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## جلسه اول پروژه درس عملیات واحد صنعتی

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# Fundamentals

خروجی‌ها	ورودی‌ها
Number of Theoretical Stages ( $\geq 1$ )	VLE Equilibrium (NIST)
N_Feed ( $\geq 1$ )	F
D	$z$ ( $1 > z > 0$ )
B	$q$
$R_{\min}$ ( $> 0$ )	$R/R_{\min}$
$N_{\min}$ ( $\geq 1$ )	$x_D$ ( $1 > x > 0$ )
McCabe Diagram	$x_B$ ( $1 > x > 0$ )

VLE Diagram From NIST Database

- MeOH : Water
- O-Xylene : P-Xylene
- AcOH : AcOEt



# Fundamentals

خروجی‌ها	ورودی‌ها
Number of Theoretical Stages ( $\geq 1$ )	VLE Equilibrium (NIST)
$N_{\text{Feed}} (\geq 1)$	F
D	$z (1 > z > 0)$
B	q
$R_{\text{min}} (> 0)$	$R/R_{\text{min}}$
$N_{\text{min}} (\geq 1)$	$x_{\text{D}} (1 > x > 0)$
McCabe Diagram	$x_{\text{B}} (1 > x > 0)$

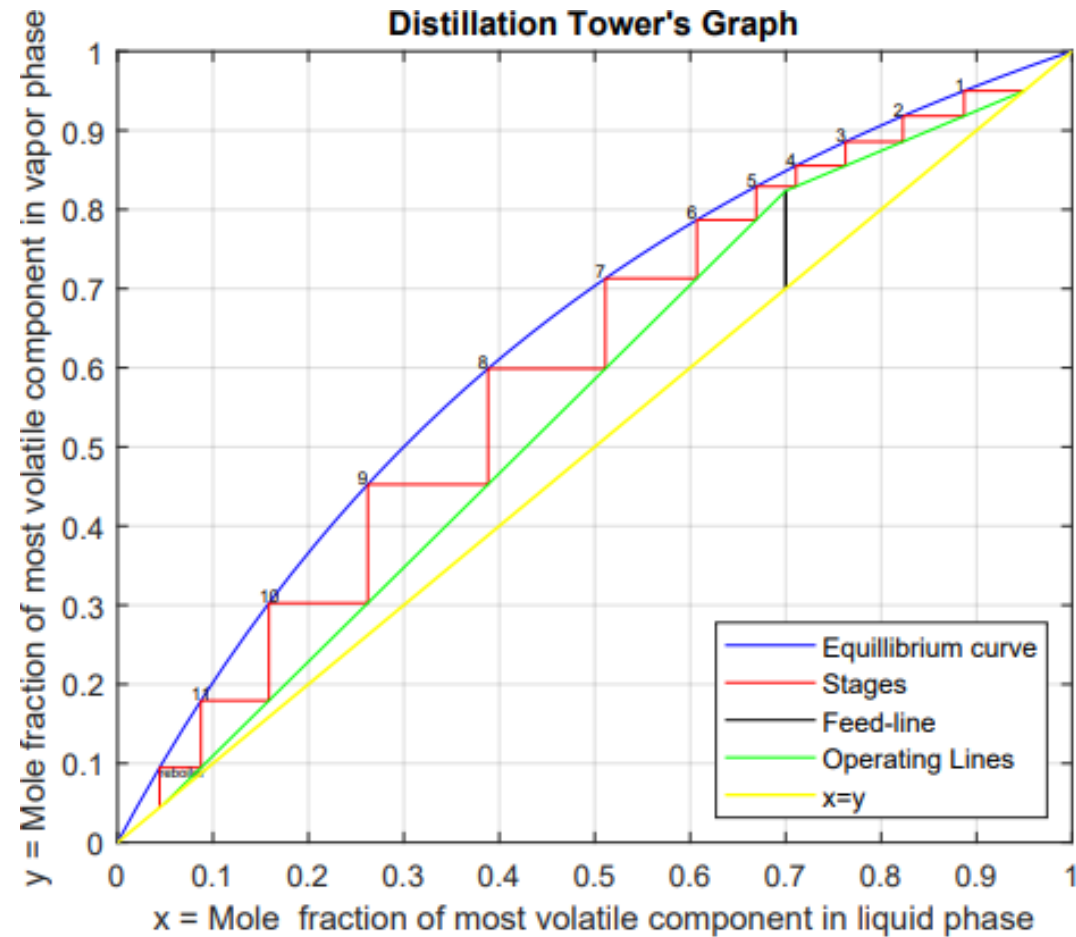
VLE Diagram From NIST Database

- MeOH : Water
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Algorithm to McCabe (Or Panchon-Savarit) Method:

1. D and B Calculation
2. VLE Curve Fitting
3. Feedline Equation
4. Calculation of  $R_{\text{min}}$
5. Calculation of  $N_{\text{min}}$
6. Rectifying and Stripping Section Lines
7. Counting (& Drawing) of Stages

# McCabe Diagram Example



# 1) D and B Calculation

Equations:

$$F = D + B \quad ; \quad Fz_F = Dx_D + Bx_B$$

$$\rightarrow \begin{cases} D + B = F \\ Dx_D + Bx_B = Fz_F \end{cases} \rightarrow \begin{bmatrix} 1 & 1 \\ x_D & x_B \end{bmatrix} \begin{bmatrix} D \\ B \end{bmatrix} = \begin{bmatrix} F \\ Fz_F \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} D \\ B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ x_D & x_B \end{bmatrix}^{-1} \begin{bmatrix} F \\ Fz_F \end{bmatrix}$$

# 2) VLE Curve Fitting

1. Data Extraction From NIST (Aspen Plus)
2. Curve Fitting in MATLAB/Python

# Line Equations in MATLAB

- Symbolic Functions
- Numerical Functions

## 3) Feedline Equation

$$y = \frac{q}{q-1}x - \frac{1}{q-1}z_F$$

## 4) Calculation of $R_{min}$

- Intersect Rectifying Section Line to Feedline and Fitted Equilibrium Curve Intersection:

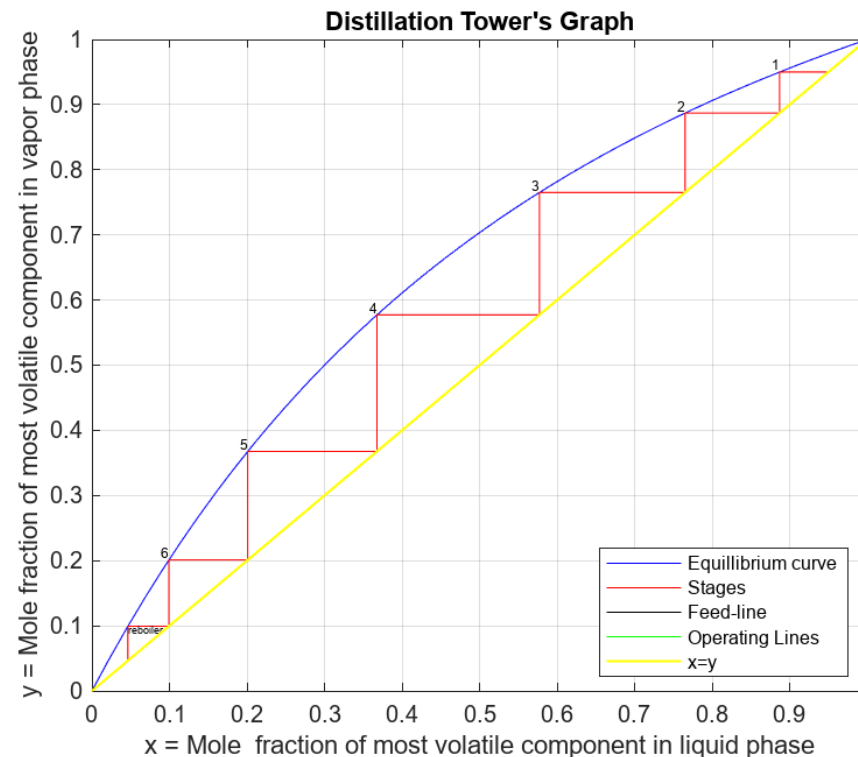
$$y_{in} = \frac{q}{q-1}x_{in} - \frac{1}{q-1}z_F ; (x_{in}, y_{in}) \in VLE$$

Minimum Reflux Rectifying Section Operating Line:

$$y_{in} = \frac{R_{min}}{R_{min}+1}x_{in} + \frac{1}{R_{min}+1}x_D \rightarrow R_{min}$$

## 5) Calculation of $N_{\min}$

- Only  $x=y$  Line and Equilibrium Curve Needed
- For Each Stage, Draw Vertical and Horizontal Lines Starting From Point ( $x_D, x_D$ ) to Connect VLE Curve and Diagonal  $x=y$  Line



## 6) Rectifying and Stripping Section Lines

Rectifying Section Operating Line:

$$R = \frac{R}{R_{min}} \times R_{min}$$
$$y = \frac{R}{R+1}x + \frac{1}{R+1}x_D$$

Stripping Section Operating Line:

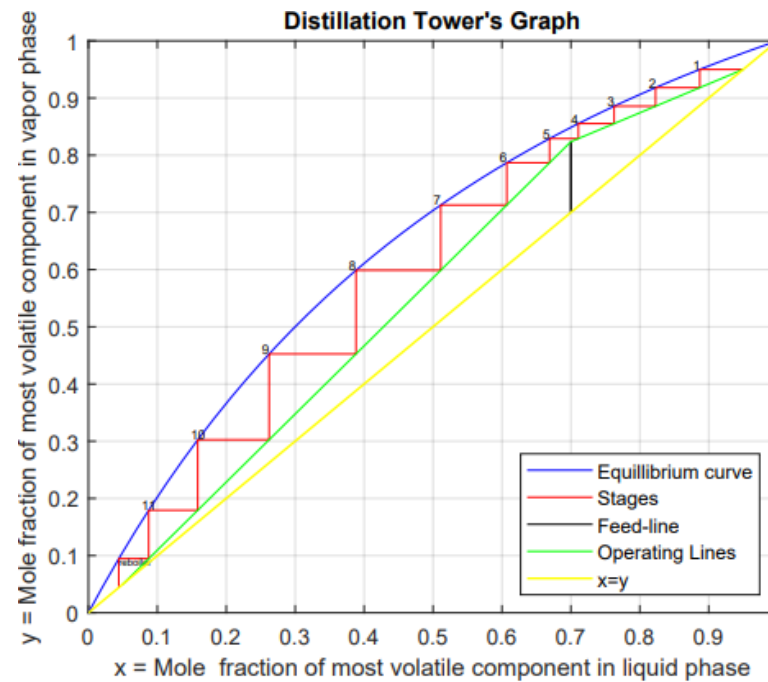
$(x_B, x_B)$  &  $(x_{in}, y_{in}) \in \text{Stripping Section}$  ;  $x_{in} > x_B$

$$\rightarrow y = \frac{y_{in} - x_B}{x_{in} - x_B}x + \frac{x_{in} - y_{in}}{x_{in} - x_B}$$



## 7) Counting (& Drawing) of Stages

- Use While Loop with Breaking Condition of  $x < x_B$
- Define 2 Arrays (or 1 Dictionary) to Store x's and y's of Intersections
  - Append 2 more Coordinates for Reboiler Stage
  - Connect Points in Graphing





# Graphing

x=y Line ; x=(0,1)

VLE Fitted Curve ; x=(0,1)

Feedline:

$$if: \begin{cases} q = 1 \rightarrow y = (z_F, y_{in}) \\ q \neq 1 \rightarrow \text{Equation with } x = (z_F, x_{in}) \end{cases}$$

Rectifying Section Line Equation with x=(x\_in, x\_D)

Stripping Section Line Equation with x=(x\_B, x\_in)

Stage Drawer, Coordinates of Connecting Lines in Arrays (or Dictionary)

Lim of Graph: x=(0, 1) ; y=(0, 1)

Graph and Axis Titles

0.1 Grid

Legend