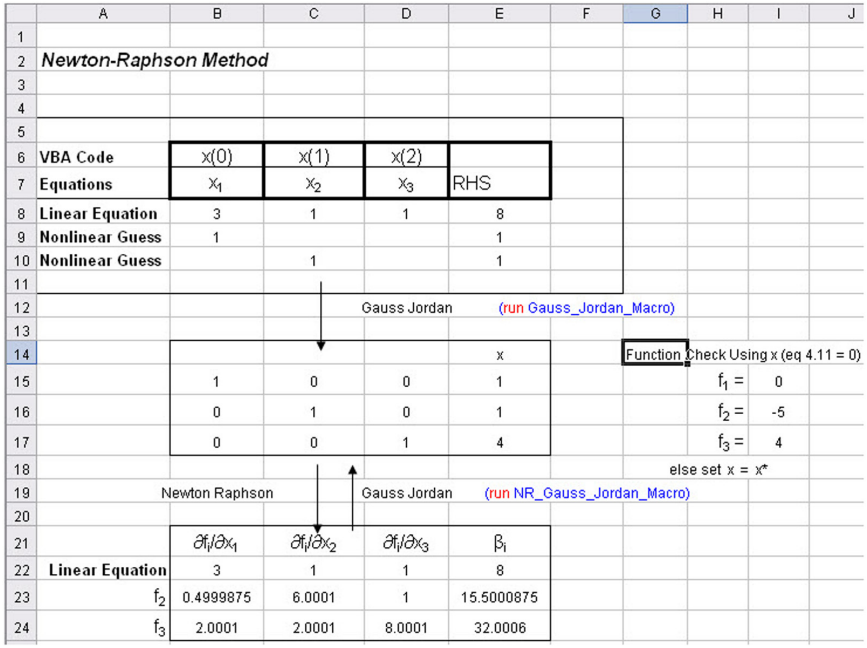

| | A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | | | | | | | | | |
| 2 | *Newton-Raphson Method* | | | | | | | | | |
| 3 | | | | | | | | | | |
| 4 | | | | | | | | | | |
| 5 | | | | | | | | | | |
| 6 | **VBA Code** | x(0) | x(1) | x(2) | | | | | | |
| 7 | **Equations** | $x_1$ | $x_2$ | $x_3$ | RHS | | | | | |
| 8 | **Linear Equation** | 3 | 1 | 1 | 8 | | | | | |
| 9 | **Nonlinear Guess** | 1 | | | 1 | | | | | |
| 10 | **Nonlinear Guess** | | 1 | | 1 | | | | | |
| 11 | | | | | | | | | | |
| 12 | | | | Gauss Jordan | (run Gauss_Jordan_Macro) | | | | | |
| 13 | | | | | | | | | | |
| 14 | | | | | x | | Function | Check Using x (eq 4.11 = 0) | | |
| 15 | | 1 | 0 | 0 | 1 | | | $f_1$ = | 0 | |
| 16 | | 0 | 1 | 0 | 1 | | | $f_2$ = | -5 | |
| 17 | | 0 | 0 | 1 | 4 | | | $f_3$ = | 4 | |
| 18 | | | | | | | else set x = x* | | | |
| 19 | | Newton Raphson | | Gauss Jordan | (run NR_Gauss_Jordan_Macro) | | | | | |
| 20 | | | | | | | | | | |
| 21 | | $\partial f_i/\partial x_1$ | $\partial f_i/\partial x_2$ | $\partial f_i/\partial x_3$ | $\beta_i$ | | | | | |
| 22 | **Linear Equation** | 3 | 1 | 1 | 8 | | | | | |
| 23 | $f_2$ | 0.4999875 | 6.0001 | 1 | 15.5000875 | | | | | |
| 24 | $f_3$ | 2.0001 | 2.0001 | 8.0001 | 32.0006 | | | | | |

**FIGURE 4.10**

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | ***Styrene Material Balance Nonlinear Specification*** | | | | | | | | | | | | | | | | | | |
| 2 | | | | | | | | | | | | | | | | | | | |
| 3 | Reactio | $C_8H_{10}$ ---> $C_8H_8$ + $H_2$ | | | Conversion | | 0.65 | | | | | | | | | | | | |
| 4 | | | | | | | | | | | | | | | | | | | |
| 5 | | x0 | x1 | x2 | x3 | x4 | x5 | x6 | x7 | x8 | x9 | x10 | x11 | x12 | x13 | x14 | x15 | x16 | |
| 6 | | Feed | | | Reactor In | | | Reactor Out | | | Water Out | Organic Out | | Vapor | Product | | Recycle | | |
| 7 | | N(C8H10) | N(H2O) | N(C8H10) | N(H2O) | N(C8H8) | N(C8H10) | N(H2O) | N(H2) | N(C8H8) | N(H2O) | N(C8H10) | N(C8H8) | N(H2) | N(C8H10) | N(C8H8) | N(C8H10) | N(C8H8) | RHS |
| 8 | Feed | | 1 | | | | | | | | | | | | | | | | 3000 |
| 9 | Specs | 1 | | | | | | | | | | | | | | | | | 100 |
| 10 | Mixer | 1 | | -1 | | | | | | | | | | | | | 1 | | 0 |
| 11 | Material | | 1 | | -1 | | | | | | | | | | | | | | 0 |
| 12 | Balances | | | | | -1 | | | | | | | | | | | | 1 | 0 |
| 13 | Reactor | | | 0.35 | | | -1 | | | | | | | | | | | | 0 |
| 14 | Balances | | | | 1 | | | -1 | | | | | | | | | | | 0 |
| 15 | | | | 0.65 | | | | | -1 | | | | | | | | | | 0 |
| 16 | | | | 0.65 | | 1 | | | | -1 | | | | | | | | | 0 |
| 17 | Separator 1 | | | | | | 1 | | | | | -1 | | | | | | | 0 |
| 18 | | | | | | | | 1 | | | -1 | | | | | | | | 0 |
| 19 | | | | | | | | | 1 | | | | | -1 | | | | | 0 |
| 20 | | | | | | | | | | 1 | | | -1 | | | | | | 0 |
| 21 | Separator 2 | | | | | | | | | | | 1 | | | -1 | | -1 | | 0 |
| 22 | | | | | | | | | | | | | 1 | | | -1 | | -1 | 0 |
| 23 | | | | | | | | | | | | 0.01 | | | -1 | | | | 0 |
| 24 | | | | | | | | | | | | | 0.99 | | | -1 | | | 0 |

(a)

| | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 30 | | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | N(C8H10) | Feed |
| 31 | | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Feed |
| 32 | | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 153.02 | N(C8H10) | Reactor In |
| 33 | | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Reactor In |
| 34 | | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1.00469 | N(C8H8) | Reactor In |
| 35 | | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 53.5578 | N(C8H10) | Reactor Out |
| 36 | | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Reactor Out |
| 37 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 99.4644 | N(H2) | Reactor Out |
| 38 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100.469 | N(C8H8) | Reactor Out |
| 39 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Water Out |
| 40 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 53.5578 | N(C8H10) | Organic Out |
| 41 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 100.469 | N(C8H8) | Organic Out |
| 42 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 99.4644 | N(H2) | Vapor Out |
| 43 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0.53558 | N(C8H10) | Product |
| 44 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 99.4644 | N(C8H8) | Product |
| 45 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 53.0222 | N(C8H10) | Recycle |
| 46 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1.00469 | N(C8H8) | Recycle |

(b)

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 50 | | | 1 | | | | | | | | | | | | | | | | 3000 |
| 51 | | 1 | | | | | | | | | | | | | | | | | 100 |
| 52 | | 1 | | -1 | | | | | | | | | | | | | 1 | | 0 |
| 53 | | | 1 | | -1 | | | | | | | | | | | | | | 0 |
| 54 | | | | | | -1 | | | | | | | | | | | | 1 | 0 |
| 55 | | | | 0.35 | | | -1 | | | | | | | | | | | | 0 |
| 56 | | | | | 1 | | | -1 | | | | | | | | | | | 0 |
| 57 | | | | 0.65 | | | | | -1 | | | | | | | | | | 0 |
| 58 | | | | 0.65 | | 1 | | | | -1 | | | | | | | | | 0 |
| 59 | | | | | | | 1 | | | | | -1 | | | | | | | 0 |
| 60 | | | | | | | | 1 | | | -1 | | | | | | | | 0 |
| 61 | | | | | | | | | 1 | | | | | -1 | | | | | 0 |
| 62 | | | | | | | | | | 1 | | | -1 | | | | | | 0 |
| 63 | | | | | | | | | | | | 1 | | | -1 | | -1 | | 0 |
| 64 | | | | | | | | | | | | | 1 | | | -1 | | -1 | 0 |
| 65 | | | | | | | | | | | | 0.01 | | | -1 | | | | 0 |
| 66 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -0.0099 | 5E-05 | -0.0001 | 0.0187 | -1E-13 |

(c)

**FIGURE 4.12a-c**

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 29 | | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | N(C8H10) | Feed |
| 30 | | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Feed |
| 31 | | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 153.02 | N(C8H10) | Reactor In |
| 32 | | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Reactor In |
| 33 | | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.2855 | N(C8H8) | Reactor In |
| 34 | | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 53.558 | N(C8H10) | Reactor Out |
| 35 | | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Reactor Out |
| 36 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 99.464 | N(H2) | Reactor Out |
| 37 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 99.75 | N(C8H8) | Reactor Out |
| 38 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Water Out |
| 39 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 53.558 | N(C8H10) | Organic Out |
| 40 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 99.75 | N(C8H8) | Organic Out |
| 41 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 99.464 | N(H2) | Vapor Out |
| 42 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0.5356 | N(C8H10) | Product |
| 43 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 99.464 | N(C8H8) | Product |
| 44 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 53.022 | N(C8H10) | Recycle |
| 45 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0.2855 | N(C8H8) | Recycle |

(d)

**FIGURE 4.12d**

```
Option Explicit                                                                  line 1

    Public Sub Gauss_Jordan_Macro()                                              line 2
        Dim C() As Double                                                        line 3
        Dim Nrows, Ncolumns As Long                                              line 4

        Nrows = 3                                                                line 5
        Ncolumns = 4                                                             line 6
        ReDim C(Nrows, Ncolumns)                                                 line 7

 'Read augmented matrix from Excel sheet                                         line 8
        Dim i As Integer                                                         line 9
        Dim j As Integer                                                         line 10
        For i = 0 To Nrows - 1                                                   line 11
            For j = 0 To Ncolumns - 1                                            line 12
                If Sheet1.Cells(i + 8, j + 2) = " " Then                         line 13
                    C(i, j) = 0                                                  line 14
                Else                                                             line 15
                    C(i, j) = Sheet1.Cells(i + 8, j + 2)                         line 16
                End If                                                           line 17
            Next j                                                               line 18
        Next i                                                                   line 19

  ' Call Gauss-Jordan matrix elimination method                                  line 20
        GJ_Elimination(C, Nrows)                                                 line 21

  ' Place solution from Gauss-Jordan matrix elimination method on Excel Sheet    line 22
        For i = 0 To Nrows - 1                                                   line 23
            For j = 0 To Ncolumns - 1                                            line 24
                Sheet1.Cells(i + 12, j + 2) = C(i, j)                            line 25
            Next j                                                               line 26
        Next i                                                                   line 27
    End Sub                                                                      line 28

    Public Sub GJ_Elimination(A, row)                                            line 29

        Dim col As Long                                                          line 30
        col = row + 1                                                            line 31

        Dim nonZerIdx As Integer                                                 line 32
        nonZerIdx = 0                                                            line 33

  ' We first to check if the diagnol element is zero                            line 34
        Dim i As Integer                                                         line 35
        For i = 0 To row - 1                                                     line 36
            If A(i, i) = 0 Then                                                  line 37
   ' If the diagnol element = 0 we need to look at following rows
   ' to find a nonzero element in the i column                                   line 38
                Dim i2 As Integer                                                line 39
                For i2 = i + 1 To row - 1                                        line 40

                    If A(i2, i) <> 0 Then                                        line 41
                        nonZerIdx = i2                                           line 42
                        Exit For                                                 line 43
                    Else                                                         line 44
                    End If                                                       line 45
                Next i2                                                          line 46

  ' Here we exchange the row with the diagnol element = 0 with the
  ' first following row in which the i column has a nonzero value               line 47
                Dim j1 As Integer                                                line 48
                For j1 = 0 To col - 1                                            line 49
                    Dim tmp As Double                                            line 50
                    tmp = A(i, j1)                                               line 51
                    A(i, j1) = A(nonZerIdx, j1)                                  line 52
                    A(nonZerIdx, j1) = tmp                                       line 53
                Next j1                                                          line 54

            Else                                                                 line 55
            End If                                                               line 56
```

**FIGURE 4.1a**

```
' Here we divide every element of the pivot row
' by the the diagnol element (the pivot element)                    line 57
         Dim tmpAii As Double                                       line 58
          tmpAii = A(i, i)                                          line 59
          Dim j As Integer                                          line 60
          For j = 0 To (col - 1)                                    line 61
              A(i, j) = A(i, j) / tmpAii                            line 62
          Next j                                                    line 63

' Here we eliminate (make zero) all elements in the pivot column.  This is
'  not done for the pivot row.  See equation (4.2) aij = aij - aik akj   line 64
        Dim i1 As Integer                                           line 65
          For i1 = 0 To (row - 1)                                   line 66
              If i1 <> i Then                                       line 67
                  Dim tmpAi1 As Double                              line 68
                  tmpAi1 = A(i1, i)                                 line 69
                  For j = 0 To (col - 1)                            line 70
                      A(i1, j) = A(i1, j) - tmpAi1 * A(i, j)        line 71
                  Next j                                            line 72
              Else                                                  line 73

              End If                                                line 74
          Next i1                                                   line 75
      Next i                                                        line 76
  End Sub                                                           line 77
```

**FIGURE 4.1b**

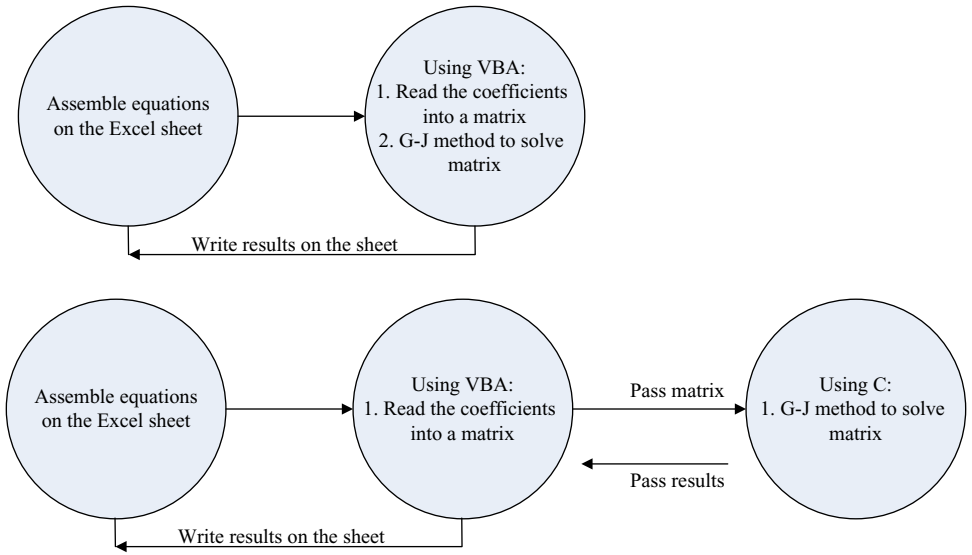
Assemble equations on the Excel sheet
Using VBA:
1. Read the coefficients into a matrix
2. G-J method to solve matrix
Write results on the sheet
Assemble equations on the Excel sheet
Using VBA:
1. Read the coefficients into a matrix
Pass matrix
Using C:
1. G-J method to solve matrix
Pass results
Write results on the sheet

**FIGURE 4.3**

(a)

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | *Styrene Material Balance using Gauss Jordan Elimination - VBA program* | | | | | | | | | | | | | | | | | | |
| 2 | | | | | | | | | | | | | | | | | | | |
| 3 | Reactio | $C_8H_{10}$ ---> $C_8H_8$ + $H_2$ | | | Conversion | | 0.65 | | | | | | | | | | | | |
| 4 | | | | | | | | | | | | | | | | | | | |
| 5 | | | | | | | | | | | | | | | | | | | |
| 6 | | Feed | | | Reactor In | | | Reactor Out | | | Water Out | Organic Out | | Vapor | Product | | Recycle | | |
| 7 | | N(C8H10) | N(H2O) | N(C8H10) | N(H2O) | N(C8H8) | N(C8H10) | N(H2O) | N(H2) | N(C8H8) | N(H2O) | N(C8H10) | N(C8H8) | N(H2) | N(C8H10) | N(C8H8) | N(C8H10) | N(C8H8) | RHS |
| 8 | Feed | | 1 | | | | | | | | | | | | | | | | 3000 |
| 9 | Specs | 1 | | | | | | | | | | | | | | | | | 100 |
| 10 | Mixer | 1 | | -1 | | | | | | | | | | | | | 1 | | 0 |
| 11 | Material | | 1 | | -1 | | | | | | | | | | | | | | 0 |
| 12 | Balances | | | | | -1 | | | | | | | | | | | | 1 | 0 |
| 13 | Reactor | | | 0.35 | | | -1 | | | | | | | | | | | | 0 |
| 14 | Balances | | | | 1 | | | -1 | | | | | | | | | | | 0 |
| 15 | | | | 0.65 | | | | | -1 | | | | | | | | | | 0 |
| 16 | | | | 0.65 | | 1 | | | | -1 | | | | | | | | | 0 |
| 17 | Separator 1 | | | | | | 1 | | | | | -1 | | | | | | | 0 |
| 18 | | | | | | | | 1 | | | -1 | | | | | | | | 0 |
| 19 | | | | | | | | | 1 | | | | | -1 | | | | | 0 |
| 20 | | | | | | | | | | 1 | | | -1 | | | | | | 0 |
| 21 | Separator 2 | | | | | | | | | | | 1 | | | -1 | | -1 | | 0 |
| 22 | | | | | | | | | | | | | 1 | | | -1 | | -1 | 0 |
| 23 | | | | | | | | | | | | 0.01 | | | -1 | | | | 0 |
| 24 | | | | | | | | | | | | | 0.99 | | | -1 | | | 0 |

Row 8 Column 2

(b)

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 30 | | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | N(C8H10) | Feed |
| 31 | | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Feed |
| 32 | | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 153.02 | N(C8H10) | Reactor In |
| 33 | | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Reactor In |
| 34 | | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1.0047 | N(C8H8) | Reactor In |
| 35 | | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 53.558 | N(C8H10) | Reactor Out |
| 36 | | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Reactor Out |
| 37 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 99.464 | N(H2) | Reactor Out |
| 38 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100.47 | N(C8H8) | Reactor Out |
| 39 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3000 | N(H2O) | Water Out |
| 40 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 53.558 | N(C8H10) | Organic Out |
| 41 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 100.47 | N(C8H8) | Organic Out |
| 42 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 99.464 | N(H2) | Vapor Out |
| 43 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0.5356 | N(C8H10) | Product |
| 44 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 99.464 | N(C8H8) | Product |
| 45 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 53.022 | N(C8H10) | Recycle |
| 46 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1.0047 | N(C8H8) | Recycle |

Row 30 Column 2

**FIGURE 4.5**

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | *Styrene Material Balance with Alternative Specification - Augmented Matrix* | | | | | | | | | | | | | | | | | | |
| 2 | | | | | | | | | | | | | | | | | | | |
| 3 | Reactio | $C_8H_{10}$ ---> $C_8H_8$ + $H_2$ | | | Conversion | | 0.65 | | | | | | | | | | | | |
| 4 | | | | | | | | | | | | | | | | | | | |
| 5 | | | | | | | | | | | | | | | | | | | |
| 6 | | Feed | | | Reactor In | | | Reactor Out | | | Water Out | Organic Out | | Vapor | Product | | Recycle | | |
| 7 | | N(C8H10) | N(H2O) | N(C8H10) | N(H2O) | N(C8H8) | N(C8H10) | N(H2O) | N(H2) | N(C8H8) | N(H2O) | N(C8H10) | N(C8H8) | N(H2) | N(C8H10) | N(C8H8) | N(C8H10) | N(C8H8) | RHS |
| 8 | Feed | 1 | | | | | | | | | | | | | | | | | 100 |
| 9 | Mixer | 1 | | -1 | | | | | | | | | | | | | 1 | | 0 |
| 10 | Material | | 1 | | -1 | | | | | | | | | | | | | | 0 |
| 11 | Balances | | | | | -1 | | | | | | | | | | | | 1 | 0 |
| 12 | Reactor | | | 0.35 | | | -1 | | | | | | | | | | | | 0 |
| 13 | Balances | | | | 1 | | | -1 | | | | | | | | | | | 0 |
| 14 | | | | 0.65 | | | | | -1 | | | | | | | | | | 0 |
| 15 | | | | 0.65 | | 1 | | | | -1 | | | | | | | | | 0 |
| 16 | Separator 1 | | | | | | 1 | | | | | -1 | | | | | | | 0 |
| 17 | | | | | | | | 1 | | | -1 | | | | | | | | 0 |
| 18 | | | | | | | | | 1 | | | | | -1 | | | | | 0 |
| 19 | | | | | | | | | | 1 | | | -1 | | | | | | 0 |
| 20 | Separator 2 | | | | | | | | | | | 1 | | | -1 | | -1 | | 0 |
| 21 | | | | | | | | | | | | | 1 | | | -1 | | -1 | 0 |
| 22 | | | | | | | | | | | | 0.01 | | | -1 | | | | 0 |
| 23 | | | | | | | | | | | | | 0.99 | | | -1 | | | 0 |
| 24 | Alternative Spec | | | -0.9 | 0.1 | -0.9 | | | | | | | | | | | | | 0 |

(a)

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 30 | | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | N(C8H10) | Feed |
| 31 | | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Feed |
| 32 | | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 153.02 | N(C8H10) | Reactor In |
| 33 | | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Reactor In |
| 34 | | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1.00469 | N(C8H8) | Reactor In |
| 35 | | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 53.5578 | N(C8H10) | Reactor Out |
| 36 | | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Reactor Out |
| 37 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 99.4644 | N(H2) | Reactor Out |
| 38 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100.469 | N(C8H8) | Reactor Out |
| 39 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1386.24 | N(H2O) | Water Out |
| 40 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 53.5578 | N(C8H10) | Organic Out |
| 41 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 100.469 | N(C8H8) | Organic Out |
| 42 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 99.4644 | N(H2) | Vapor Out |
| 43 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0.53558 | N(C8H10) | Product |
| 44 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 99.4644 | N(C8H8) | Product |
| 45 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 53.0222 | N(C8H10) | Recycle |
| 46 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1.00469 | N(C8H8) | Recycle |

(b)

**FIGURE 4.6**

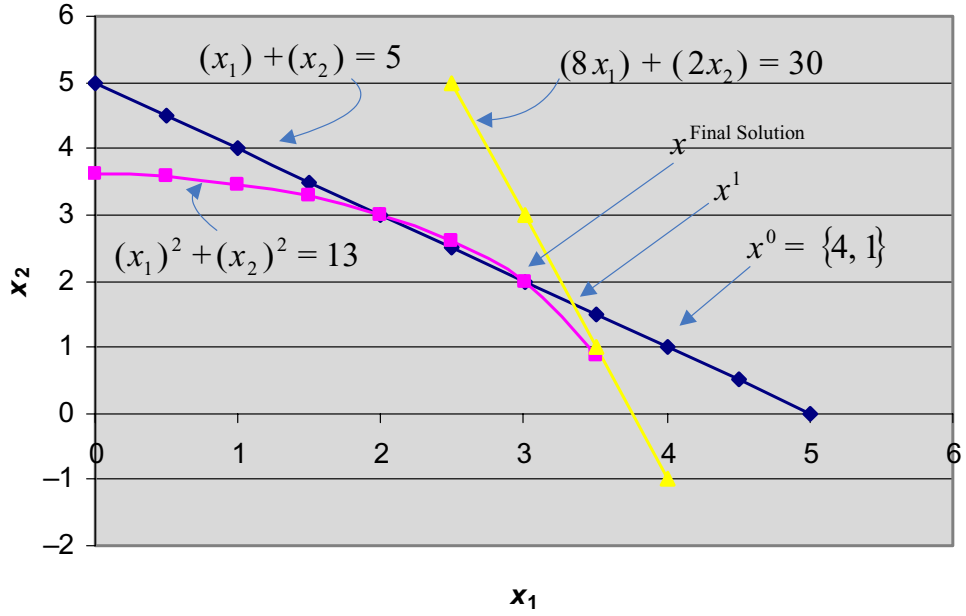
$(x_1) + (x_2) = 5$
$(8x_1) + (2x_2) = 30$
$x^{\text{Final Solution}}$
$x^1$
$x^0 = \{4, 1\}$
$(x_1)^2 + (x_2)^2 = 13$
$x_2$
$x_1$
6
5
4
3
2
1
0
–1
–2
0
1
2
3
4
5
6

**FIGURE 4.7**

```
Option Explicit
'path to the Gauss-Jordan matrix elimination method
Public Declare Sub GJ_Elimination_Main Lib "C:\POEA\Bridging Excel and C
Codes\Examples\Simple_C_Matrix_dll\Debug\Simple_C_Matrix_dll.dll" (ByRef Matrix As
Double, ByVal Nrows As Long, ByVal Ncolumns As Long)

Dim Nrows, Ncolumns, cntNLeq, RowStartFirstMatrix, RowStartSecondMatrix,
RowStartThirdMatrix, RowStartNLEqsThirdMatrix As Long

Public Sub Gauss_Jordan_Macro()
    Dim C() As Double

    'The user must specify the number of rows (Nrows);
    'the number of nonlinear equations (cntNLeq);
    'and the row where the first matrix begins on the Excel sheet (RowStartFirstMatrix)
    'we assume all matrices will begin in column 2 - use column one for comments
    Nrows = 3
    Ncolumns = Nrows + 1
    cntNLeq = 2
    RowStartFirstMatrix = 8

    'Here we are keeping a gap of 4 rows between matrices on the Excel sheet
    RowStartSecondMatrix = RowStartFirstMatrix + Nrows + 4
    RowStartThirdMatrix = RowStartSecondMatrix + Nrows + 4

    'Here we identify the starting row in the thrid matrix for the nonlinear equations
    RowStartNLEqsThirdMatrix = RowStartThirdMatrix + Nrows - cntNLeq


    'Here we read the first matrix on the Excel sheet into the VBA matrix C
    ' if the entry on the Excel sheet is blank " " we set the entry to zero
    ReDim C(Nrows, Ncolumns)
    Dim i As Integer
    Dim j As Integer
    For i = 0 To Nrows - 1
        For j = 0 To Ncolumns - 1
            If Sheet1.Cells(i + RowStartFirstMatrix, j + 2) = " " Then
                C(i, j) = 0
            Else
                C(i, j) = Sheet1.Cells(i + RowStartFirstMatrix, j + 2)
            End If
        Next j
    Next i

    ' We call the Gauss-Jordan matrix elimination method which is a C program
    ' and we palce the results in the second matrix on the Excel sheet
    GJ_Elimination_Main C(0, 0), Nrows, Ncolumns

    For i = 0 To Nrows - 1
        For j = 0 To Ncolumns - 1
            Sheet1.Cells(i + RowStartSecondMatrix, j + 2) = C(i, j)
        Next j
    Next i
End Sub
Public Sub NR_Gauss_Jordan_Macro()
'Here we will use the Newton Raphson method to linearize the NL equations.

    Dim x() As Double
    Dim F() As Double
    Dim D() As Double

    Dim i, j As Integer

    Dim DELTA As Double
    DELTA = 0.0001

'First we copy all the current coeficients from the first matrix (the all linear matrix)
    'to the third matrix
    'Eventually we will then need to substitute in the linearized NL equations

    For i = 0 To Nrows - 1
        For j = 0 To Ncolumns - 1
            Sheet1.Cells(i + RowStartThirdMatrix, j + 2) = Sheet1.Cells(i +
RowStartFirstMatrix, j + 2)
        Next j
    Next i

 'Get the current solution x = x* from the second matrix
    ReDim x(Nrows)
    Get_X_Values(Nrows, x)

 'The Newton Raphson Method for the NL equations
    ReDim F(cntNLeq)
    ReDim D(cntNLeq, Nrows)
```

**FIGURE 4.9a**

```
 ' Evaluate each NL equation at x*
    For i = 0 To cntNLeq - 1
        F(i) = NLFunc(i, x)
    Next i

 ' Determine partial derivative for each NL equation wrt each variable at x*
    For i = 0 To cntNLeq - 1
        For j = 0 To Nrows - 1
            x(j) = x(j) + DELTA
            D(i, j) = (NLFunc(i, x) - F(i)) / DELTA
            x(j) = x(j) - DELTA
        Next j
    Next i
' Place the partial derivatives at x* for each NL equation on the Excel sheet - third
' matrix
    For i = 0 To cntNLeq - 1
        For j = 0 To Nrows - 1
            Sheet1.Cells(i + RowStartNLEqsThirdMatrix, j + 2) = D(i, j)
        Next j
    Next i

' Calculate Beta for each NL equation and place on Excel sheet - third matrix
    Dim TempSum As Double
    For i = 0 To cntNLeq - 1
        TempSum = 0
        For j = 0 To Nrows - 1
            TempSum = TempSum + x(j) * D(i, j)
        Next j
        Sheet1.Cells(i + RowStartNLEqsThirdMatrix, Ncolumns + 1) = TempSum - F(i)
    Next i

  ' Read coefficients from the third matrix into the VBA matrix C
    Dim C() As Double

    ReDim C(Nrows, Ncolumns)

    For i = 0 To Nrows - 1
        For j = 0 To Ncolumns - 1
            If Sheet1.Cells(i + RowStartThirdMatrix, j + 2) = " " Then
                C(i, j) = 0
            Else
                C(i, j) = Sheet1.Cells(i + RowStartThirdMatrix, j + 2)
            End If
        Next j
    Next i

  'Call the Gauss-Jordan matrix elimination mathod
  'and place the results on the Excel sheet in the second matrix
    GJ_Elimination_Main C(0, 0), Nrows, Ncolumns

    For i = 0 To Nrows - 1
        For j = 0 To Ncolumns - 1
            Sheet1.Cells(i + RowStartSecondMatrix, j + 2) = C(i, j)
        Next j
    Next i

End Sub

Private Sub Get_X_Values(ByVal N As Integer, ByRef x() As Double)
  ' Get the current solution x = x*
    Dim i As Integer

    For i = 0 To N - 1
        x(i) = Sheet1.Cells(i + RowStartSecondMatrix, Ncolumns + 1)
    Next i
End Sub

Private Function NLFunc(ByVal Idx As Long, ByRef x() As Double) As Double
  ' The NL equations
  ' --- Remember Index on Functions AND x(i) BOTH start at Zero
    If Idx = 0 Then
        NLFunc = x(0) ^ (1 / 2) + (x(1)) ^ 2 + x(1) * x(2) - 11
    End If
    If Idx = 1 Then
        NLFunc = x(0) * x(0) + x(1) * x(1) + x(2) * x(2) - 14
    End If

End Function
```

**FIGURE 4.9b**

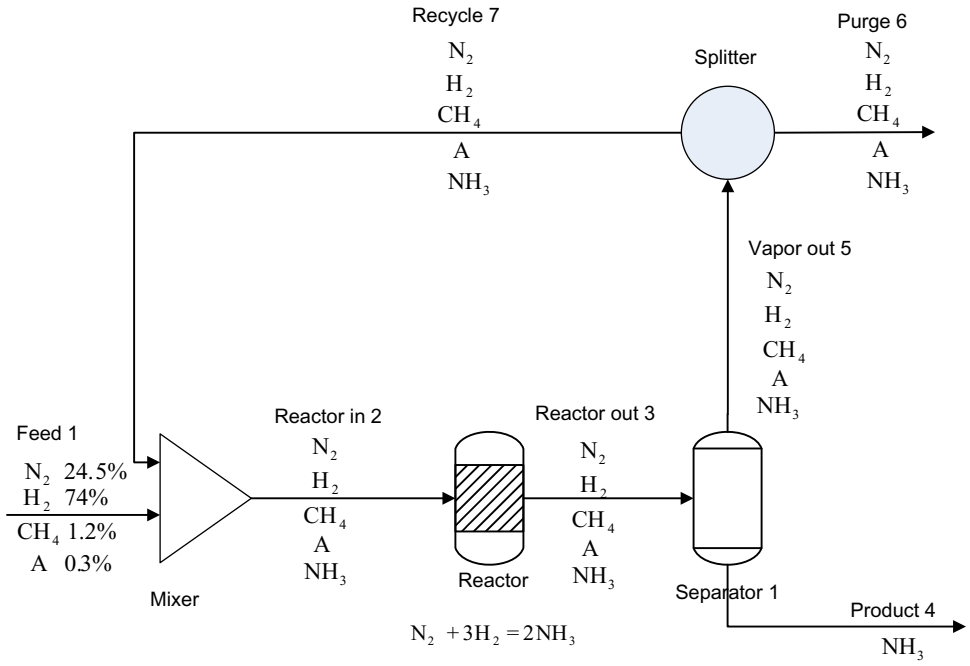
Recycle 7
$N_2$
$H_2$
$CH_4$
A
$NH_3$
Splitter
Purge 6
$N_2$
$H_2$
$CH_4$
A
$NH_3$
Vapor out 5
$N_2$
$H_2$
$CH_4$
A
$NH_3$
Feed 1
$N_2$ 24.5%
$H_2$ 74%
$CH_4$ 1.2%
A 0.3%
Mixer
Reactor in 2
$N_2$
$H_2$
$CH_4$
A
$NH_3$
Reactor
Reactor out 3
$N_2$
$H_2$
$CH_4$
A
$NH_3$
Separator 1
Product 4
$NH_3$
$N_2 + 3H_2 = 2NH_3$

**FIGURE p4.10**