Multicomponent Isothermal Flash and Partial condensation Calculations:

Given
- ▲ Feed data (F, T_F, P_F, C-1 values of $\vec{z}$)
- ▲ T_V (or T_L)
- ▲ P_V (or P_L)

Required: $\underbrace{V, L, Q, \vec{y}, \vec{x}, T_L (\text{or } T_V), P_L (\text{or } P_V), Z_c}$ (remaining)

Remaining unknowns: 2C+6

<u>Procedure:</u> The solution procedure is sequential.

Step 1:

Solve equations containing one variable.

$$T_L = T_V$$
$$P_L = P_V$$
$$Z_k = 1 - \sum_{\substack{i=1 \\ i \neq k}}^{c} z_i \qquad c: \text{no of components.}$$

Step 2: Solution of Material Balance and Eqm Relations

- ▲ Material Balances are non linear → computational procedure is not straightforward and many solution strategies can be adopted
- ▲ K_i values may be function of composition or independent of composition. This influences the solution strategy.

Case: K_i values independent of composition.

$$F z_i = V y_i + L x_i$$

+

$$F = V + L$$

$$F z_i = V y_i + (F - V) \cdot x_i$$

Substitute $y_i = K_i \cdot x_i$ for y_i or x_i

solve for y_i | solve for x_i

Solve for y_i:

$$F z_i = V y_i + (F - V) \cdot \frac{y_i}{x_i}$$

$$y_i \left[V + \frac{(F-V)}{K_i} \right] = F z_i$$

$$y_i = \frac{F z_i K_i}{V K_i + (F - V)}$$

$$y_i = \frac{z_i \cdot K_i}{\left(\frac{V}{F}\right) K_i + \left(1 - \frac{V}{F}\right)}$$

$$\psi = \frac{V}{F}$$

$$y_i = \frac{K_i \cdot z_i}{1 + \psi (K_i - 1)}$$

Solve for x_i:

$$F z_i = V K_i x_i + (F - V) x_i$$

$$x_i \left[V K_i + (F - V) \right] = F z_i$$

$$x_i = \frac{F z_i}{V K_i + (F - V)}$$

$$x_i = \frac{z_i}{\frac{V}{F} K_i + \left(1 - \frac{V}{F}\right)}$$

$$\psi = \frac{V}{F}$$

$$x_i = \frac{z_i}{1 + \psi (K_i - 1)}$$

($y_i = K_i x_i$ →)

Constraints $\quad \sum y_i = 1 \qquad \sum x_i = 1$

In iterative solutions:

$\sum < 1$ reduce ψ

$\sum > 1$ increase ψ

One strategy consists of

- Finding K_i's at T_V
- Guessing values of ψ until $\sum y_i = 1$ OR $\sum x_i = 1$

Another strategy:

The equations for y_i and x_i can be combined to give a non linear equation in ψ only.

$$\sum_{i=1}^{c} y_i - \sum_{i=1}^{c} x_i = 0$$

$$\sum^{c} \frac{K_i z_i}{1+\psi(K_i-1)} - \sum \frac{z_i}{1+\psi(K_i-1)} = 0$$

$$\boxed{\sum \frac{z_i (K_i-1)}{1+\psi(K_i-1)} = 0}$$

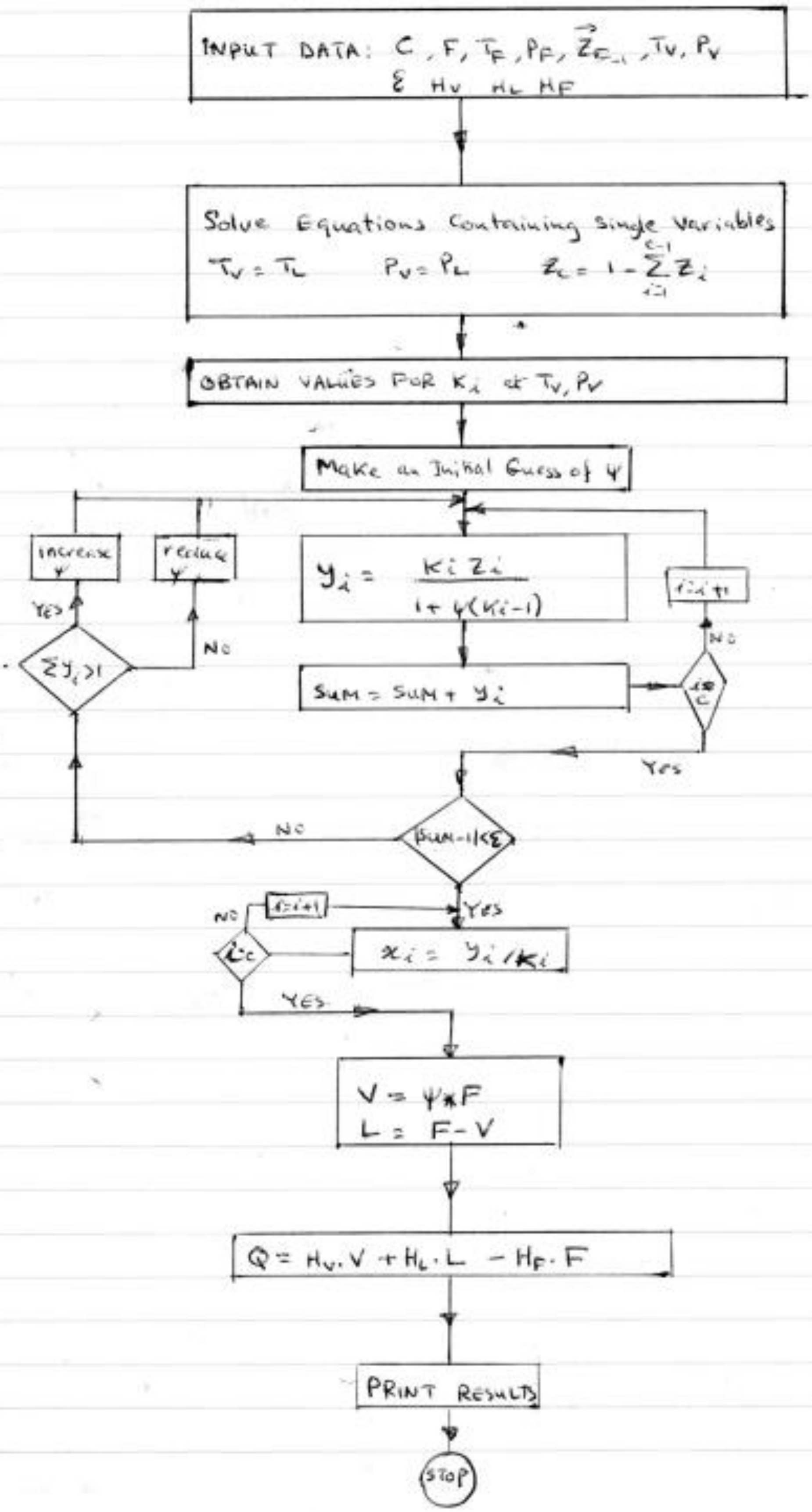
This equation can be solved for ψ.

Step 3:

- $V = \psi F \Rightarrow L = F - V$
- $x_i = \dfrac{z_i}{1+\psi(K_i-1)}$
- $y_i = K_i x_i$

$$Q = H_V \cdot V + H_L \cdot L - H_F \cdot F.$$

Note: If T_F or/and P_F are not specified, then Q cannot be calculated. In this case eqm phase conditions are calculated only.


INPUT DATA: C, F, T_F, P_F, $\vec{Z}_{F_{c-1}}$, T_V, P_V
ε H_V H_L H_F
Solve Equations Containing single Variables
$T_V = T_L$ $P_V = P_L$ $Z_c = 1 - \sum_{i=1}^{c-1} Z_i$
OBTAIN VALUES FOR K_i at T_V, P_V
Make an Initial Guess of ψ
increase ψ
reduce ψ
YES
NO
$\sum y_i > 1$
$y_i = \frac{K_i Z_i}{1 + \psi(K_i - 1)}$
SUM = SUM + y_i
i = i+1
NO
YES
NO
$|SUM - 1| < \varepsilon$
YES
NO
i = i+1
$x_i = y_i / K_i$
YES
$V = \psi * F$
$L = F - V$
$Q = H_V \cdot V + H_L \cdot L - H_F \cdot F$
PRINT RESULTS
STOP

Bubble and dew Point Calculations:

Q: Does a Feed give a two phase equilibrium mixture at a given T and P?

A: • As a first estimate

If all K values > 1 ⇒ exit phase above dew point (superheated Vapor)

If all K values < 1 ⇒ exit phase below bubble point (subcooled liquid).

• Use of parameter ψ (more precise).

- $\psi \in [0,1]$ $\quad f(\psi) = \sum \frac{z_i(1-K_i)}{1+\psi(K_i-1)}$

- Bubble point.

$$\psi = 0 \Rightarrow f[\psi=0] = 1 - \Sigma \underbrace{z_i K_i}_{y_i}$$

If $f[\psi=0] > 0 \Rightarrow$ exit mixture below bubble. Vapor is not rich enough $\Sigma y_i < 1$

If $f[\psi=0] = 0 \Rightarrow$ exit mixture at bubblepoint

∴ Bubble point criterion is

$$\boxed{\sum_{i=1}^{c} z_i K_i = 1}$$

with $x_i = z_i$, $y_i = z_i K_i$ } In first bubble

Note:

$$y_i = \frac{\alpha_{ij} z_i}{\Sigma \alpha_{kj} z_k} \Rightarrow \Sigma \alpha_{kj} z_k = \frac{\alpha_{ij} z_i}{y_i} = \frac{K_i}{K_j}\frac{1}{K_i} = \frac{1}{K_j}$$

$$\therefore \quad \Sigma \frac{K_k}{K_j} z_k = \frac{1}{K_j}$$

j: reference component

Dew Point:

$$\psi = 1 \Rightarrow f[\psi=1] = \sum \frac{z_i}{K_i} - 1 \qquad \Sigma z_i = 1$$

if $f[\psi=1] < 0$ exit stream above its dew point [super heated Vapor $K>1$]

if $f[\psi=1] = 0$ exit stream is at its Dew point

∴ Dew point criterion is

$$\sum \left(\frac{z_i}{K_i}\right) = 1 \qquad \text{with } \left.\begin{matrix} y_i = z_i \\ x_i = \frac{z_i}{x_i} \end{matrix}\right\} \Sigma x_i = 1$$

Note: $$x_i = \frac{y_i/\alpha_{ij}}{\Sigma y_K/\alpha_{Kj}} \Rightarrow \sum \frac{y_K}{\alpha_{Kj}} = \frac{y_i}{x_i}\frac{1}{\alpha_{ij}} = K_j$$

$$\text{Assume } T \text{ find } \frac{y_K}{\alpha_{Kj}} \Rightarrow \Sigma \frac{y_K}{\alpha_{Kj}} \overset{?}{=} K_j$$

Note:

Bubble point and Dew point Calculations are used to determine saturatio conditions for liquid and vapor streams respectively.

in VLE
- → Vap is at its dew point (saturated)
- → Liq is at its bubble point (saturated).

Adiabatic Flash:

Given: ▲ Feed data.
▲ P_V
▲ $Q = 0$.

Reqd: $V, L, \vec{y}, \vec{x}$ T_V, T_L, P_L, z_c

Remaining unknowns $2C+6$

Procedure: The solution procedure is simultaneous.

- T_V is unknown ∴ K values cannot be obtained.
- To find T_V – solve enthalpy balance.
- Since EB depends on composition and ψ it cannot be solved alone
- net result → simultaneous soln.

One strategy:

Step 1: solve equations containing one variable.

$P_L = P_V$

$z_c = 1 - \sum^{c-1} z_i$

Step 2: Estimate T_V.

Step 3: use isothermal flash procedure at T_V, P_V.

- obtain K_i at T_V, P_V
- Solve for ψ,
- Solve for $\vec{y}, \vec{x}$
- Solve for V, L.

Step 4: Calculate H_L, H_V

step 5: Check T_v.

From Enthalpy balance $Q=0$ and M.B. $L=F-V$

$$Q = H_V V + H_L(F-V) - H_F \cdot F$$

$$\Psi H_V + (1-\Psi)\cdot H_L - H_F = 0 = f\{T_V\}$$

$f\{T_V\} = 0$ at eqm.

$\therefore$ Calculate $\frac{f\{T_V\}}{1000} = \frac{\Psi H_V - (1-\Psi)H_L - H_F}{1000} \overset{?}{=} 0$.

step 6: if $f\{T_V\} \neq 0$ reestimate T_V and
Go back to step 3.

step 7: stop and print results.