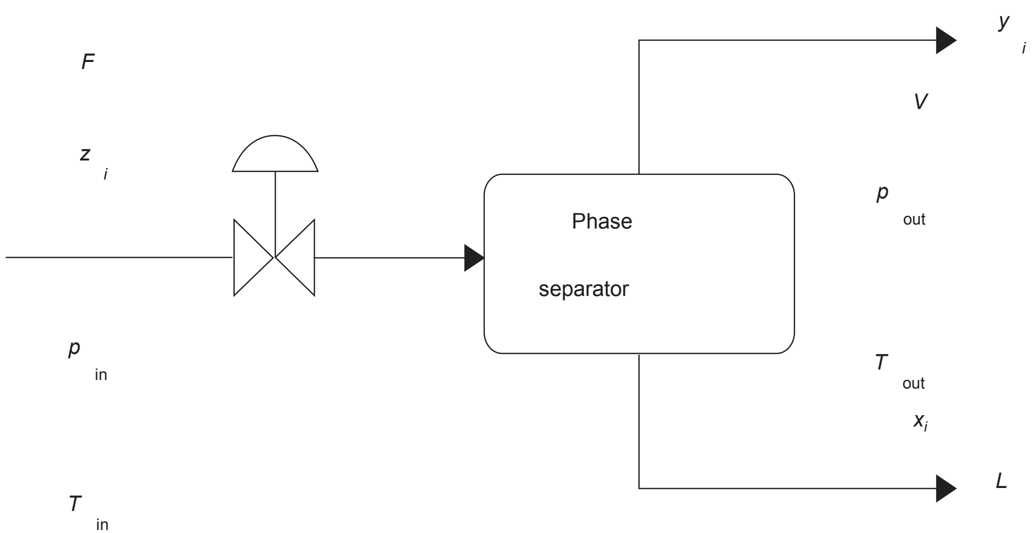
KING SAUD UNIVERSITY

CHE406: Numerical Methods In Chemical Engineering

(Week 5-6 Lecture)

Numerical solutions of Single non-linear equations

Multi-Component Flash Distillation



Multi-Component Flash Distillation

Equilibrium Relationship:

$$y_i = K_i x_i \qquad \text{N equations} \qquad \text{Eq. (1)}$$

$$K_i = K_i(T_d, P_d, \text{all } x_i) \qquad \text{N equations} \qquad \text{Eq. (2)}$$

Stoichiometric (mole fraction) Relationships:

$$\sum_{i=1}^{C} x_i = 1.0 \qquad \sum_{i=1}^{C} y_i = 1.0 \qquad \text{2 equations} \qquad \text{Eq. (3)}$$

Mass Balance Equations:

$$Fz_i = Vy_i + Lx_i \qquad \text{N equations} \qquad \text{Eq. (4)}$$

$$F = V + L \qquad \text{Eq. (5)}$$

Energy Balance:

$$Fh_F + Q_{flash} = VH_V + Lh_L \qquad \text{Eq. (6)}$$

Multi-Component Flash Distillation

- We could define all N equations, and solve the N simultaneous equations simultaneously.

- This may or may not be possible – if we are dealing with a large number of simultaneous equations, and one may experience convergence problems in a numerical solution.

- How can we "enhance" the convergence? One method is to partially solve the set of equations for a parameter which is tightly bounded – that is its values cannot vary widely.

- A convenient choice is the fraction of feed vaporized, f = V/F, which varies between 0 and 1.

Multi-Component Flash Distillation

Substituting the equilibrium relationship, Eq. (1), for y_i, into the component mass balance, Eq. (4), we obtain

$$Fz_i = Lx_i + VK_i x_i \qquad i = 1, 2, ..., C \qquad \text{Eq. (4a)}$$

Substituting the overall mass balance, Eq. (5), for L into Eq. (4a), solving for x_i, and dividing through by F yields

$$x_i = \frac{z_i}{1 + (K_i - 1)\frac{V}{F}} \qquad i = 1, 2, ..., C \qquad \text{Eq. (7)}$$

Since $y_i = K_i x_i$, from Eq. (7), we also obtain

$$y_i = \frac{K_i z_i}{1 + (K_i - 1)\frac{V}{F}} \qquad i = 1, 2, ..., C \qquad \text{Eq. (8)}$$

Multi-Component Flash Distillation

Substituting Eqs. (7) and (8) into the respective mole fraction relationships, Eqs.(3-20), yields:

$$\sum_{i=1}^{C} \frac{z_i}{1+(K_i-1)\frac{V}{F}} = 1 \qquad \text{Eq.(9)}$$

$$\sum_{i=1}^{C} \frac{K_i z_i}{1+(K_i-1)\frac{V}{F}} = 1 \qquad \text{Eq. (10)}$$

Subtracting Eq. (9) from Eq. (10) term by term yields

$$\sum_{i=1}^{C} \frac{(K_i-1)z_i}{1+(K_i-1)\frac{V}{F}} = 0 \qquad \text{Eq. (11)}$$

Eq. (11) is known as the Rachford-Rice equation. It has excellent conversion properties for use in numerical solutions of multi-component flash distillations.

Multi-Component Flash Distillation

Once one solves the Rachford-Rice equation and determines all of the vapor and liquid mole fractions, the accompanying energy balances can then solved.

$$H_V = \sum_{i=1}^{C} y_i \tilde{H}_{V_i}(T_d, P_d) \qquad \text{Eq. (12)}$$

$$h_L = \sum_{i=1}^{C} x_i \tilde{h}_{L_i}(T_d, P_d) \qquad \text{Eq. (13)}$$

Multi-Component Flash Distillation

```
% vapor-liquid equilibrium
% output: vapor fraction of flash

function vf = vpequil(v)
global z K nc

sum = 0.0;
for i=1:nc
    num = (K(i)-1)*z(i);
    denom = 1 + (K(i)-1)*v;
    sum = sum + num/denom;
end
vf = sum;
end
```

Multi-Component Flash Distillation

```
%page34_run_VLEquil.m
global z K nc
z = [0.1 0.3 0.4 0.2];
K = [6.8 2.2 0.8 0.052];
nc = length(z) ;

VoF = fzero(@vpequil,0.2)
for i = 1:nc
     denum = 1 + (K(i)-1)*VoF ;
     x(i) = z(i)/denum ;
     y(i) = K(i)*x(i) ;
end

xxx = sum(x)
yyy = sum(y)
% to check your answer, evaluate the function
with the output values
ans = feval(@vpequil,VoF)
```

Multi-Component Flash Distillation

FoV=

0.4258

ans =

5.5511e-17