Example of using NEQNF subroutine

Example Statement

Consider a binary system of component 1 and 2, with component 1 being the more volatile one. For a given pressure P and a vapor composition y of component 1 the dew point calculation consist in determining the Temperature T and the liquid composition x. Assuming ideal phase equilibrium the Pressure and the liquid composition are given by:

$$P = xP_1^s + (1-x)P_2^s$$

$$yP = xP_1^s$$

where P_i^s are the vapor-pressure given by the simple Antoine relation:

$$\ln P_i^s = A_i + \frac{B_i}{T} \quad (\mathrm{i} = 1,2)$$

- For specific pressure and vapor composition the objective is then to find the Temperature T and the liquid composition x that satisfy:

$$f_1(T,x) = P - xP_1^s(T) - (1-x)P_2^s = 0$$

$$f_2(T,x) = yP - xP_1^s(T) = 0$$

- Perform the calculations for a mixture of water-methanol at atmospheric and at a pressure of 3 bar. The vapor mole fraction of methanol in both cases is 0.6. solve the problem using appropriate IMSL library subroutine.
- Data:

  Methanol: $A_1 = 19.6664$, $B_1 = -4361.55$

  Water: $A_1 = 20.1735$, $B_1 = -5050.5$

The pressure should be in *mmHg* and temperature in ^{o}K.

Fortran Program Listing

```
INTEGER    N,ITMAX
REAL                  X(3), XG(3), FNORM
EXTERNAL  FCN

N=2
ERRREL=1.0e-4
ITMAX=100
XG(1)=0.5
XG(2)=100.0

CALL NEQNF (FCN, ERRREL, N, ITMAX, XG, X, FNORM)

WRITE(6,*)
WRITE(6,*)'FNORM = ',FNORM
      WRITE(6,*)'X1 = ',X(1)
      WRITE(6,*)'X2 = ',X(2)

STOP
END
```

```
SUBROUTINE FCN(X,F,N)
      INTEGER    N
      REAL                    X(N),F(N)

      P=3.0*750.6
      Y=0.6
      A1=19.6664
      B1=-4361.55
      A2=20.1735
      B2=-5050.5

      PS1=EXP(A1+B1/(X(2)+273))
      PS2=EXP(A2+B2/(X(2)+273))

      F(1)=P-X(1)*PS1-(1-X(1))*PS2
      F(2)=Y*P-X(1)*PS1

      RETURN
      END
```

Output

```
c
c          FNORM =    5.483037E-04
c          X1 =    2.966535E-01
c          X2 =      114.950700
c          Stop - Program terminated.

c          Press any key to continue
```