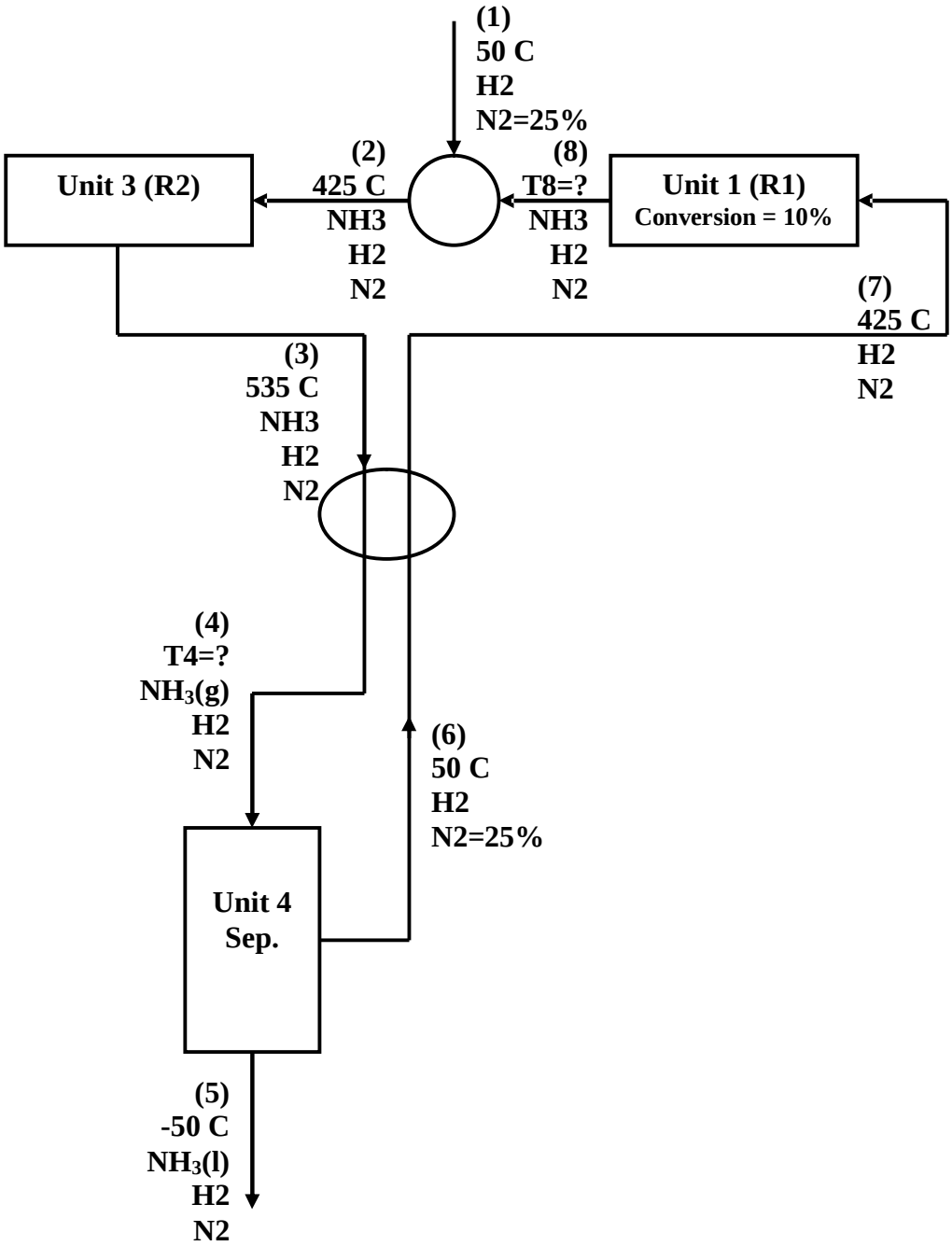
**Example 6 (Page 512)**

Consider the following flow sheet for the production of liquid ammonia from hydrogen and nitrogen according to the gas phase reaction: $N_2 + 3H_2 \rightarrow 2NH_3$. Assume the two reactors and the mixer to operate adiabatically and no heat losses in the heat exchanger.




Use the following data:

1- Constant heat capacities for:
$N_2$ (gas) = 7 cal/mol

$H_2$ (gas) = 7 cal/mol
$NH_3$ (gas) = 9.5 cal/mol
$NH_3$ (liquid) = 30 cal/mol

2- Latent heat of vaporization for $NH_3$ = 5.581 kcal/mol at –33.4 ºC.
3- Heat of formation of $NH_3$ (gas) = -10.92 kcal/mol at 25 ºC.
4- The conversion in the first reactor (reactor 1) is 10%.

**Calculate:**
1- Heat load of separator per mol of $NH_3$ produced
2- Overall conversion of $N_2$.
3- Conversion in Reactor 2.
4- Find the temperatures of stream 4 & 8

**SOLUTION**

**Degree of Freedom**

| | Mixer | | R1 | | R2 | | HE | | Separator | | Overall | | Process | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **M** | **ME** | **M** | **ME** | **M** | **ME** | **M** | **ME** | **M** | **ME** | **M** | **ME** | **M** | **ME** |
| **PV** | 8 | 8 | 5 | 5 | 6 | 6 | 5/10 | 5/10 | 8 | 8 | 5 | 5 | 16/21 | 16/21 |
| **Rx** | 0 | 0 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 1 | 1 | 2 | 2 |
| **T** | - | 3 | - | 2 | - | 2 | - | 4 | - | 3 | - | 2 | - | 8 |
| **Q** | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 5 |
| **U** | **8** | **12** | **6** | **9** | **7** | **10** | **5/10** | **10/15** | **8** | **12** | **6** | **9** | **18/23** | **31/36** |
| **MB** | 3 | 3 | 3 | 3 | 3 | 3 | 0/5 | 0/5 | 3 | 3 | 3 | 3 | 12/17 | 12/17 |
| **EB** | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 1 | - | 5 |
| **FL** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Com** | 1 | 1 | - | - | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 |
| **Rel** | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 |
| **T** | - | 2 | - | 1 | - | 2 | - | 3 | - | 2 | - | 2 | - | 6 |
| **Q** | - | 1 | - | 1 | - | 1 | - | 1 | - | 0 | - | 0 | - | 4 |
| **I** | **4** | **7** | **4** | **7** | **3** | **7** | **1/6** | **6/11** | **4** | **7** | **4** | **7** | **15/20** | **30/35** |
| **I-U** | **-4** | **-4** | **-2** | **-2** | **-4** | **-3** | **-4** | **-4** | **-4** | **-5** | **-2** | **-2** | **-3** | **-1** |

The process is solvable if a basis is assumed:

Stream variables (M.B. based)

| **Stream** | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| **P. V.** | 2 | 3 | 3 | 3 | 3 | 2 | 2 | 3 |
| **Given** | 1y | 0 | 0 | 0 | 0 | 1y | 0 | 0 |
| **Remain** | 1 | 3 | 3 | 3 | 3 | 1 | 2 | 3 |
| **Fixed** | N1 | N2, H2, NH2 | N3, H3, NH3 | N4, H4, NH4 | N5, H5, NH5 | N6 | N7, H7, NH7 | N8, H8, NH8 |
| **Defined** | H1 | | | | | H6 | | |

**Basis**: Ntotal_6= 400 mol/s

## E-ZSOLVE PROGRAM

```
// N=N2;  H=H2;  NH=NH3 ; BASIS NT6= 400
NT6 = 400
N6 = 0.25*NT6
H6 = 75/25*N6
H1 = 75/25*N1
//DATA
CPGN = 0.007
CPGH = 0.007
CPGNH = 0.0095
CPLNH = 0.030
T1=50
T2=425
T3=535
T5= -50
T6=50
T7=425
TREF = 25
TB=-33.4
HVNH=5.581              //AT -33.4 C
HRNH=  -10.92           //HEAT OF FORMATION OF NH3 (=REACTION) AT 25 C

//CONVERSION
(N7-N8)/N7=0.1

//REFERENCE  (G,25,1)
//E.B. == Q = DELTA H
// DELTA H  = OUTPUT - INPUT + ZETA*HRNH (REACTION METHOD)
// DELTA H = OUTPUT - INPUT                        (FORMATION METHOD)

// UNIT 1 (REACTOR 1)
N8 = N7 - R1
H8 = H7 - 3*R1
NH8 = 2*R1
ZETA1 = (N8-N7)/(-1)            // ZETA1=R1
HR1 = ZETA1*(2*HRNH)          // 2 MOLES OF NH3
QR1=0
QR1 = DH8 - DH7 + HR1

// UINT 2 (MIXER)
N1 + N8 = N2
H1 + H8 = H2
NH8 = NH2
QMIX = 0
QMIX = DH2 - DH1 - DH8

// UNIT 3 (REACTOR 2)
N3 = N2 - R2
H3 = H2 - 3*R2
NH3 = NH2 + 2*R2
QR2 = 0
HR2 = R2*(2*HRNH)
QR2 = DH3 - DH2 + HR2


// UNIT 4 (HEAT EXCHANGER)
N4 = N3
H4 = H3
NH4 = NH3
```

```
N6 = N7
H6 = H7
Q4 = 0
Q4 = DH4 + DH7 - DH3 - DH6

// UNIT 5 (SEPARATOR)
N4 = N5 + N6
H4 = H5 + H6
NH4 = NH5
QSEP = DH5 + DH6 - DH4

// ENTHAPLIES

DH1 = (N1*CPGN + H1*CPGH)*(T1-TREF)
DH2 = (NH2*CPGNH + N2*CPGN + H2*CPGH)*(T2-TREF)
DH3 = (NH3*CPGNH + N3*CPGN + H3*CPGH)*(T3-TREF)
DH4 = (NH4*CPGNH + N4*CPGN + H4*CPGH)*(T4 - TREF)
DH5 = (N5*CPGN + H5*CPGH)*(T5-TREF)+NH5*(CPGNH*(TB-TREF) - HVNH + CPLNH*(T5 - TB))
DH6 = (N6*CPGN + H6*CPGH)*(T6 - TREF)
DH7 = (N7*CPGN + H7*CPGH)*(T7-TREF)
DH8 = (NH8*CPGNH + N8*CPGN + H8*CPGH)*(T8 -TREF)

// ANSWERS
QREQ = QSEP/NH5
OVCONV = (N1 - N5)/N1*100
CONV2 = (N2 - N3)/N2*100
```

**E-ZSOLVE RESULTS**

| H1 | H2 | H3 | H4 | H5 | H6 | H7 | H8 |
|---|---|---|---|---|---|---|---|
| 72.69 | 342.69 | 300.38 | 300.38 | 0.38 | 300.00 | 300.00 | 270.00 |

| N1 | N2 | N3 | N4 | N5 | N6 | N7 | N8 |
|---|---|---|---|---|---|---|---|
| 24.23 | 114.23 | 100.13 | 100.13 | 0.13 | 100.00 | 100.00 | 90.00 |

| NH2 | NH3 | NH4 | NH5 | NH8 |
|---|---|---|---|---|
| 20.00 | 48.20 | 48.20 | 48.20 | 20.00 |

| T1 | T2 | T3 | T4 | T5 | T6 | T7 | T8 |
|---|---|---|---|---|---|---|---|
| 50.00 | 425.00 | 535.00 | 213.06 | -50.00 | 50.00 | 425.00 | 518.88 |

| QR1 | QMIX | QR2 | Q4 | QSEP | TB | TREF |
|---|---|---|---|---|---|---|
| 0.00 | 0.00 | 0.00 | 0.00 | -863.40 | -33.40 | 25.00 |

| R1 | R2 | ZETA1 | HRNH | HVNH | HR1 | HR2 |
|---|---|---|---|---|---|---|
| 10.00 | 14.10 | 10.00 | -10.92 | 5.58 | -218.40 | -307.99 |

| DH1 | DH2 | DH3 | DH4 | DH5 | DH6 | DH7 | DH8 |
|---|---|---|---|---|---|---|---|
| 16.96 | 1355.36 | 1663.35 | 613.35 | -320.05 | 70.00 | 1120.00 | 1338.40 |

| Heat load | Overall conv. | Conv. R2 |
|---|---|---|
| -17.91 | 99.48 | 12.35 |