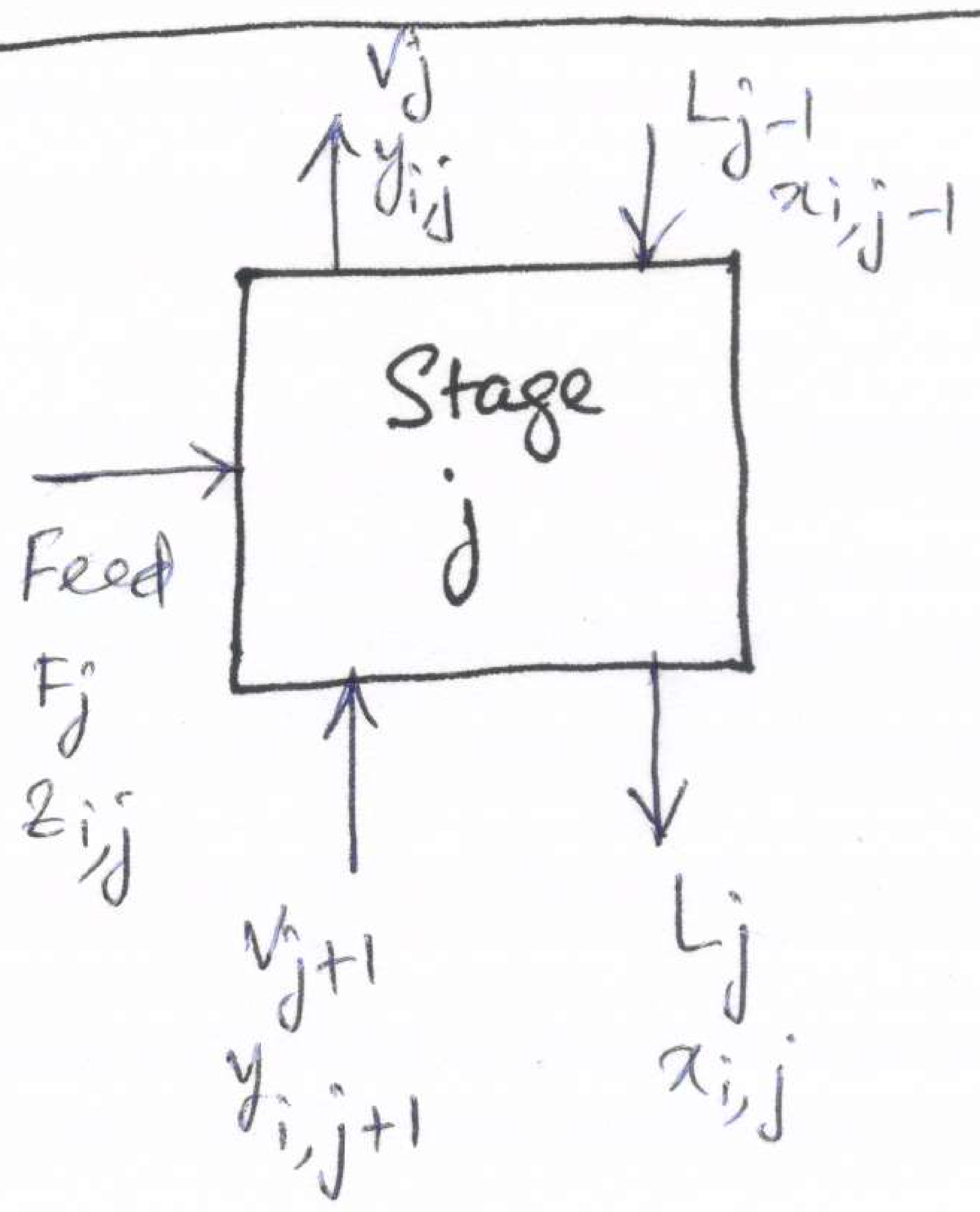
# MULTICOMPONENT MULTISTAGE EXTRACTION




## M-type Equations

(Material balance for each component

C equations for each stage)

for $i^{th}$ component, $j^{th}$ stage

$$M_{ij} = L_{j-1}\, x_{i,j-1} + V_{j+1}\, y_{i,j+1} + \cancel{F_j\, z_{ij}}$$

No feed added to $j^{th}$ stage

$$- (L_j + \cancel{V_j})\, x_{i,j} - (V_j + \cancel{W_j})\, y_{i,j} = 0$$

No Reflux   No Reflux

$$\Rightarrow M_{ij} = L_{j-1}\, x_{i,j-1} + V_{j+1}\, y_{i,j+1} - L_j\, x_{i,j} - V_j\, y_{i,j} = 0$$

.... (Eq. 1.)

## E-type Equations

(Phase equilibrium relation for each component

C-equations for each stage)

$$E_{ij} = y_{i,j} - K_{i,j}\, x_{i,j} = 0 \quad \text{.... (Eq. 2)}$$

## S-type Equations

(Mole fraction summations (one for each stage, each phase))

$$(S_y)_j = \sum_{i=1}^{c} y_{i,j} - 1.0 = 0$$

$$(S_x)_j = \sum_{i=1}^{c} x_{i,j} - 1.0 = 0$$

... (Eq. 3)

Material balance over the train, comprising of stages $1, 2, \dots, j-1, j$

(including the block shown above for $j^{th}$ stage):

$$L_j = V_{j+} + \left[\sum_{m=1}^{j} F_m\right] - V_1 + L_0 \quad \text{...... (Eq. 4)}$$

This expression for $L_j$ can be substituted in M-eqn. Referring (Eq. 1)

From Eq. 2
$= K_{i,j+1} x_{i,j+1}$

$$M_{ij} = \left[ V_j + \sum_{m=1}^{j-1} F_m - V_1 + L_0 \right] x_{i,j-1} + V_{j+1}\, y_{i,j+1} + F_j\, z_{i,j}$$

$$- \left[ V_{j+1} + \sum_{m=1}^{j} F_m - V_1 + L_0 \right] x_{i,j} - V_j\, y_{i,j} = 0$$

From Eq. 2
$= K_{i,j}\, x_{i,j}$

$$\Rightarrow \quad M_{ij} = A_j\, x_{i,j-1} + B_j\, x_{i,j} + C_j\, x_{i,j+1} - D_j = 0 \quad \text{---- (Eq. 5)}$$

where

$$A_j = V_j + \sum_{m=1}^{j-1} F_m - V_1 + L_0 \qquad \text{for } 2 \le j \le N$$

$$B_j = -\left[ V_{j+1} + \sum_{m=1}^{j} F_m - V_1 + L_0 + V_j K_{i,j} \right] \qquad \text{for } 1 \le j \le N$$

$$C_j = V_{j+1} K_{i,j+1} \qquad \text{for } 1 \le j \le N-1$$

$$D_j = -F_j\, z_{i,j} \qquad \text{for } 1 \le j \le N$$

with $\left. \begin{array}{l} x_{i,0} = 0 \\ V_{N+1} = 0 \end{array} \right\}$

If the $V_j$ and $L_j$ are known for each stage, the Equation 5 forms a tri-diagonal matrix equation system that can be solved to obtain $x_{i,j}$ for every component and every stage.

Solution of tri-diagonal matrix equation by Thomas Algorithm

$$\begin{bmatrix} B_1 & C_1 & 0 & \cdots & 0 & \cdots \\ A_2 & B_2 & C_2 & 0 & \cdots & \\ 0 & A_3 & B_3 & C_3 & 0 & \cdots \\ 0 & 0 & A_4 & B_4 & C_4 & 0 \cdots \\ & & \ddots & \ddots & \ddots & \\ & & & A_{N-1} & B_{N-1} & C_{N-1} \\ & & & 0 & A_N & B_N \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ \\ x_{N-1} \\ x_N \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ \vdots \\ \\ \\ D_{N-1} \\ D_N \end{bmatrix}$$

Essentially Gaussian Elimination without operating on 'zeros'!

$$B_1 x_1 + C_1 x_2 = D_1$$

$$\Rightarrow x_1 = \frac{D_1 - C_1 x_2}{B_1} = \left(\frac{D_1}{B_1}\right) - \left(\frac{C_1}{B_1}\right) x_2 = q_1 - p_1 x_2$$

$$A_2 x_1 + B_2 x_2 + C_2 x_3 = D_2$$

$$\Rightarrow x_2 = \frac{D_2 - A_2 q_1}{B_2 - A_2 p_1} - \left(\frac{C_2}{B_2 - A_2 p_1}\right) x_3$$

$$= q_2 - p_2 x_3$$

General Form

$$x_j = q_j - p_j x_{j+1}$$

where $p_j = \dfrac{C_j}{B_j - A_j p_{j-1}}$

$$q_j = \frac{D_j - A_j q_{j-1}}{B_j - A_j p_{j-1}}$$

$$\begin{bmatrix} 1 & p_1 & 0 & 0 & \cdots & & \\ 0 & 1 & p_2 & 0 & \cdots & & \\ 0 & 0 & 1 & p_3 & 0 \cdots & & \\ \vdots & & \ddots & \ddots & & & \\ \vdots & & & & & & \\ 0 & 0 & \cdots & & 0 & 1 & p_{N-1} \\ 0 & 0 & \cdots & & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ \\ x_{N-1} \\ x_N \end{bmatrix} = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ \\ \\ q_{N-1} \\ q_N \end{bmatrix}$$

$$\Rightarrow x_N = q_N$$

And recursive back substitution from the bottom-most row

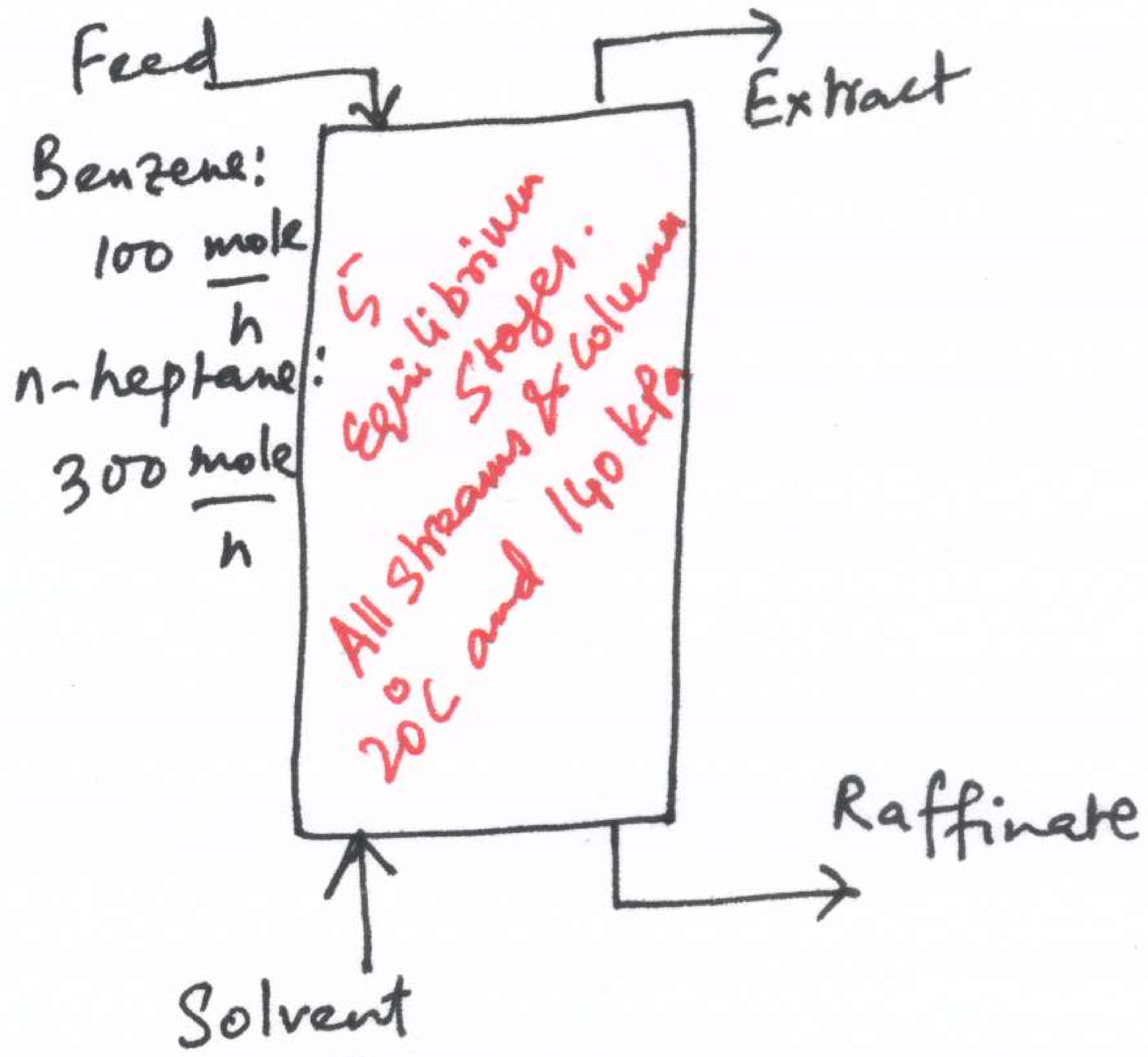
$$x_j = q_j - p_j x_{j+1}$$

$$x_{j-1} = q_{j-1} - p_{j-1} x_j$$

$$\vdots$$

# Isothermal Sum Rates Method

# Example Problem




Given NRTL Equation

$$\ln \gamma_i = \frac{\sum_{j=1}^{C} \tau_{ji} G_{ji} x_j}{\sum_{k=1}^{C} G_{kj} x_k} + \sum_{j=1}^{C} \left[ \frac{x_j G_{ij}}{\sum_{k=1}^{C} G_{kj} x_k} \left( \tau_{ij} - \frac{\sum_{k=1}^{C} x_k \tau_{kj} G_{kj}}{\sum_{k=1}^{C} G_{kj} x_k} \right) \right]$$

where $G_{ji} = e^{-\alpha_{ji} \tau_{ji}}$

$G_{ii} = G_{jj} = 1$

$\tau_{ii} = \tau_{jj} = 1$

| Binary Pair (i, j) | $\tau_{ij}$ | $\tau_{ji}$ | $\alpha_{ji} = \alpha_{ij}$ |
|---|---|---|---|
| DMF – Heptane | 2.036 | 1.910 | 0.25 |
| Water – Heptane | 7.038 | 4.806 | 0.15 |
| Benzene – Heptane | 1.196 | −0.355 | 0.30 |
| Water – DMF | 2.506 | −2.128 | 0.253 |
| Benzene – DMF | −0.240 | 0.676 | 0.425 |
| Benzene – Water | 3.639 | 5.750 | 0.203 |

| Stage $j$ | $V_j$ | $y_{i,j}$ Heptane | Benzene | DMF | Water | $x_{i,j}$ Heptane | Benzene | DMF | Water |
|---|---|---|---|---|---|---|---|---|---|
| 1 | ~~1100~~ 1113.1 | ~~0~~ 0.0263 | ~~0.0909~~ 0.0866 | ~~0.6818~~ 0.6626 | 0.2273 | 0.7895 | 0.2105 | 0 | 0 |
| 2 | 1080 | 0 | 0.0741 | 0.6944 | 0.2315 | 0.8333 | 0.1667 | 0 | 0 |
| 3 | 1060 | 0 | 0.0566 | 0.7076 | 0.2359 | 0.8824 | 0.1176 | 0 | 0 |
| 4 | 1040 | 0 | 0.0385 | 0.7211 | 0.2404 | 0.9375 | 0.0625 | 0 | 0 |
| 5 | ~~1020~~ 1028.2 | ~~0~~ 0.019 | ~~0.0196~~ 0.0062 | ~~0.7353~~ 0.7316 | 0.2451 | 1.0 | 0 | 0 | 0 |

Converged Solution.