degree of freedom to compensate for having subtracted the same relation twice, to finally obtain 7 overall degrees of freedom (A student who gets this one has done very well indeed!)

- b. The catalyst circulation rate is not included in any equations other than the catalyst balance ( $n_9 = n_{10}$ ). It may therefore not be determined unless either  $n_9$  or  $n_{10}$  is specified.

**10.6**  $n - C_4H_{10} \rightarrow i - C_4H_{10} \quad (n - B = i - B)$



**a. Mixer:** 5 variables ( $n_1, n_2, n_3, n_r, x_r$ )  
 -2 material balances  


---

 3 degrees of freedom

**Reactor:** 4 variables ( $n_2, n_3, n_4, n_5$ )  
 -2 material balances  
 +1 reaction  


---

 3 degrees of freedom

**Still:** 6 variables ( $n_4, n_5, n_6, x_6, n_r, x_r$ )  
 -2 material balances  


---

 4 degrees of freedom

**Process:** 10 Local degrees of freedom  
 - 6 ties  


---

 4 overall degrees of freedom

**b.**  $n_1 = 100 \text{ mol } n - C_4H_{10}, \quad x_6 = 0.115 \text{ mol } n - C_4H_{10} / \text{mol}, \quad x_r = 0.85 \text{ mol } n - C_4H_{10} / \text{mol}$

Overall C balance:  $(100)(4) = n_6[(0.115)(4) + (0.885)(4)] \text{ mol C} \Rightarrow n_6 = 100 \text{ mol overhead}$

Overall conversion  $= \frac{100 \text{ mol } n - B \text{ fed} - (100)(0.115) \text{ mol } n - B \text{ unreacted}}{100 \text{ mol } n - B \text{ fed}} \times 100\% = \underline{\underline{88.5\%}}$

Mixer n-B balance:  $100 + 0.85n_r = n_2 \quad (1)$

35% S.P. conversion:  $n_4 = 0.65n_2 \Rightarrow n_4 = 65 + 0.5525n_r \quad (2)$

Still n - B balance:

$n_4 = n_6x_6 + n_rx_r \Rightarrow 65 + 0.5525n_r = (0.115)(100) + 0.85n_r \Rightarrow n_r = 179.83 \text{ mol}$

Recycle ratio  $= (179.83 \text{ mol recycle}) / (100 \text{ mol fresh feed}) = 1.79 \frac{\text{mol recycle}}{\text{mol fresh feed}}$

### 10.6 (cont'd)

c.

	$k = 1$	$k = 2$	$k = 3$
$n_r$	100.0	132.3	151.5
$n_2 = 100 + 0.85n_r$	185.0	212.5	228.8
$n_3 = n_r(1 - 0.85)$	15.0	19.85	22.73
$n_4 = 0.65n_2$	120.25	138.1	148.7
$n_5 = n_2 + n_3 - n_4$	79.75	94.21	102.8
$n_4 + n_5 = n_6 + n_r$	67.69	80.76	88.55
$n_4 = 0.115n_6 + 0.85n_r$			
$\Rightarrow$	$n_6 =$	$n_r =$	
	132.3	151.5	163.0

Error:  $\frac{179.83 - 163.0}{179.83} \times 100 = \underline{\underline{9.3\% \text{ error}}}$

d.  $w = \frac{151.5 - 132.3}{132.3 - 100.0} = 0.595$

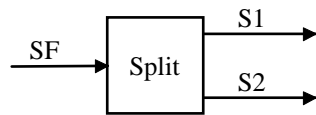
$q = \frac{0.595}{0.595 - 1} = -1.470$

$n_r^{(3)} = -1.470(132.3) + (1 - (-1.470))(151.5) = 179.8$

Error:  $\frac{179.8 - 179.8}{179.8} \times 100 = \underline{\underline{< 0.1\% \text{ error}}}$

e. Successive substitution, Iteration 32:  $n_r = 179.8319 \rightarrow n_r = 179.8319$   
Wegstein, Iteration 3:  $n_r = 179.8319 \rightarrow n_r = 179.8319$

### 10.7



a.

	A	B	C	D
1	X1 = 0.6			
2	Molar flow rates (mol/h)			
3		SF	S1	S2
4	nA	85.5	51.3	34.2
5	nB	52.5	31.5	21.0
6	nC	12.0	7.2	4.8
7	nD	0.0	0.0	0.0
8	T(deg.C)	315	315	315

Formula in C4: = \$B\$1\*B4

Formula in D4: = B4-C4

### 10.7 (cont'd)

```
b. C  **CHAPTER 10 -- PROBLEM 7
      DIMENSION SF(8), S1(8), S2(8)
      FLOW = 150.
      N = 3
      SF(1) = 0.35*FLOW
      SF(2) = 0.57*FLOW
      SF(3) = 0.08*FLOW
      SF(8) = 315.
      X1 = 0.60
      CALL SPLIT (SF, S1, S2, X1, N)
      WRITE (6, 900)' STREAM 1', S1(1), S1(2), S1(3), S1(8)
      WRITE (6, 900)' STREAM 2', S2(1), S2(2), S2(3), S2(8)
900   FORMAT (A10, F8.2, ' mols/h n-octane', /,
      *10X, F8.2, ' mols/h iso-octane', /,
      *10X, F8.2, ' mols/h inerts', /,
      *10X, F8.2, ' K')
      END

C
C  SUBROUTINE SPLIT
C
      SUBROUTINE SPLIT (SF, S1, S2, X1, N)
      DIMENSION SF(8), S1(8), S2(8)
      DO 100 J = 1, N
      S1(J) = X1*SF(J)
100   S2(J) = SF(J) - S1(J)
      S1(8) = SF (8)
      S2(8) = SF (8)
      RETURN
      END
```

Program Output: Stream 1 31.50 mols/h n-octane  
51.30 mols/h iso-octane  
7.20 mols/h inerts  
315.00 K  
Stream 2 21.00 mols/h n-octane  
34.20 mols/h iso-octane  
4.80 mols/h inerts  
315.00 K

## 10.8

- a. Let Bz = benzene, Tl = toluene

Antoine equations:  $\underline{\underline{p_{Bz}^*}} = 10^{6.89272 - 1211.033 / (T + 220.790)} (=1350.491)$

$\underline{\underline{p_{Tl}^*}} = 10^{6.95805 - 1346.773 / (T + 219.693)} (=556.3212)$

Raoult's law:  $\underline{\underline{x_{Bz}}} = (P - p_{Tl}^*) / (p_{Bz}^* - p_{Tl}^*) (=0.307)$ ,  $\underline{\underline{y_{Bz}}} = x_{Bz} p_{Bz}^* / P (=0.518)$

Total mole balance:  $100 = n_v + n_l$

Benzene balance:  $40 = y_{Bz} n_v + x_{Bz} n_l$

$$\Rightarrow \underline{\underline{n_v}} = \frac{40 - 100 x_{Bz}}{y_{Bz} - x_{Bz}} (=44.13), \underline{\underline{n_l}} = 100 - n_v (=55.87)$$

Fractional benzene vaporization:  $\underline{\underline{f_B}} = n_v y_{Bz} / 40 (=0.571)$

Fractional toluene vaporization:  $\underline{\underline{f_T}} = n_v (1 - y_{Bz}) / 60 (=0.354)$

The specific enthalpies are calculated by integrating heat capacities and (for vapors) adding the heat of vaporization.

$\underline{\underline{Q}} = \sum n_{out} \hat{H}_{out} - \sum n_{in} \hat{H}_{in} (= 1097.9)$

- b. Once the spreadsheet has been prepared, the goalseek tool can be used to determine the bubble-point temperature (find the temperature for which  $n_v=0$ ) and the dew-point temperature (find the temperature for which  $n_l=0$ ). The solutions are

$\underline{\underline{T_{bp}}} = 96.9^\circ \text{C}$ ,  $\underline{\underline{T_{dp}}} = 103.2^\circ \text{C}$

- c. C \*\*CHAPTER 10 PROBLEM B

DIMENSION SF(3), SL(3), SV(3)

DATA A1, B1, C1/6.90565, 1211.033, 220.790/

DATA A2, B2, C2/6.95334, 1343.943, 219.377/

DATA CP1, CP2, HV1, HV2/ 0.160, 0.190, 30.765, 33.47/

COMMON A1, B1, C1, A2, B2, C2, CP1, CP2, NV1, NV2

FLOW = 1.0

SF(1) = 0.30\*FLOW

SF(2) = 0.70\*FLOW

T = 363.0

P = 512.0

CALL FLASH2 (SF, SL, SV, T, P, Q)

WRITE (6, 900) 'Liquid Stream', SL(1), SL(2), SL(3)

WRITE (6, 900) 'Vapor Stream', SV(1), SV(2), SV(3)

900 FORMAT (A15, F7.4, ' mol/s Benzene', /,

\* 15X, F7.4, ' mol/s Toluene', /,

\* 15X, F7.2, 'K')

WRITE (6, 901) Q



## 10.8 (cont'd)

```

901  FORMAT ('Heat Required', F7.2, ' kW')
      END
      C
      SUBROUTINE FLASN2 (SF, SL, SV, T, P, Q)
      REAL NF, NL, NV
      DIMENSION SF(3), SL(3), SV(3)
      COMMON A1, B1, C1, C2, CP1, CP2, NV1, NV2
      C  Vapor Pressure
      PV1 = 10.**(A1 - B1/(T - 273.15 + C1))
      PV2 = 10.**(A2 - B2/(T - 273.15 + C2))
      C  Product fractions
      XL1 = (P - PV2)/(PV1 - PVS)
      XV1 = XL1*PM/P
      C  Feed Variables
      NF = SF(1) + SF(2)
      XF1 = SF(1)/NF
      C  Product flows
      NL = NF*(XF1 - XV1)/(XL1 - XV1)
      NV = NF - NL
      SL(1) = XL1*NL
      SL(2) = NL - SL(1)
      SY(1) = XY1*NY
      SY(2) = NV - SY(1)
      SL(3) = T
      SV(3) = T
      C  Energy Balance
      Q = CP1*SF(1)*SF(1) + CP2*SF(2)
      Q = Q*(T - SF(3)) + (NV1*XV1 + HV2*(1 - XV1))*NV
      RETURN
      END

```

**10.9 a. Mass Balance:**  $NF = NL + NV$  (1)

$$XF(I) * NF = XL(I) * NL + XV(I) * NV \quad I = 1, 2, \dots, n-1 \quad (2)$$

**Energy Balance:**  $Q = (T - TF) * \sum_{I=1}^N CP(I) * (XL(I) * NL + XV(I) * NV)$

$$+ NV * \sum_{I=1}^N HV(I) * XV(I) \quad (3)$$

where:  $XL(N) = 1 - \sum_{I=1}^{N-1} XL(I)$   $XV(N) = 1 - \sum_{I=1}^{N-1} XV(I)$

**Raoult's law:**  $P = \sum_{I=1}^N XL(I) * PV(I)$  (4)

$$XV(I) * P = XL(I) * PV(I) \quad I = 1, 2, \dots, N-1 \quad (5)$$

## 10.9 (cont'd)

where:  $PV(I) = 10 * (A(I) - B(I) / (C(I) + T))$   $I = 1, 2, \dots, N - 1$

$3 + 3(N - 1) + N + 4$  variables ( $NF, NL, NV, XF(I), XL(I), XV(I), PV(I), TF, T, P, Q$ )

–  $N$  mass balance

– 1 energy balances

–  $N$  equilibrium relations

–  $N$  Antoine equations

$N + 3$  degrees of freedom

Design Set  $\{TF, T, P, NF, XF(I)\}$

Eliminate  $NL$  from (2) using (1)

Eliminate  $XV(I)$  from (2) using (5)

Solve (2) for  $XL(I)$

$$XL(I) = XF(I) * NF / (NF + NV * (PV(I) / P - 1)) \quad (6)$$

Sum (6) over  $I$  to Eliminate  $XL(I)$

$$f(NV) = -1 + NF * \sum_{I=1}^N XF(I) / (NF + NV * (PV(I) / P - 1)) = 0 \quad (7)$$

Use Newton's Method to solve (7) for  $NV$

Calculate  $NL$  from (1)

$XL(I)$  from (2)

$XV(I)$  from (5)

$Q$  from (3)

b. C \*\*CHAPTER 10 - - PROBLEM 9  
 DIMENSION SF(8), SL(8), SV(8)  
 DIMENSION A(7), B(7), C(7), CP(7), HV(7)  
 COMMON A, B, C, CP, NV  
 DATA A/6.85221, 6.87776, 6.402040, 0., 0., 0., 0./  
 DATA B/1064.63, 1171.530, 1268.115, 0., 0., 0., 0./  
 DATA C/232.00, 224.366, 216.900, 0., 0., 0., 0./  
 DATA CP/0.188, 0.216, 0.213, 0., 0., 0., 0./  
 DATA NV/25.77, 28.85, 31.69, 0., 0., 0., 0./  
 FLOW = 1.0  
 N\*3  
 SF(1) = 0.348\*FLOW  
 SF(2) = 0.300\*FLOW  
 SF(3) = 0.352\*FLOW  
 SF(4) = 363  
 SL(4) = 338  
 SV(4) = 338  
 P\*611  
 CALL FLASHN (SF, SL, SV, N, P, Q)  
 WRITE (6, 900)' Liquid Stream', (SL(I), I = 1, N + 1)  
 WRITE (6, 900)' Vapor Stream', (SV(I), I = 1, N + 1)

## 10.9 (cont'd)

```
900  FORMAT (A15, F7.4, ' mols/s n-pentane', /,  
      *15X, F7.4, ' mols/s n-hexane', /,  
      *15X, F7.4, ' mols/s n-hephane', /,  
      15X, F7.2, ' K')  
      WRITE (6, 901) Q  
901  FORMAT ('Heat Required', F7.2, ' kW')  
      END  
      C  SUBROUTINE FLASHIN (SF, SL, SV, N, P, Q)  
          REAL NF, NL, NV, NVP  
          DIMENSION SF(8), SL(8), SV(8)  
          DIMENSION XF(7), XL(7), XV(7), PV(7)  
          DIMENSION A(7), B(7), C(7), CP(7), HV(7)  
          COMMON A, B, C, CP, HV  
          TOL = 1,5 - 6  
      C  Feed Variables  
          NF = 0.  
          DO 100 I = 1, N  
100    NF = NF + SF(I)  
          DO 200 I = 1, N  
200    XF(I) = SF(I)/NF  
          TF = SF (N + 1)  
          T = SL (N + 1)  
          TC = T - 273.15  
      C  Vapor Pressures  
          DO 300 I = 1, N  
300    PV(I) = 10.**((A(I) - B(I)/(TC + C(I)))  
      C  Find NV -- Initial Guess = NF/2  
          NVP = NF/2  
          DO 400 ITER = 1, 10  
          NV = NVP  
          F = -1.  
          FP = 0.  
          DO 500 I = 1, N  
          PPM1 = PV(I)/P - 1.  
          F = F + NF*XF(I)/(NF + NV*PPM1)  
500    FP = FP - PPM1*XF(I)/(NF + NV*PPM1)**2.  
          NVP = NV - F/FP  
          IF (ABS((NVP - NV)/NVP).LT.TOL) GOTO 600  
400    CONTINUE  
          WRITE (6, 900)  
900    FORMAT ('FLASHN did not converge on NV')  
          STOP  
      C  Other Variables
```

### 10.9 (cont'd)

```

600  NL = NF - NVP
      DO 700 I = 1, N
        XL(I) = XF(I)*NF/(NF + NV**(PV(I)/P - 1))
        SL(I) = XL(I)*NL
        XV(I) = XL(I)*PV(I)/P
700  SV(I) = SF(I) - SL(I)
      Q1 = 0.
      Q2 = 0.
      DO 800 I = 1, N
        Q1 = Q1 + CP(I)*SF(I)
800  Q2 = Q2 + HV(I)*XV(I)
      Q = Q1*(T - TF) + Q2*NVP
      RETURN
      END

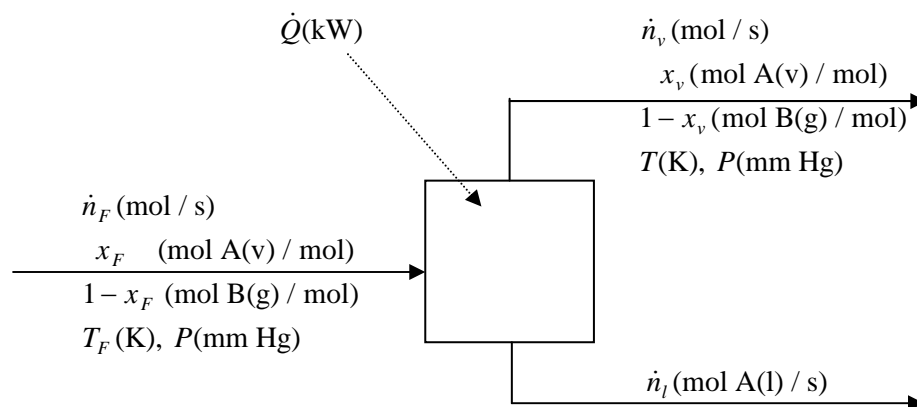
```

Program Output:

<u>Liquid Stream</u>	0.0563 mols/s n-pentane
	0.1000 mols/s n-hexane
	0.2011 mols/s n-heptane
	338.00 K
<u>Vapor Stream</u>	0.2944 mols/s n-pentane
	0.2000 mols/s n-hexane
	0.1509 mols/s n-heptane
	338.00 K
<u>Heat Required</u>	13.01 kW

### 10.10

a.



### 10.10 (cont'd)

- 10 variables ( $\dot{n}_F, x_F, T_F, P, \dot{n}_v, x_v, T, \dot{n}_l, p_A^*, \dot{Q}$ )
- 2 material balances
- 1 Antoine equation
- 1 Raoult's law
- 1 energy balance
- 5 degrees of freedom

b.

References: A(l), B(g) at 25°C

Substance	$\dot{n}_{in}$	$\hat{H}_{in}$	$\dot{n}_{out}$	$\hat{H}_{out}$
A(l)	—	—	$\dot{n}_l$	$\hat{H}_3$
A(v)	$\dot{n}_F x_F$	$\hat{H}_1$	$\dot{n}_v x_v$	$\hat{H}_4$
B(g)	$\dot{n}_F (1 - x_F)$	$\hat{H}_2$	$\dot{n}_v (1 - x_v)$	$\hat{H}_5$

Given  $\dot{n}_F$  and  $x_F$  (or  $\dot{n}_{AF}$  and  $\dot{n}_{BF}$ ),  $T_F, P, y_c$  (fractional condensation),

Fractional condensation  $\Rightarrow \underline{\dot{n}_l} = y_c \dot{n}_F x_F$

Mole balance  $\Rightarrow \underline{\dot{n}_v} = \dot{n}_F - \dot{n}_l$

A balance  $\Rightarrow \underline{x_v} = (\dot{n}_F x_F - \dot{n}_l) / \dot{n}_v$

Raoult's law  $\Rightarrow \underline{p_A^*} = x_v P$

Antoine's equation  $\Rightarrow \underline{T} = \frac{B}{A - \log_{10} p_A^*} - C$

Enthalpies:  $\underline{\hat{H}_1} = \Delta \hat{H}_v + C_{pv} (T_F - 25), \underline{\hat{H}_2} = C_{pg} (T_F - 25), \underline{\hat{H}_3} = C_{pl} (T - 25),$

$\underline{\hat{H}_4} = \Delta \hat{H}_v + C_{pv} (T - 25), \underline{\hat{H}_5} = C_{pg} (T - 25)$

Energy balance:  $\underline{\dot{Q}} = \sum \dot{n}_{out} \hat{H}_{out} - \sum \dot{n}_{in} \hat{H}_{in}$

c.

$\underline{n_{AF}}$	$\underline{n_{BF}}$	$\underline{n_F}$	$\underline{x_F}$	$\underline{T_F}$	$\underline{P}$	$\underline{y_c}$	$\underline{n_L}$
0.704	0.296	1.00	0.704	333	760	0.90	0.6336
$\underline{n_V}$	$\underline{x_V}$	$\underline{A}$	$\underline{B}$	$\underline{C}$	$\underline{p_A^*}$	$\underline{T}$	$\underline{C_{pl}}$
0.3664	0.1921	7.87863	1473.11	230	146.0	300.8	0.078
$\underline{C_{pv}}$	$\underline{C_{pg}}$	$\underline{H_1}$	$\underline{H_2}$	$\underline{H_3}$	$\underline{H_4}$	$\underline{H_5}$	$\underline{Q}$
0.050	0.030	37.02	1.05	0.2183	35.41	0.0839	-23.7

Greater fractional methanol condensation ( $y_c$ )  $\Rightarrow$  lower temperature ( $T$ ). ( $y_c = 0.10 \Rightarrow T = 328^\circ\text{C}$ .)

## 10.10 (cont'd)

```
e.  C  **CHAPTER 10 -- PROBLEM 10
      DIMENSION SF(3), SV(3), SL(2)
      COMMON A, B, C, CPL, HV, CPV, CPG
      DATA A, B, C / 7.87863, 1473.11, 230.0/
      DATA CPL, HV, CPV, CPG, / 0.078, 35.27, 0.050, 0.029/
      FLOW = 1.0
      SF(1) = 0.704*FLOW
      SF(2) = FLOW - SF(1)
      YC = 0.90
      P = 1.
      SF(3) = 333.
      CALL CNDNS (SF, SV, SL, P, YC, Q)
      WRITE (6, 900) SV(3)
      WRITE (6, 401) 'Vapor Stream', SV(1), SV(2)
      WRITE (6, 401) 'Liquid Stream', SL(1)
      WRITE (6, 902) Q
900  FORMAT ('Condenser Temperature', F7.2, ' K')
901  FORMAT (A15, F7.3, ' mols/s Methyl Alcohol', /,
      *15X, F7.3, ' mols/s air')
902  FORMAT ('Heat Removal Rate', F7.2, ' kW')
      END
      C  SUBROUTINE CNDNS (SF, SV, SL, P, YC, Q)
      REAL NF, NL, NV
      DIMENSION SF(3), SV(3), SL(2)
      COMMON A, B, C, CPL, HV, CPV, CPG
      C  Inlet Stream Variables
      NF = SF(1) + SF(2)
      TF = SF(3)
      XF = SF(1)/NF
      C  Solve Equations
      NL = YC * XF * NF
      NV = NF - NL
      XV = (XF*NF - NL)/NV
      PV = P * XV * 760.
      T = B/(A - LOG(N)/LOG (10.)) - C
      T = T + 273.15
      Q = ((CPV * XV + CPG * (1 - XY)) * NV + CPL * NL) * (T - TF) - NL * HV
      C  Output Variables
      SL(1) = NL
      S2(2) = T
      SV(1) = XV*NV
      SV(2) = NV - SV(1)
      SV(3) = T
      RETURN
      END
```

$$10.11 \quad \eta_1 A_1 + \eta_2 A_2 + \eta_3 A_3 + \dots \eta_m A_m = 0$$

a. Extent of reaction equations:

$$\xi = -[SF(IX) * X] / NU(IX)$$

$$SP(I) = SF(I) + NU(I) * \xi \quad I = 1, 2, \dots, N$$

Energy Balance: Reference states are molecular species at 298K.

$$TF = SF(N+1) \quad TP = SP(N+1)$$

$$\Delta \hat{H}_r = \sum_{I=1}^N HF(I) * NU(I)$$

$$Q = \xi * \Delta \hat{H}_r + (TP - 298) * \sum_{I=1}^N SP(I) * CP(I) - (TF - 298) * \sum_{I=1}^N SF(I) * CP(I)$$

b.  $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

Subscripts: 1 =  $C_3H_8$ , 2 =  $O_2$ , 3 =  $N_2$ , 4 =  $CO_2$ , 5 =  $H_2O$

$$\frac{270 \text{ m}^3}{\text{h}} \bigg| \frac{1 \text{ atm}}{273 \text{ K}} \bigg| \frac{\text{mol} \cdot \text{K}}{0.08206 \text{ liter} \cdot \text{atm}} \bigg| \frac{1000 \text{ liter}}{\text{m}^3} \bigg| \frac{\text{h}}{3600 \text{ s}} = 3.348 \text{ mol } C_3H_8 / \text{s} [=SF(1)]$$

$$\frac{3.348 \text{ mol } C_3H_8}{\text{sec}} \bigg| \frac{1.2(5 \text{ mol } O_2)}{\text{mol } C_3H_8} = 20.09 \text{ mol } O_2 / \text{s} [=SF(2)] \Rightarrow 75.54 \text{ mol } N_2 / \text{s} [=SF(3)]$$

$$X_{C_3H_8} = 0.90 \Rightarrow \dot{n}_{C_3H_8} = 0.10(3.348) = 0.3348 \text{ mol } C_3H_8 / \text{s} \text{ in product gas} [=SP(1)]$$

$$\xi = -[SF(IX) * X] / NU(IX) = -(3.348 \text{ mol/s})(0.90) / (-1) = 3.013 \text{ mol/s}$$

	1-C3H8	2-O2	3-N2	4-CO2	5-H2O(v)
Nu	-1	-5	0	3	4
nin (SF)	3.348	20.09	75.54		
X	0.90				
Xi	3.01				
nout (SP)	0.3348	5.024	75.54	9.0396	12.0528
Cp	0.1431	0.033	0.0308	0.0495	0.0375
Tin	423				
Hin	17.9	4.1	3.9	6.2	4.7
Tout	1050				
Hout	107.6	24.8	23.2	37.2	28.2
HF	-103.8	0	0	-393.5	-241.83
DHr	-2044				
Q	-4006				

For the given conditions,  $Q = -4006 \text{ kJ} / \text{s}$ . As  $T_{\text{stack}}$  increases, more heat goes into the stack gas so less is transferred out of the reactor: that is, Q becomes less negative.

## 10.11 (cont'd)

```

C  **CHAPTER 10 PROBLEM 11
    DIMENSION SF(8), SP(8), CP(7), HF(7)
    REAL NU(7)
    DATA NU/-1., -5, 0., 3., 4., 0., 0./
    DATA CP/0.1431, 0.0330, 0.0308, 0.0495, 0.0375, 0., 0./
    DATA HF/-103.8, 0., 0., -393.5, -241.83, 0., 0./
    COMMON CP, HF
    SF(1) = 3.348
    SF(2) = 20.09
    SF(3) = 75.54
    SF(4) = 0.
    SF(5) = 0.
    SF(6) = 423.
    SP(6) = 1050.
    IX = 1
    X = 0.90
    N = 5
    CALL REACTS (SF, SP, NU, N, X, IX, Q)
    WRITE (6, 900) (SP(I), I = 1, N + 1), Q
900  FORMAT ('Product Stream', F7.3, ' mols/s propane', /,
    *15X, F7.3, ' mols/s oxygen', /,
    *15X, F7.3, ' mols/s nitrogen', /,
    *15X, F7.3, ' mols/s carbon dioxide', /,
    *15X, F7.3, ' mols/s water', /,
    *15X, F7.2, 'K', /,
    Heat required', F8.2, 'kW')
    END
C  SUBROUTINE REACTS (SF, SP, NU, N, X, IX, Q)
    DIMENSION SF(8), SP(8), CP(7), HF(7)
    REAL NU(7)
    COMMON CP, HF
C  Extent of Reaction
    EXT = -SF(IX)*X/NU(IX)
C  Solve Material Balances
    DO 100 I = 1, N
100  SP(I) = SF(I) + EXT = NU(I)
C  Heat of Reaction
    HR = 0
    DO 200 I = 1, N
200  HR = HR + NF(I)*NU(I)
C  Product Enthalpy (ref * inlet)
    HP = 0.
    DO 300 I = 1, N
300  HP = HP + SP(I)*CP(I)
    HP = HP + (SP(N + 1) - SF (N + 1))
    Q = EXT * HR + HP
    RETURN
    END

```



**10.12 a.** Extent of reaction equations:

$$\xi = -SF(IX) * X / NU(IX)$$

$$SP(I) = SF(I) + NU(I) * \xi \quad I = 1, N$$

Energy Balance: Reference states are molecular species at feed stream temperature.

$$Q = \Delta H = \xi \Delta \hat{H}_r + \sum n_{\text{out}} \hat{H}_{\text{out}} = 0 \Rightarrow 0 = \xi \sum_{i=1}^N NU(I) HF(I) + \sum_{I=1}^N SP(I) \int_{T_{\text{feed}}}^T CP(I) dT$$

$$\Downarrow \quad CP(I) = ACP(I) + BCP(I) * T + CCP(I) * T^2 + DCP(I) * T^3$$

$$f(T) = \xi * \sum_{I=1}^N NU(I) * HF(I) + AP * (T - T_{\text{feed}}) + \frac{BP}{2} * (T^2 - T_{\text{feed}}^2) + \frac{CP}{3} * (T^3 - T_{\text{feed}}^3) + \frac{DP}{4} * (T^4 - T_{\text{feed}}^4) = 0$$

$$\text{where: } AP = \sum_{I=1}^N SP(I) * ACP(I), \text{ and similarly for BP, CP, \& DP}$$

Use goalseek to solve  $f(T) = 0$  for  $T [= SP(N+1)]$

**b.**  $2\text{CO} + \text{O}_2 \rightarrow 2\text{CO}_2$

Temporary basis: 2 mol CO fed

$$\frac{2 \text{ mol CO}}{2 \text{ mol CO}} \left| \frac{1.25(1 \text{ mol O}_2)}{2 \text{ mol CO}} \right| = 1.25 \text{ mol O}_2 \Rightarrow 4.70 \text{ mol N}_2$$

$$\Rightarrow \text{Total moles fed} = (2.00 + 1.25 + 4.70) \text{ mol} = 7.95 \text{ mol}$$

Scale to given basis:

$$\frac{(23.0 \frac{\text{kmol}}{\text{h}})(\frac{1 \text{ h}}{3600 \text{ s}})(\frac{10^3 \text{ mol}}{1 \text{ kmol}})}{7.95 \text{ mol}} = 0.8036 \Rightarrow \begin{aligned} SF(1) &= 1.607 \text{ mol CO fed/s} \\ SF(2) &= 1.004 \text{ mol O}_2 \text{ fed/s} \\ SF(3) &= 3.777 \text{ mol N}_2 \text{ fed/s} \end{aligned}$$

## 10.12 (cont'd)

### Solution to Problem 10.12

	1-CO	2-O2	3-N2	4-CO2
Nu	-2	-1	0	2
nin (SF)	1.607	1.004	3.777	0
X	0.45			
Xi	0.36			
nout (SP)	0.88385	0.642425	3.777	0.72315
ACP	0.02895	0.0291	0.029	0.03611
BCP	4.11E-06	1.16E-05	2.20E-06	4.23E-05
CCP	3.55E-09	-6.08E-09	5.72E-09	-2.89E-08
DCP	-2.22E-12	1.31E-12	-2.87E-12	7.46E-12
AP	0.1799			
BP	5.00E-05			
CP	-2.90E-11			
DP	-6.57E-12			
Tfeed	650			
DHF	-110.52	0	0	-393.5
DHr	-566			
T	1560			
f(T)	-4.7E-08			

The adiabatic reaction temperature is 1560°C.

As  $X$  increases,  $T$  increases. (The reaction is exothermic, so more reaction means more heat released.)

d.

```

C **CHAPTER 10 -- PROBLEM 12
  DIMENSION SF(8), SP(B), NU(7), ACP(7), BCP(7), CCP(7), DCP(7), HF(7)
  COMMON ACP, BCP, CCP, DCP, NF
  DATA NU / -2., -1., 0., 2., 0., 0., 0./
  DATA ACP/ 28.95E-3, 29.10E-3, 29.00E-3, 36.11E-3, 0., 0., 0./
  DATA BCP/ 0.4110E-5, 1.158E-5, 0.2199E-5, 4.233E-6, 0., 0., 0./
  DATA CCP/ 0.3548E-8, -0.6076E-8, 0.5723E-8, -2.887E-8, 0., 0., 0./
  DATA DCP/ -2.220 E-12, 1.311E-12, -2.871E-12, 7.464E-12, 0., 0., 0./
  DATA HF / -110.52, 0., 0., -393.5, 0., 0., 0./
  SF(1) = 1.607
  SF(2) = 1.004
  SF(3) = 3.777
  SF(4) = 0.
  SF(5) = 650.
  IX = 1
  X = 0.45
  N = 4
  CALL REACTAD (SF, SP, NU, N, X, IX)
  WRITE (6, 900) (SP(I), I = 1, N + 1)

```

## 10.12 (cont'd)

```
900  FORMAT ('Product Stream', F7.3, ' mols/s carbon monoxide', /,  
      *15X, F7.3, 'mols/s oxygen', /,  
      *15X, F7.3, 'mols/s nitrogen', /,  
      *15X, F7.3, 'mols/s carbon dioxide', /,  
      15X, F7.2, 'C')  
      END  
C    SUBROUTINE REACTAD (SF, SP, NU, N, X, IX)  
      DIMENSION SF(8), SP(8), NU(7), ACP(7), BCP(7), CCP(7), DCP(7), HF(7)  
      COMMON ACP, BCP, CCP, DCP, NF  
      TOL = 1.E-6  
C    Extent of Reaction  
      EXT = -SF(IX)*X/NU(IX)  
C    Solve Material Balances  
      DO 100 I = 1, N  
100   SP(I) = SF(I) + EXT*NU(I)  
C    Heat of Reaction  
      HR = 0  
      DO 200 I = 1, N  
200   HR = HR + HF(I) * NU(I)  
      HR = HR * EXT  
C    Product Heat Capacity  
      AP = 0.  
      BP = 0.  
      CP = 0.  
      DP = 0.  
      DO 300 I = 1, N  
  
      AP = AP + SP(I)*ACP(I)  
      BP = BP + SP(I)*BCP(I)  
      CP = CP + SP(I)*CCP(I)  
300   DP = DP + SP(I)*DCP(I)  
C    Find T  
      TIN = SF (N + 1)  
      TP = TIN  
      DO 400 ITER = 1, 10  
      T = TP  
      F = HR  
      FP = 0.  
      F = F + T*(AP + T*(BP/2. + T*(CP/3. + T*DP/4.)))  
      * -TIN*(AP + TIN*(BP/2. + TIN*(CP/3. + TIN*DP/4.)))  
      FP = FP + AP + T *(BP + T*(CP + T*DP))  
      TP = T - F/FP  
      IF(ABS((TP - T)/T).LT.TOL) GOTO 500  
400   CONTINUE  
      WRITE (6, 900)  
900   FORMAT ('REACTED did not converge')  
      STOP
```

### 10.12 (cont'd)

```
500    SP(N + 1) = T  
      RETURN  
      END
```

#### Program Output:

0.884 mol/s carbon monoxide

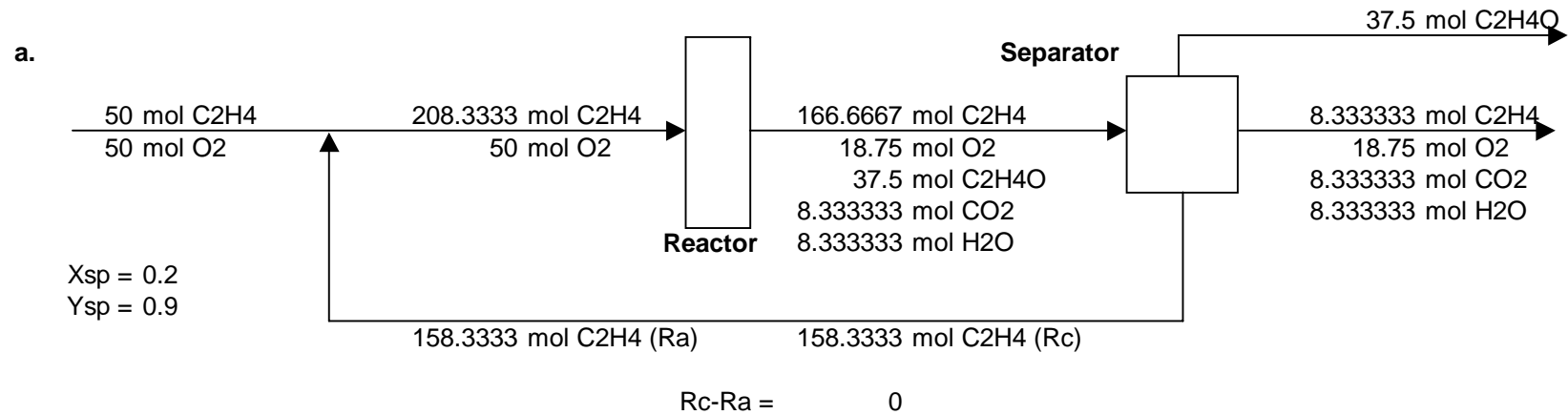
0.642 mol/s oxygen

3.777 mol/s nitrogen

0.723 mol/s carbon dioxide

$T = 1560.43\text{ C}$

10.13



Procedure: Assume  $R_a$ , perform balances on mixing point, then reactor, then separator.  $R_c$  is recalculated recycle rate. Use goalseek to find the value of  $R_a$  that drives  $(R_c - R_a)$  to zero.

b.

$X_{sp}$	$Y_{sp}$	$Y_o$	no
0.2	0.72	0.6	158.33
0.2	1	0.833	158.33
0.3	0.75333	0.674	99.25
0.3	1	0.896	99.25

The second reaction consumes six times more oxygen per mole of ethylene consumed. The lower the single pass ethylene oxide yield, the more oxygen is consumed in the second reaction. At a certain yield for a specified ethylene conversion, all the oxygen in the feed is consumed. A yield lower than this value would be physically impossible.

```

10.14 C  **CHAPTER 10 -- PROBLEM 14
        DIMENSION XA(3), XC(3)
        N = 2
        EPS = 0.001
        KMAX = 20
        IPR = 1
        XA(1) = 2.0
        XA(2) = 2.0
        CALL CONVG (XA, XC, N, KMAX, EPS, IPR)
        END
C      SUBROUTINE FUNCGEN(N, XA, XC)
        DIMENSION XA(3), XC(3)
        XC(1) = 0.5*(3. - XA(2) + (XA(1) + XA(2))**0.5)
        XC(2) = 4. - 5./(XA(1) + XA(2))
        RETURN
        END
C      SUBROUTINE CONVG (XA, XC, N, KMAX, EPS, IPR)
        DIMENSION XA(3), XC(3), XAH(3), XCM(3)
        K = 1
        CALL FUNCGEN (N, XA, XC)
        IF (IPR.EQ.1) CALL IPRNT (K, XA, XC, N)
        DO 100 I = 1, N
            XAM(I) = XA(I)
            XA(I) = XC(I)
100      XCM(I) = XC(I)
110      K = K + 1
            CALL FUNCGEN (N, XA, XC)
            IF (IPR.EQ.1) CALL IPRNT (K, XA, XC, N)
            DO 200 I = 1, N
                IF (ABS ((XA(I) - XC(I))/XC(I)).GE.EPS) GOTO 300
200      CONTINUE
C      Convergence
        RETURN
300      IF(K.EQ.KMAX) GOTO 500
            DO 400 I = 1, N
                W = (XC(I) - XCM(I))/(XA(I) - XAM(I))
                Q = W/(W - 1.)
                IF (Q.GT.0.5) Q = 0.5
                IF (Q.LT.-5) Q = -5.
                XCM(I) = XC(I)
                XAM(I) = XA(I)
400      XA(I) = Q * XAM(I) + (1. - Q)*XCM(I)
            GOTO 110
500      WRITE (6, 900)
900      FORMAT (' CONVG did not converge')
        STOP
        END

```

#### 10.14 (cont'd)

```

C    SUBROUTINE IPRNT (K, XA, XC, N)
      DIMENSION XA(3), XC(3)
      IF (K.EQ.1) WRITE (6, 400)
      IF (K.NE.1) WRITE (6, *)
      DO 100 I = 1, N
100   WRITE (6, 901) K, I, XA(I), XC(I)
      RETURN
900   FORMAT (' K Var Assumed Calculated')
901   FORMAT (I4, I4, 2E15.6)
      END

```

Program Output:	K	Var	Assumed	Calculated
	1	1	0.200000E + 01	0.150000E + 01
	1	2	0.200000E + 01	0.275000E + 01
	2	1	0.150000E + 01	0.115578E + 01
	2	2	0.275000E + 01	0.282353E + 01
	3	1	0.395135E + 00	0.482384E + 00
	3	2	0.283152E + 01	0.245041E + 01
	:	:	:	:
	8	1	0.113575E + 01	0.113289E + 01
	8	2	0.269023E + 01	0.269315E + 01
	4	1	0.113199E + 01	0.113180E + 01
	9	2	0.269186E + 01	0.269241E + 01