Distillation

Processos de Separação

LEQB

2023/2024

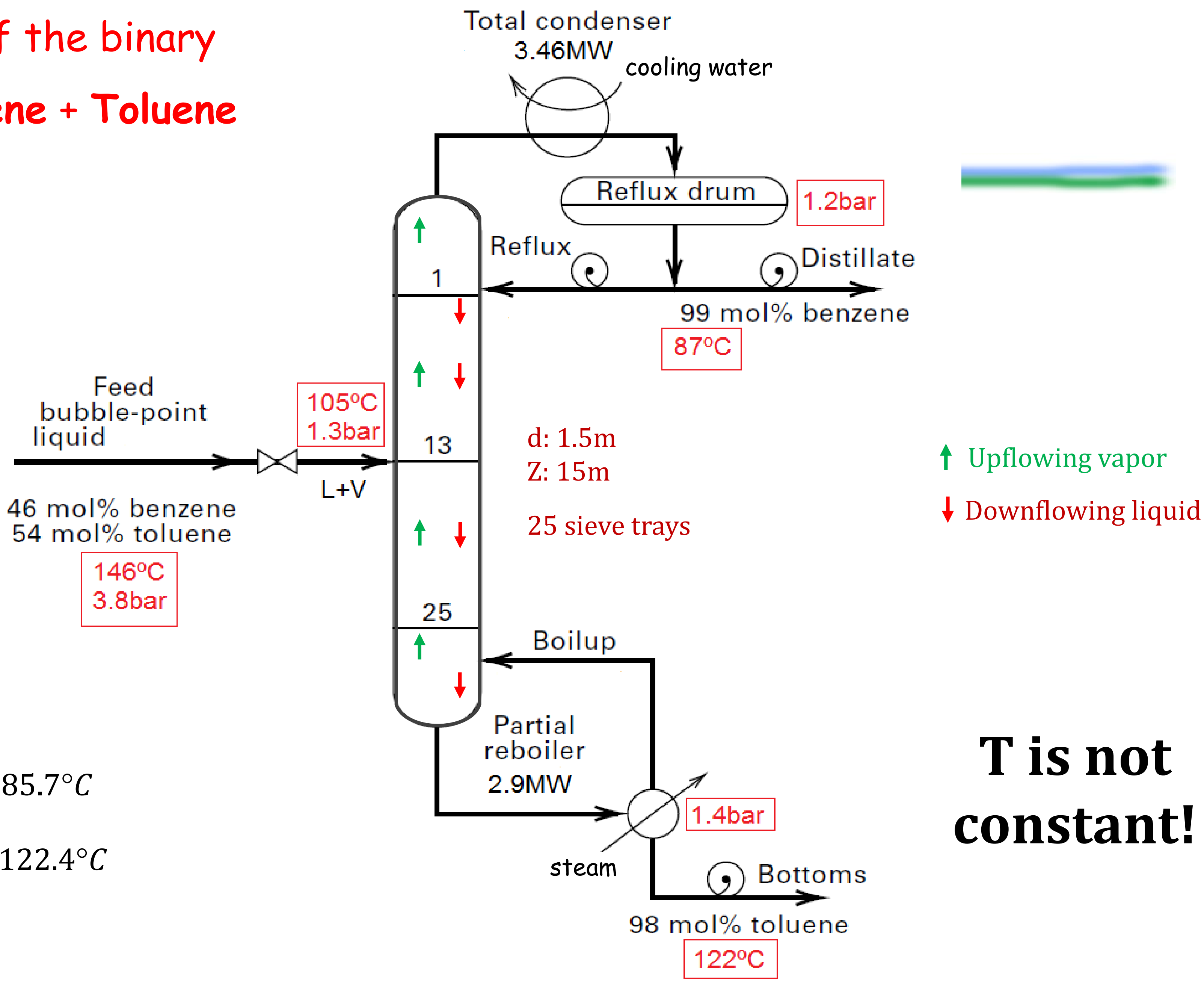
Summary

Design of Distillation Columns

- **Introducing the McCabe-Thiele method** *

* "Graphical design of fractionating columns" W.L. McCabe and E.W. Thiele, Ind. Eng. Chem. 605, June 1925

Distillation of the binary mixture **Benzene + Toluene**

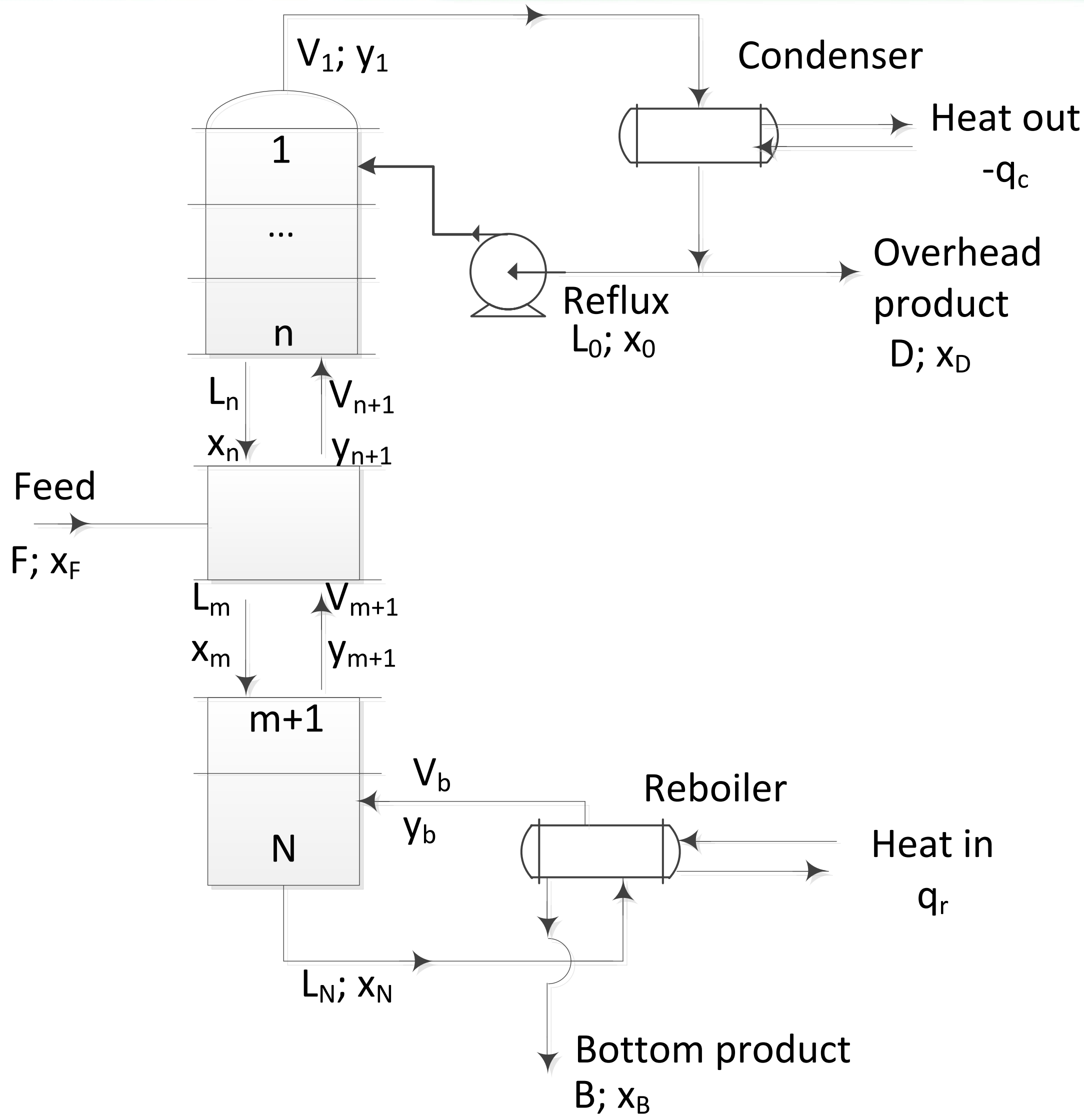


$$T_{boiling}|_{benzene}\ (1.2\ bar) = 85.7°C$$

$$T_{boiling}|_{toluene}\ (1.4\ bar) = 122.4°C$$

T is not constant!

Schematic diagram of a distillation column



Binary mixture A+C

A: more volatile species

Plate numbering nomenclature

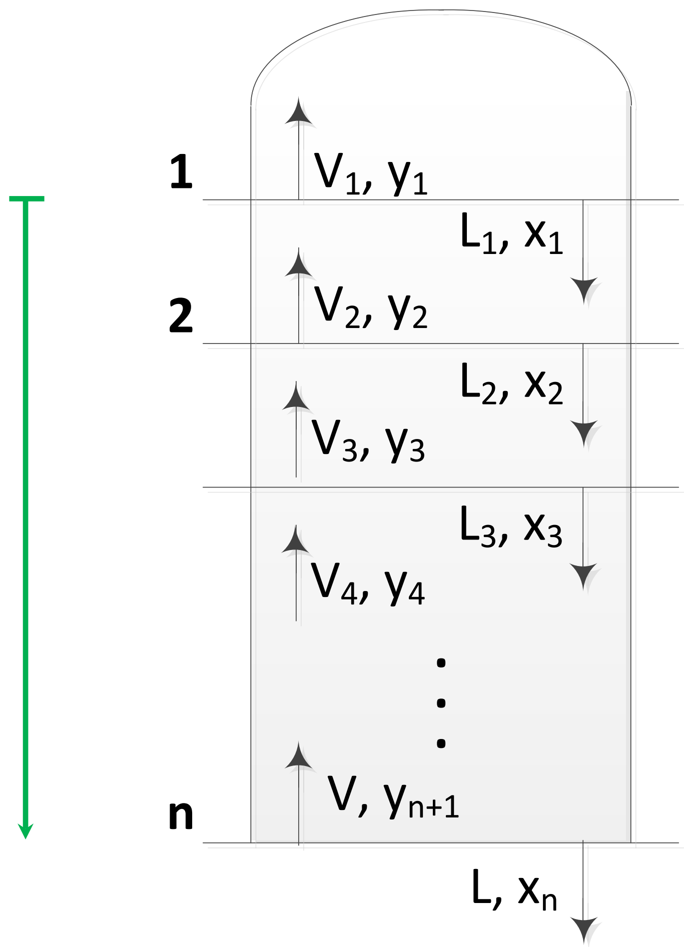
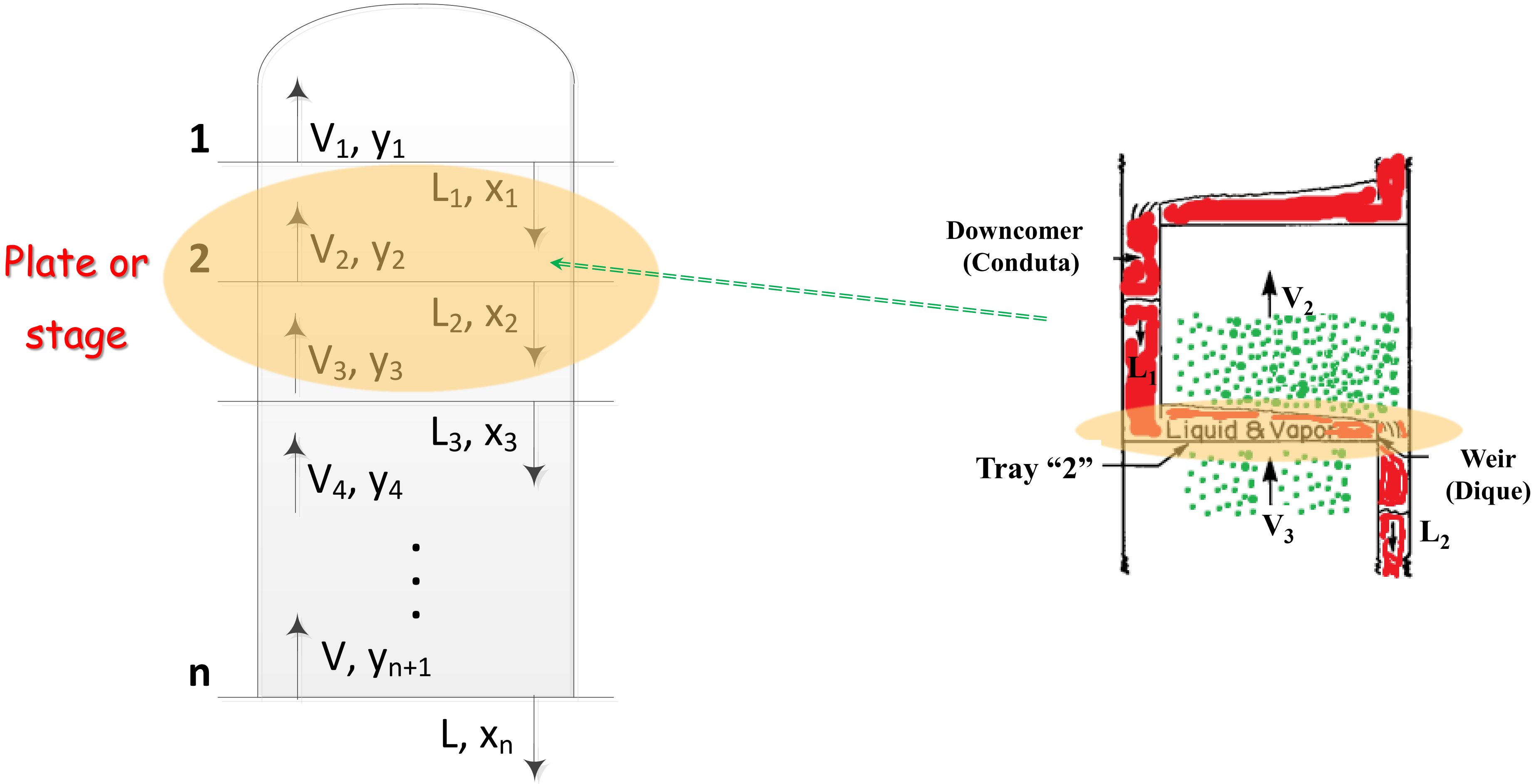
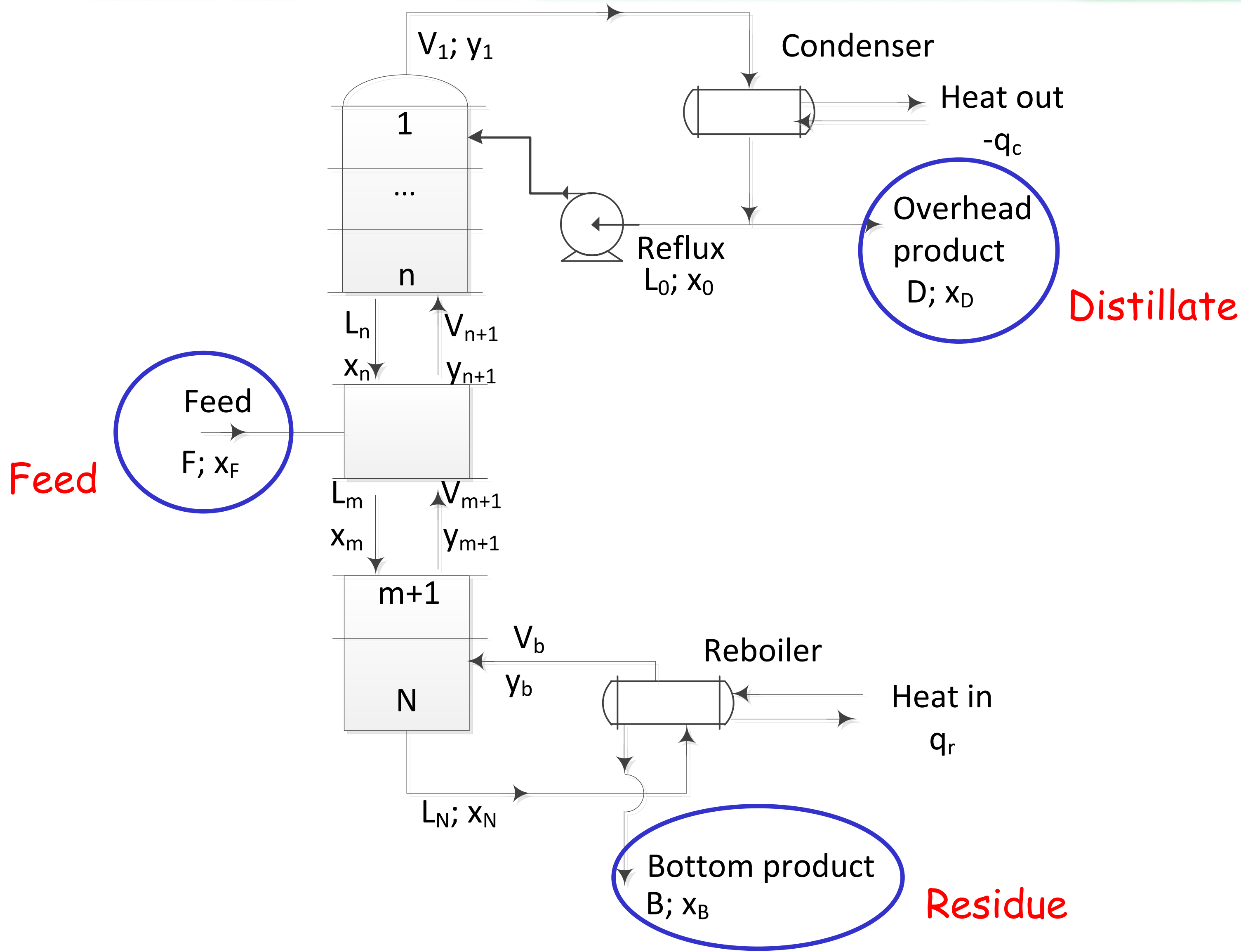


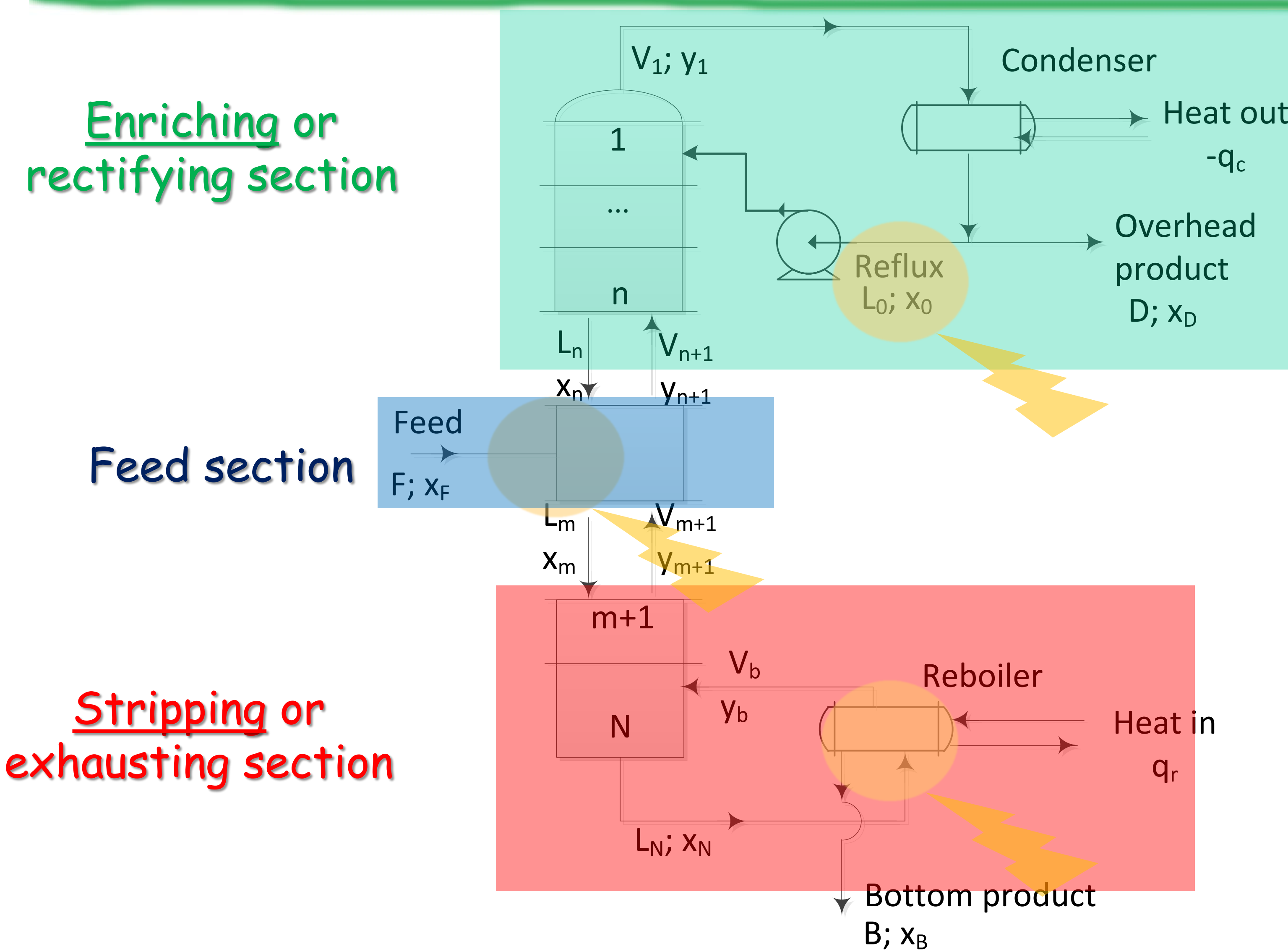
Plate numbering nomenclature

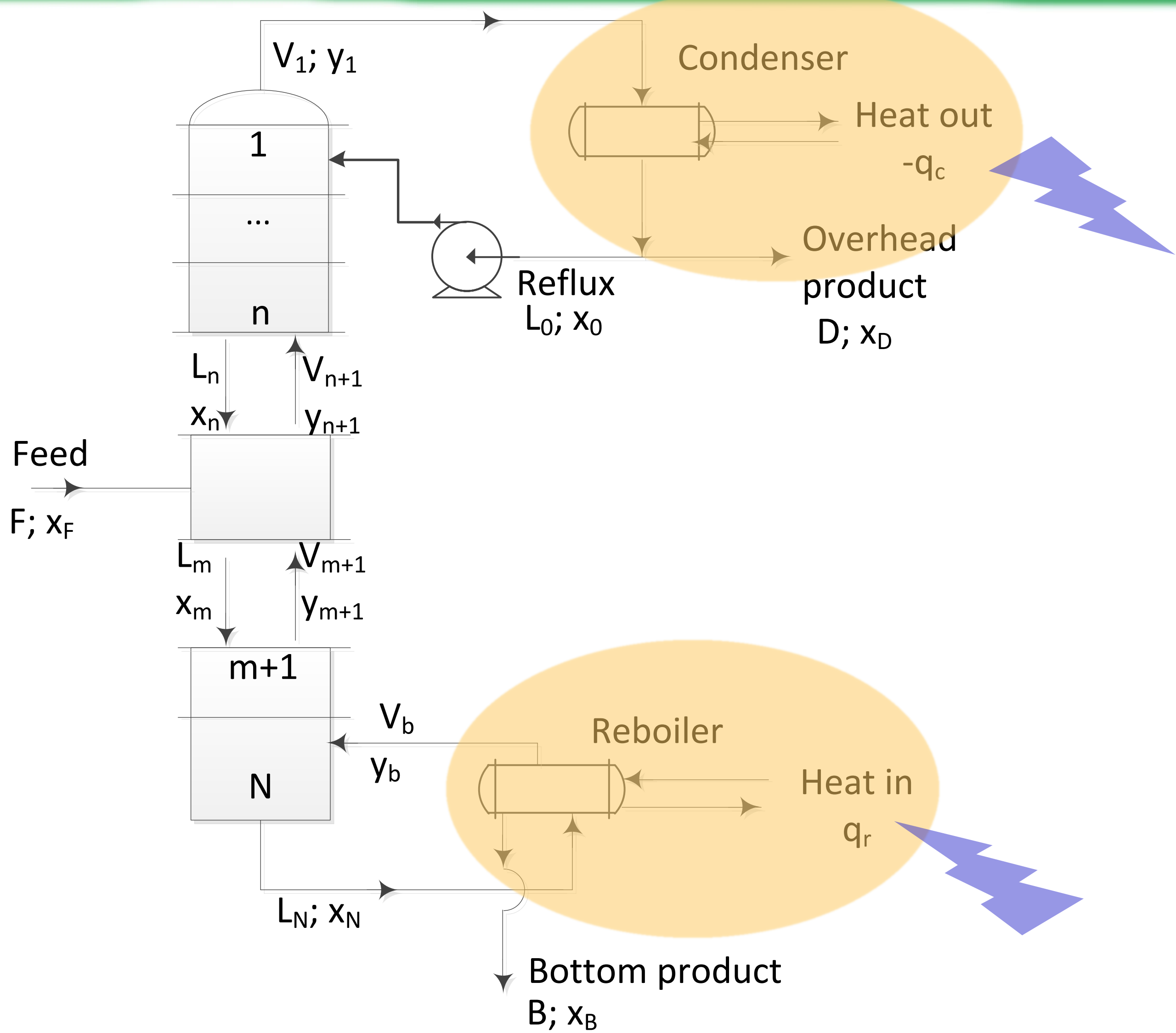


Column input and output currents



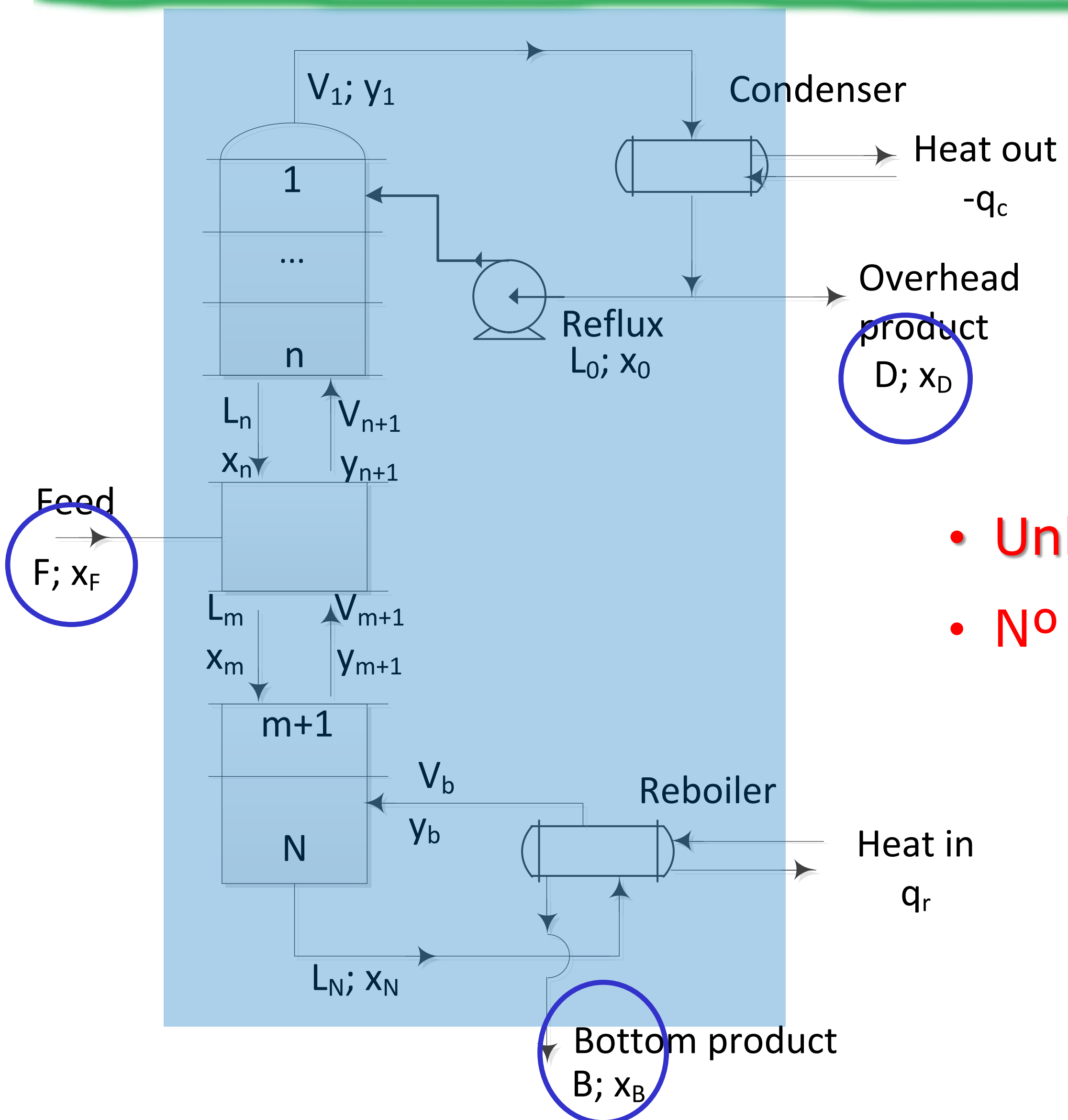
Column sections




V_1; y_1
Condenser
Heat out
$-q_c$
1
...
n
Reflux
L_0; x_0
Overhead
product
D; x_D
L_n
x_n
V_{n+1}
y_{n+1}
Feed
F; x_F
L_m
x_m
V_{m+1}
y_{m+1}
m+1
N
V_b
y_b
Reboiler
Heat in
q_r
L_N; x_N
Bottom product
B; x_B

Material balances

❑ Overall material balance



$$F = B + D$$

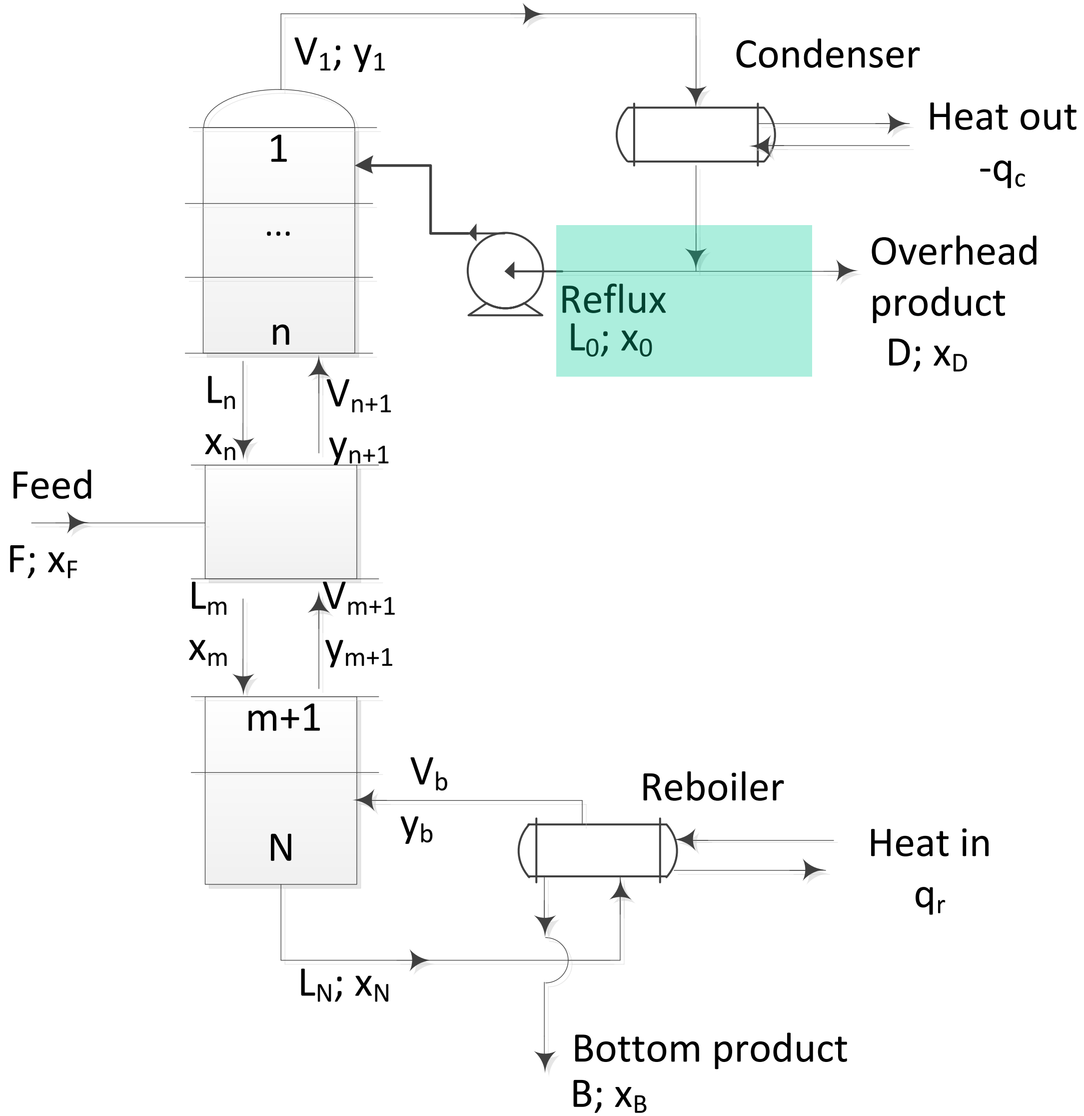
$$F\,x_F = B\,x_B + D\,x_D$$

- Unknown variables: B, D, x_B, x_D
- Nº of independente equations = 2

=> We need information on 2 of former variables

Material balances

❑ Enriching section



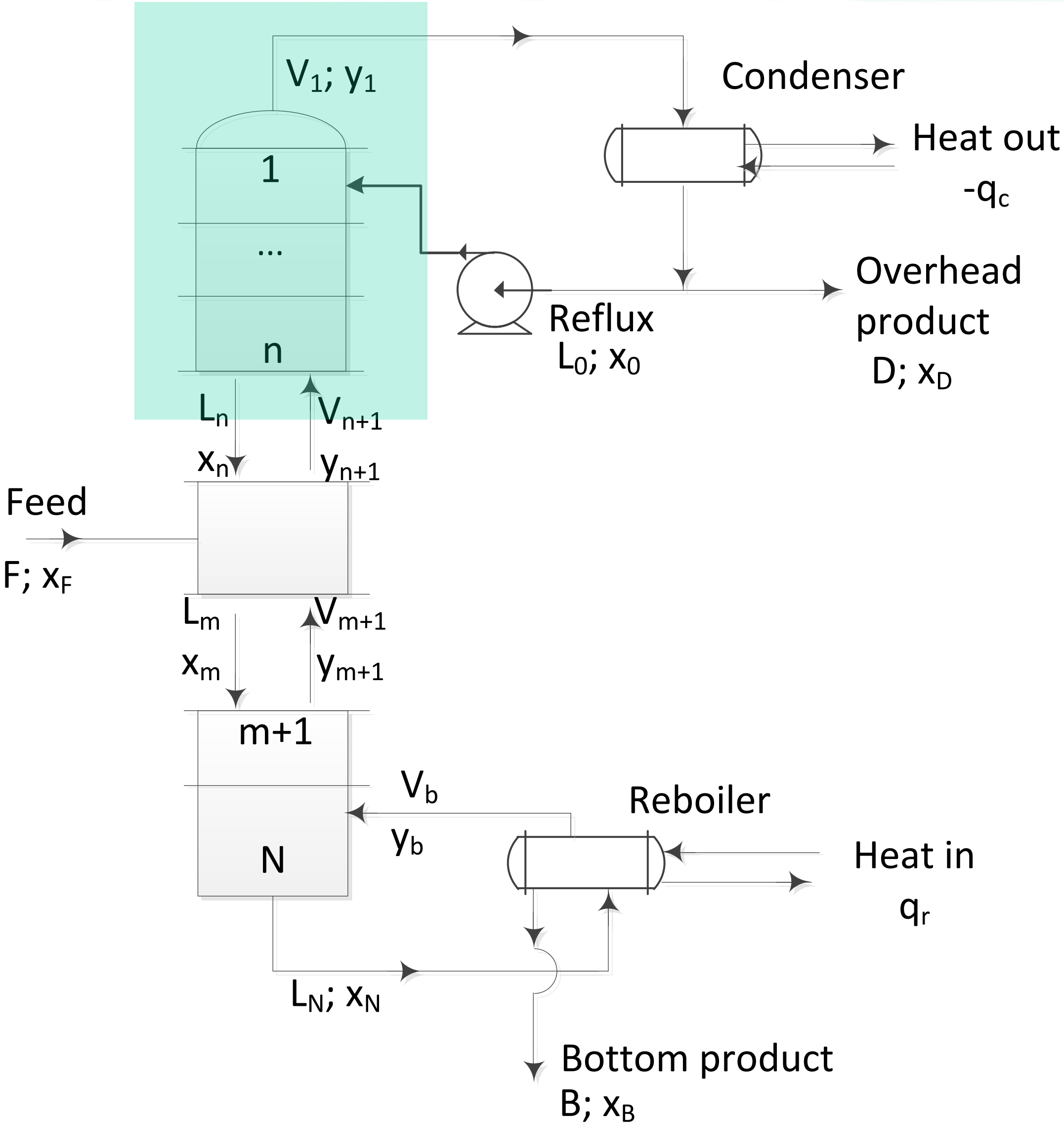
$$\boxed{\begin{aligned} V_1 &= L_0 + D \\ V_1 y_1 &= L_0 x_0 + D x_D \end{aligned}}$$

$$y_1 = x_0 = x_D$$

Why?

Material balances – Operating line

Enriching section



$$\begin{cases} L_0 + V_{n+1} = L_n + V_1 \\ L_0 x_0 + V_{n+1} y_{n+1} = L_n x_n + V_1 y_1 \end{cases}$$

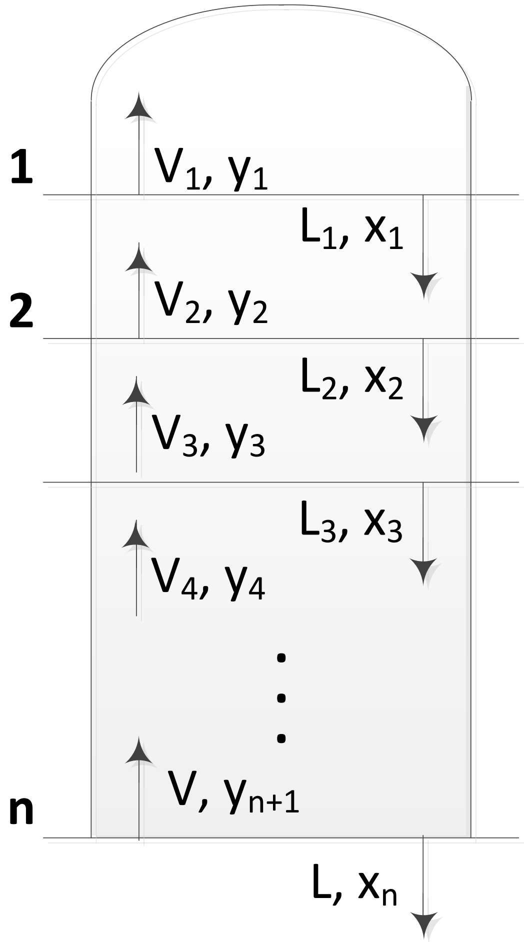
$$V_1 = L_0 + D$$

$$V_1 y_1 = L_0 x_0 + D x_D$$

$$\boxed{y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D x_D}{V_{n+1}}}$$

Rectifying Section Operating Line

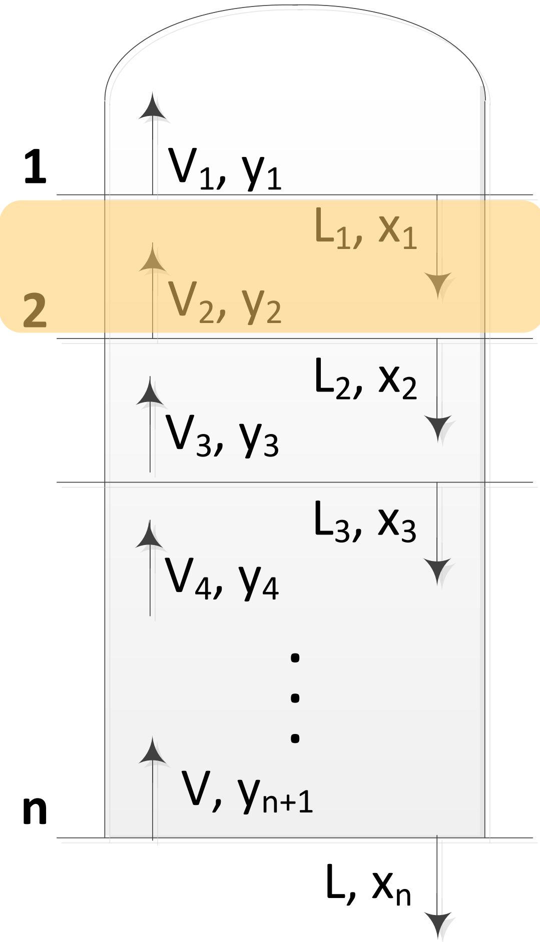
Meaning of a operating line…



Rectifying Section Operating Line

$$\boxed{y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D x_D}{V_{n+1}}}$$

Meaning of a operating line…



Rectifying Section Operating Line

$$\boxed{y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D x_D}{V_{n+1}}}$$

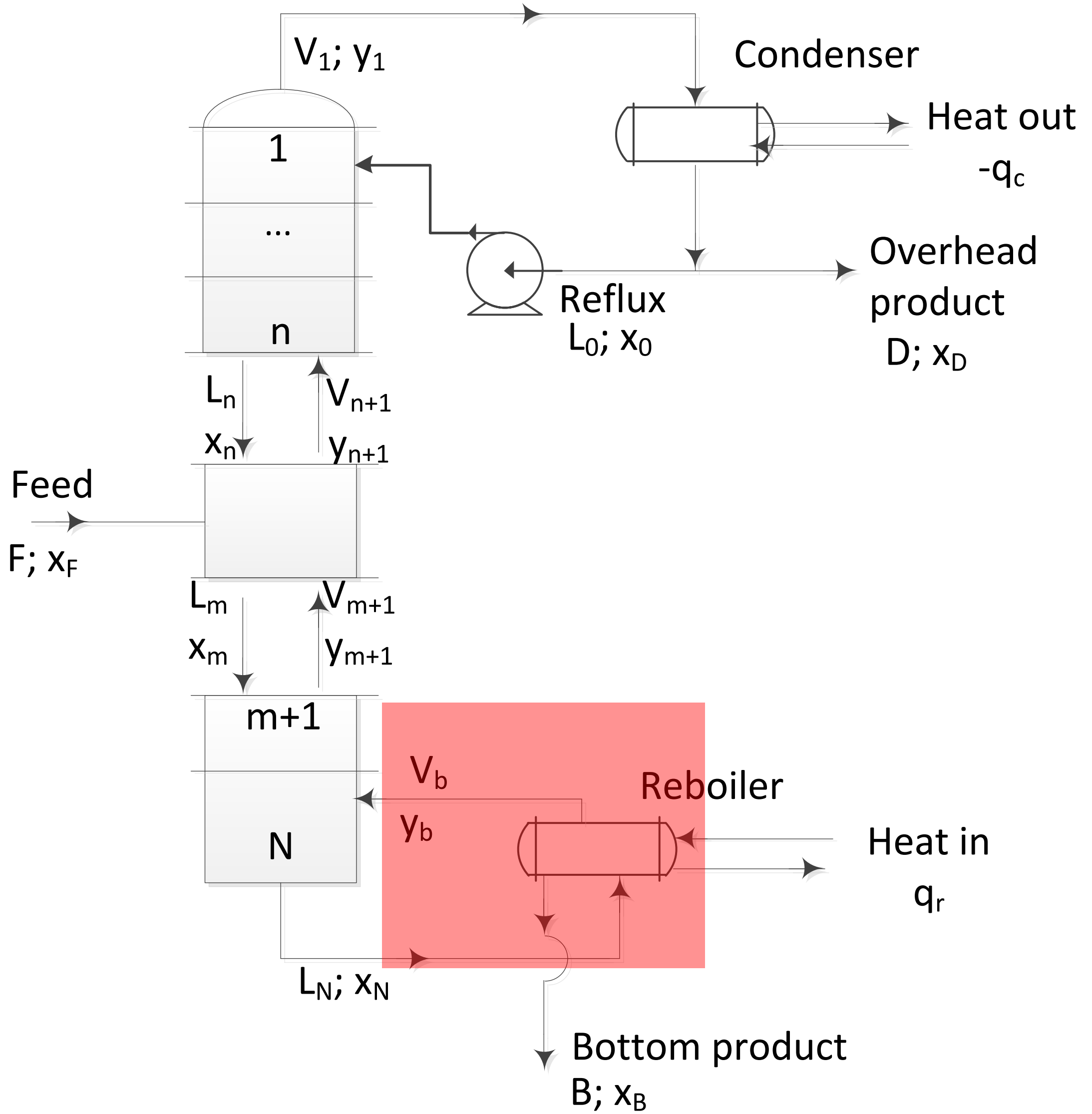
Tray 2

<u>*n* = 1</u>

$$y_2 = \frac{L_1}{V_2} x_1 + \frac{D x_D}{V_2}$$

Material balances

❑ Stripping section

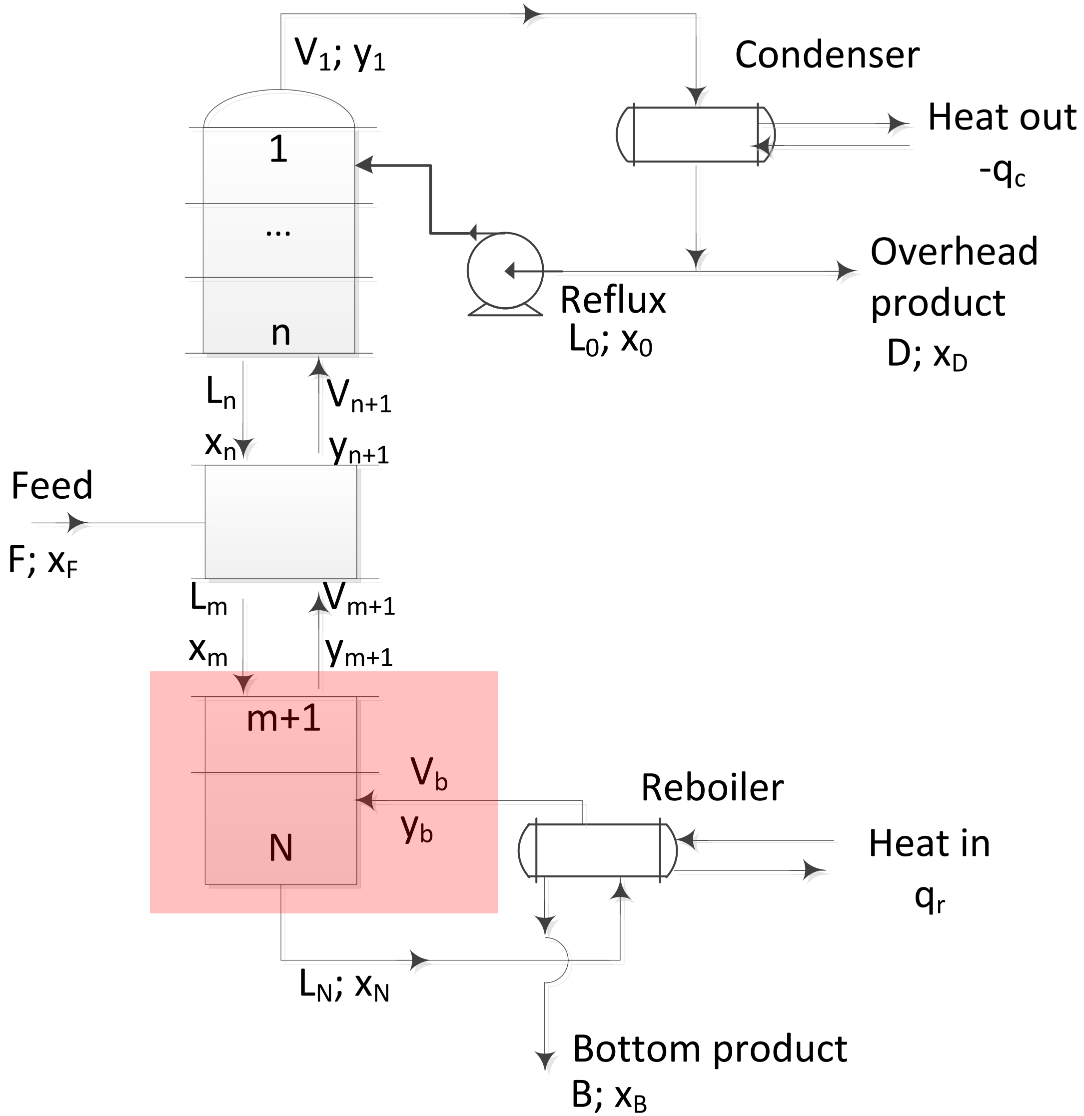


$$L_N = V_b + B$$

$$L_N x_N = V_b y_b + B x_B$$

Material balances – Operating line

Stripping section



$$\begin{cases} L_m + V_b = V_{m+1} + L_N \\ L_m x_m + V_b y_b = V_{m+1} y_{m+1} + L_N x_N \end{cases}$$

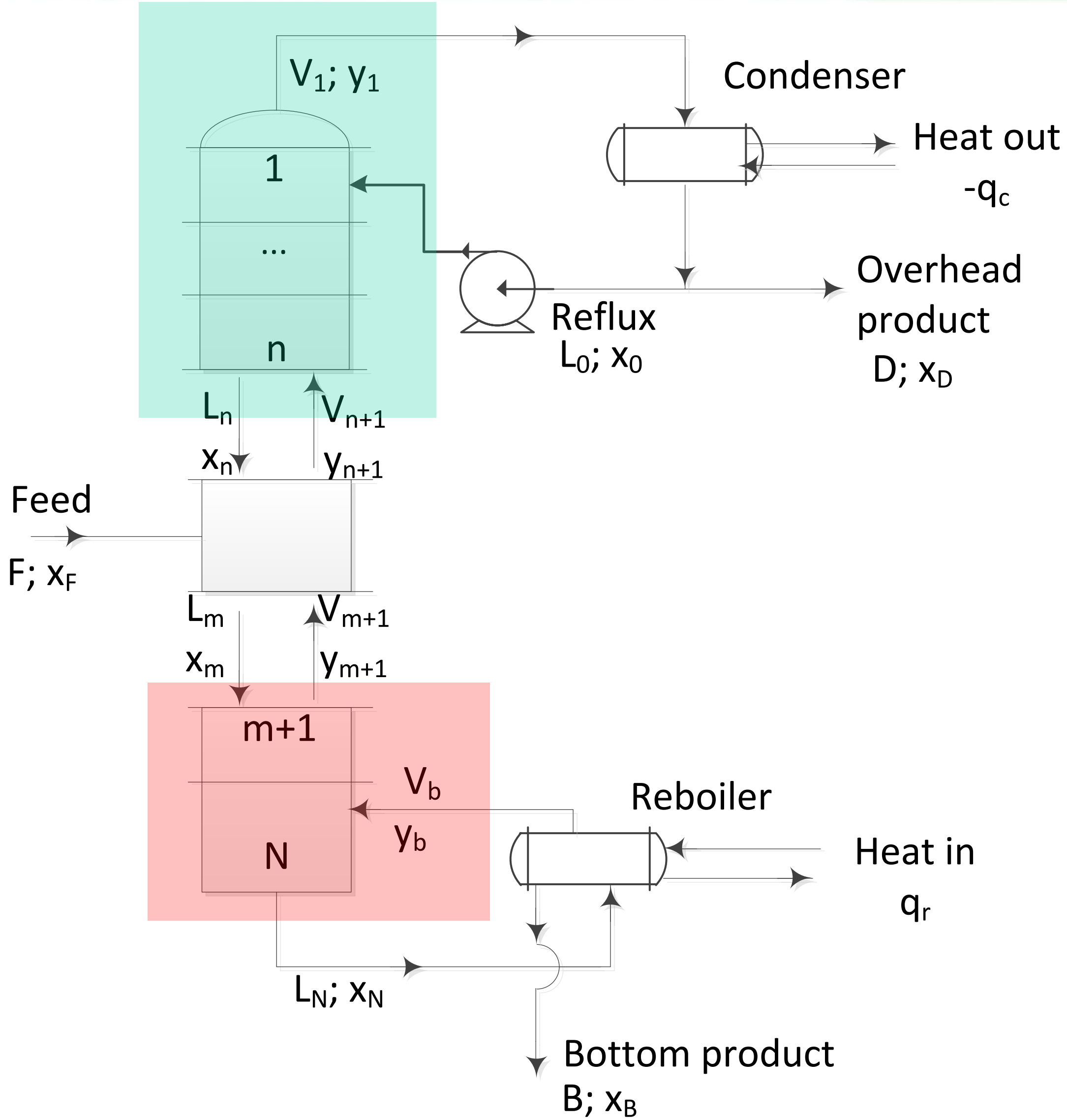
$$L_N = V_b + B$$

$$L_N x_N = V_b y_b + B x_B$$

$$\boxed{y_{m+1} = \frac{L_m}{V_{m+1}} x_m - \frac{B x_B}{V_{m+1}}}$$

Stripping Section Operating Line

Material balances – Operating lines



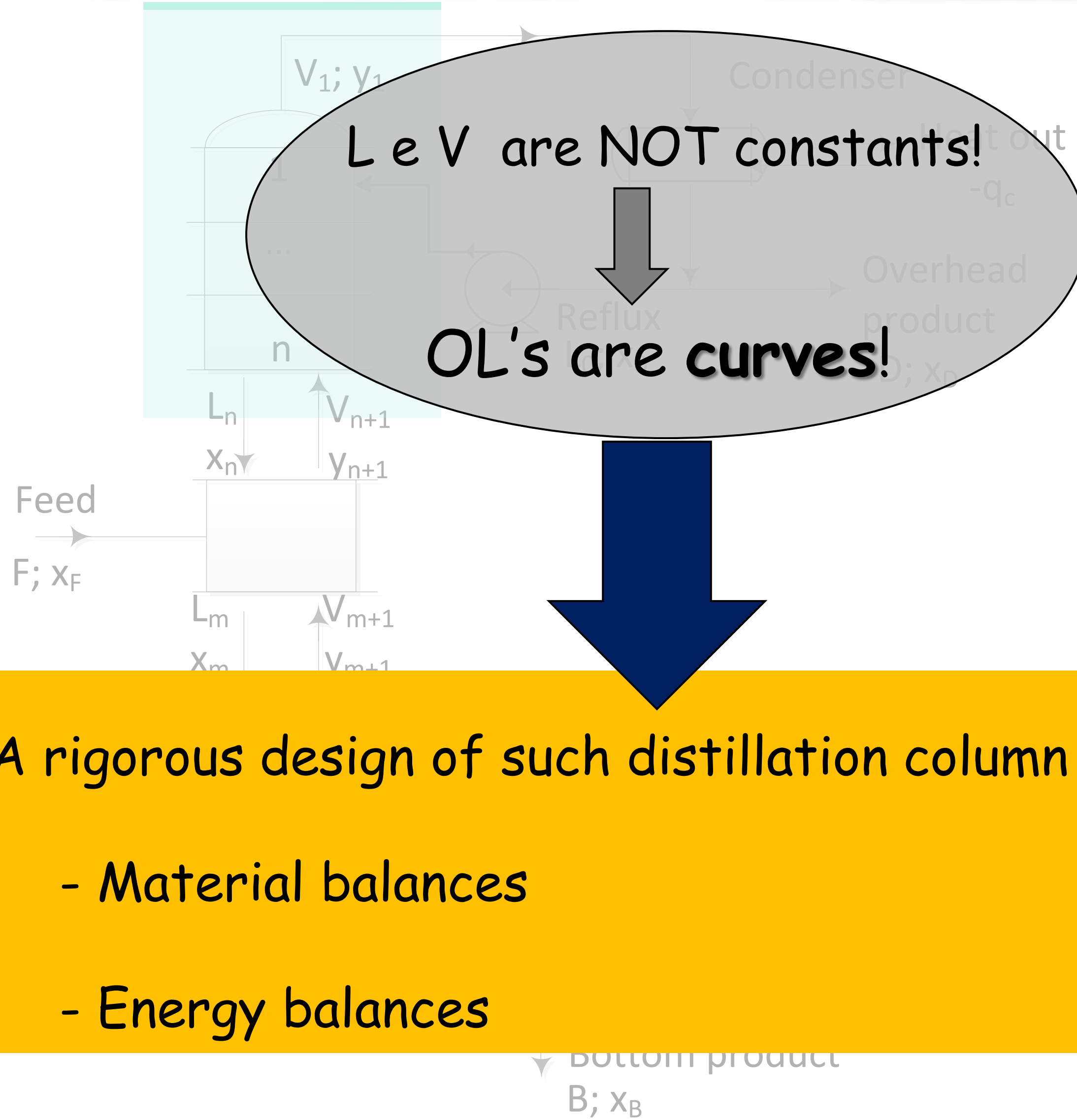
Enriching section

$$y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D x_D}{V_{n+1}}$$

Stripping section

$$y_{m+1} = \frac{L_m}{V_{m+1}} x_m - \frac{B x_B}{V_{m+1}}$$

Material balances – Operating lines



L e V are NOT constants!

OL's are **curves**!

A rigorous design of such distillation column will involve:

- Material balances
- Energy balances

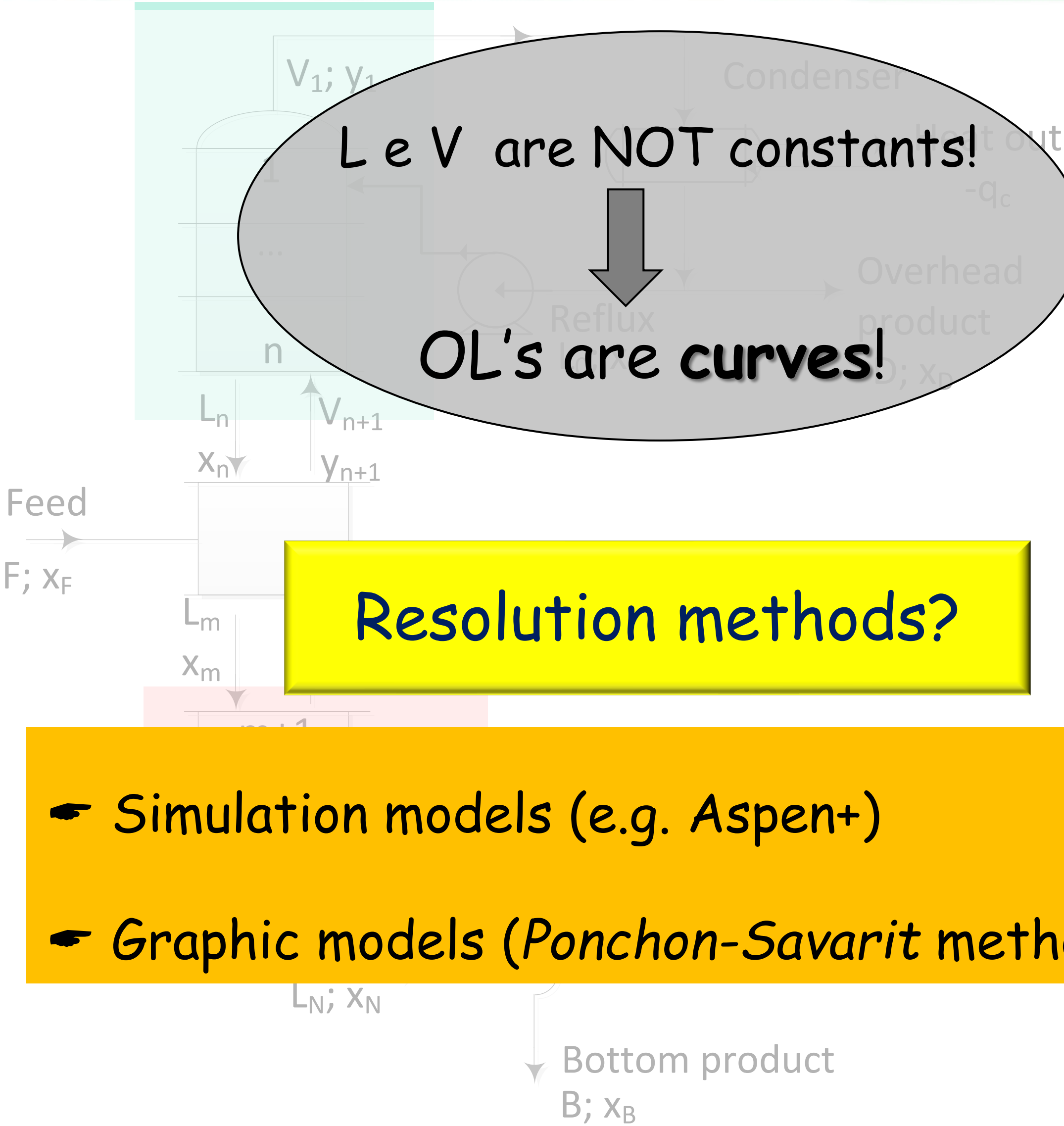
Enriching section

$$y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D x_D}{V_{n+1}}$$

Stripping section

$$y_{m+1} = \frac{L_m}{V_{m+1}} x_m - \frac{B x_B}{V_{m+1}}$$

Material balances – Operating lines



L e V are NOT constants!

OL's are **curves**!

Resolution methods?

- Simulation models (e.g. Aspen+)
- Graphic models (*Ponchon-Savarit* method)

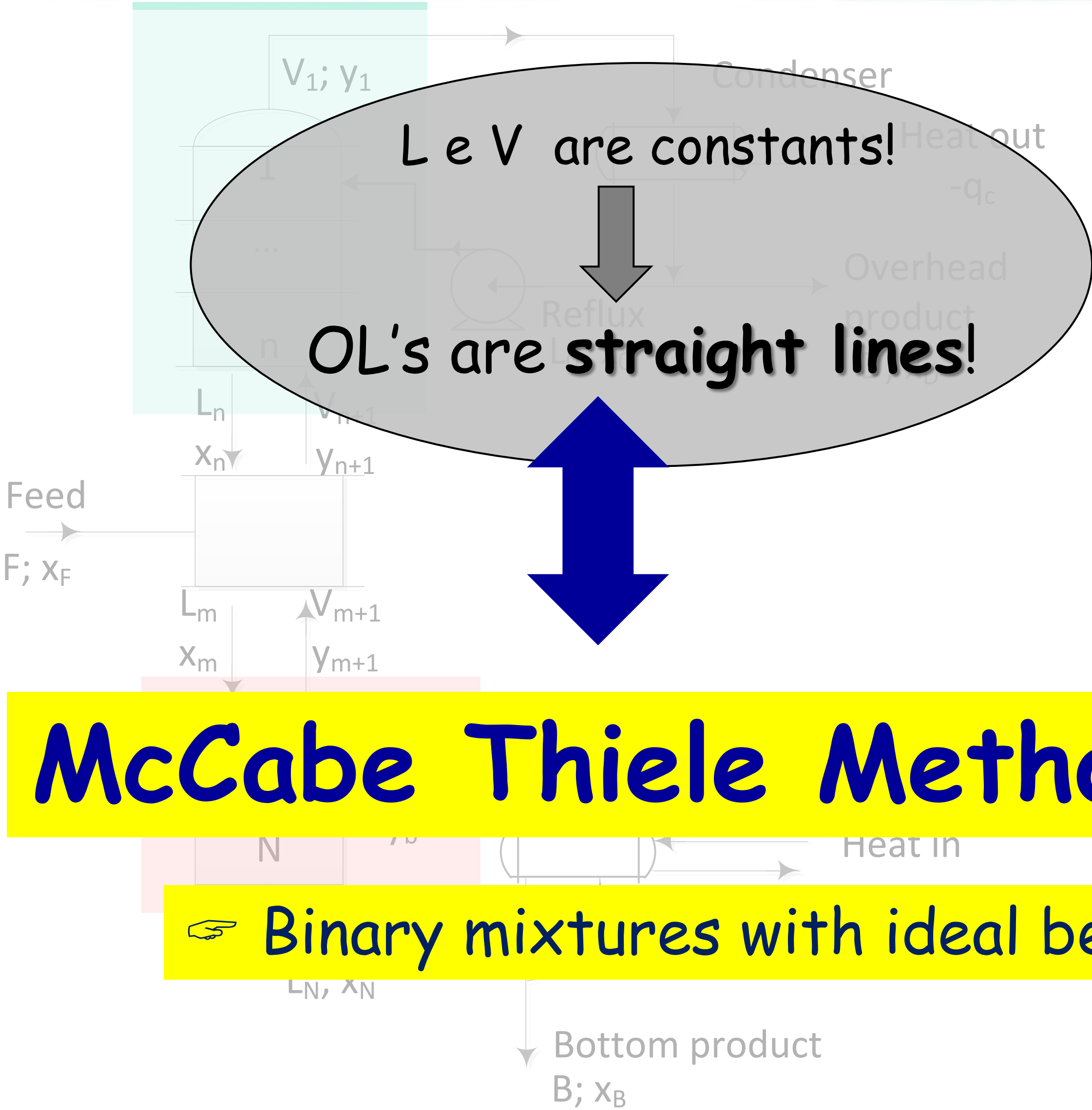
Enriching section

$$y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D x_D}{V_{n+1}}$$

Stripping section

$$y_{m+1} = \frac{L_m}{V_{m+1}} x_m - \frac{B x_B}{V_{m+1}}$$

Material balances – Operating lines



L e V are constants!

OL's are **straight lines!**

McCabe Thiele Method!

☞ Binary mixtures with ideal behaviour

Enriching section

$$y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D x_D}{V_{n+1}}$$

Stripping section

$$y_{m+1} = \frac{L_m}{V_{m+1}} x_m - \frac{B x_B}{V_{m+1}}$$

McCabe - Thiele (1925)

L and V flowrates are essentially influenced by the latent heat of vaporization/condensation of the mixture ($\Delta H_{vaporization/condensation}$)

If the **molar latent heat** of the mixture is **constant** and independent of the composition

L and V flowrates are **constants**

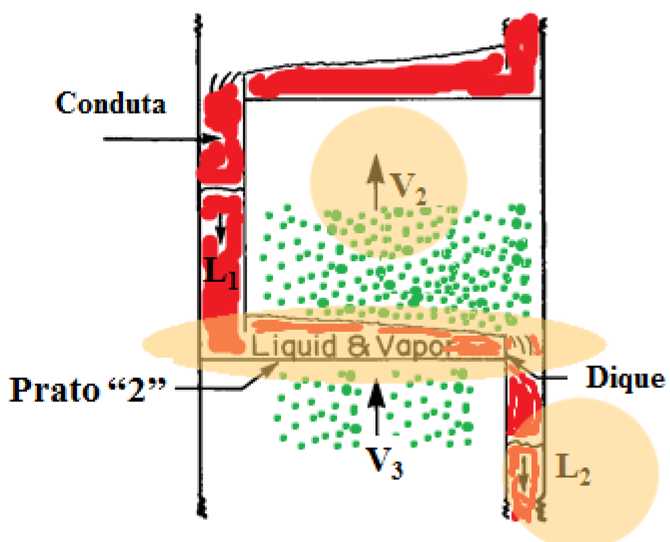
If L and V constants => the Operating lines are straight

McCabe Thiele Method !

☞ Molar units

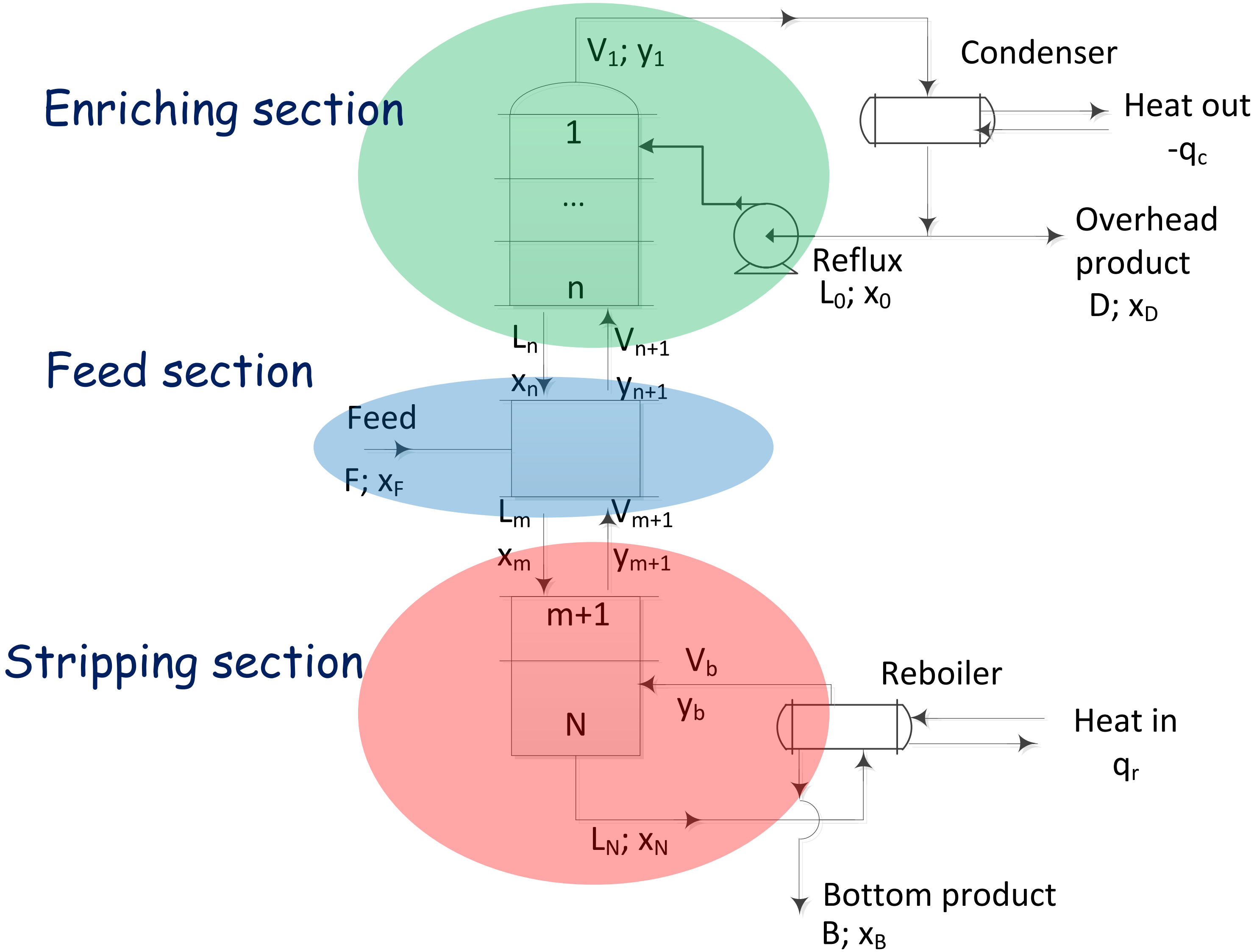
McCabe Thiele Method

- L e V flowrates constants (Rectilinear Operating lines)
- Full equilibrium between liquid and vapour phases in each plate (Equilibrium or theoretic stage)

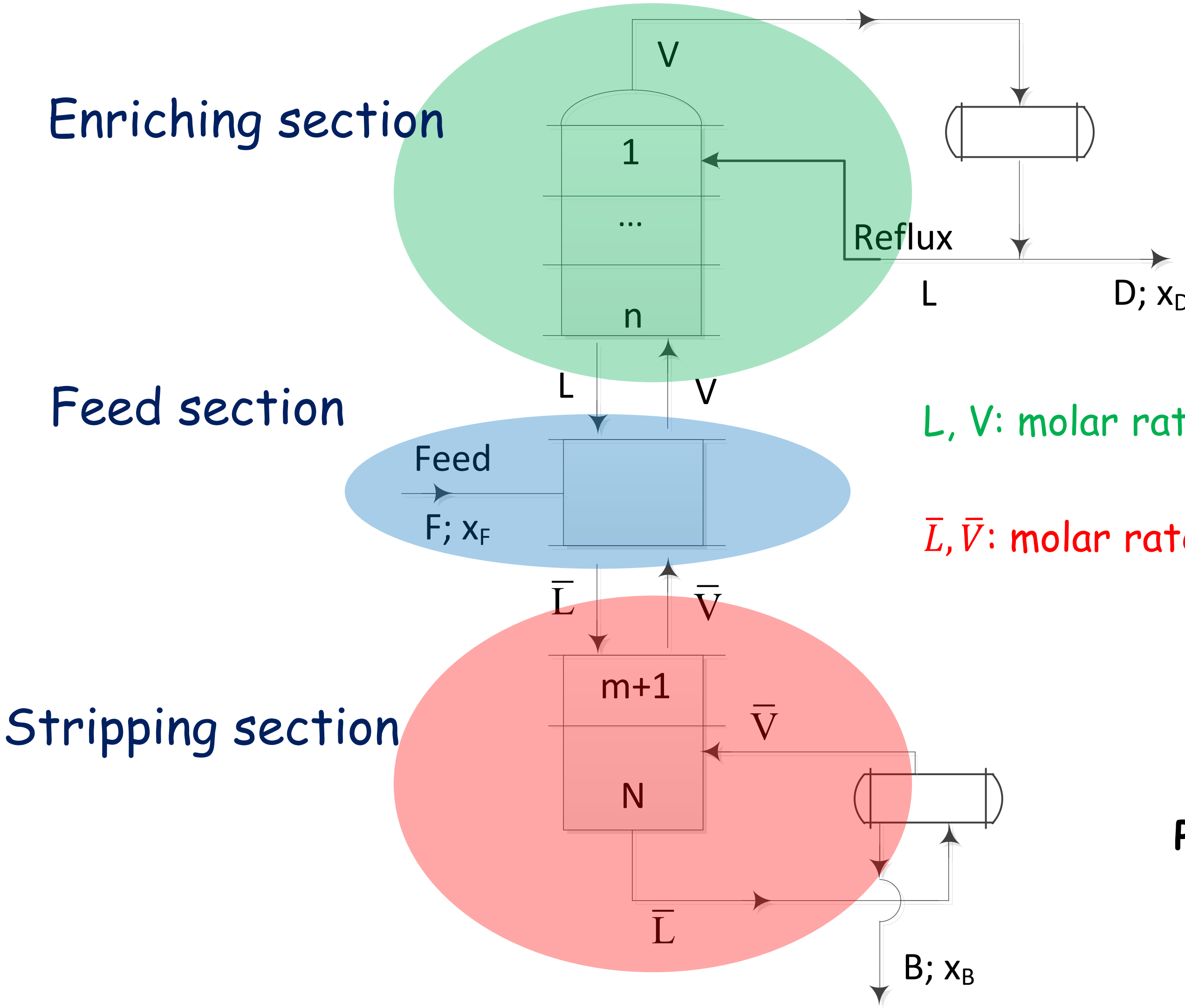


→ L_2 e V_2 are equilibrium streams

McCabe Thiele Method



McCabe Thiele Method



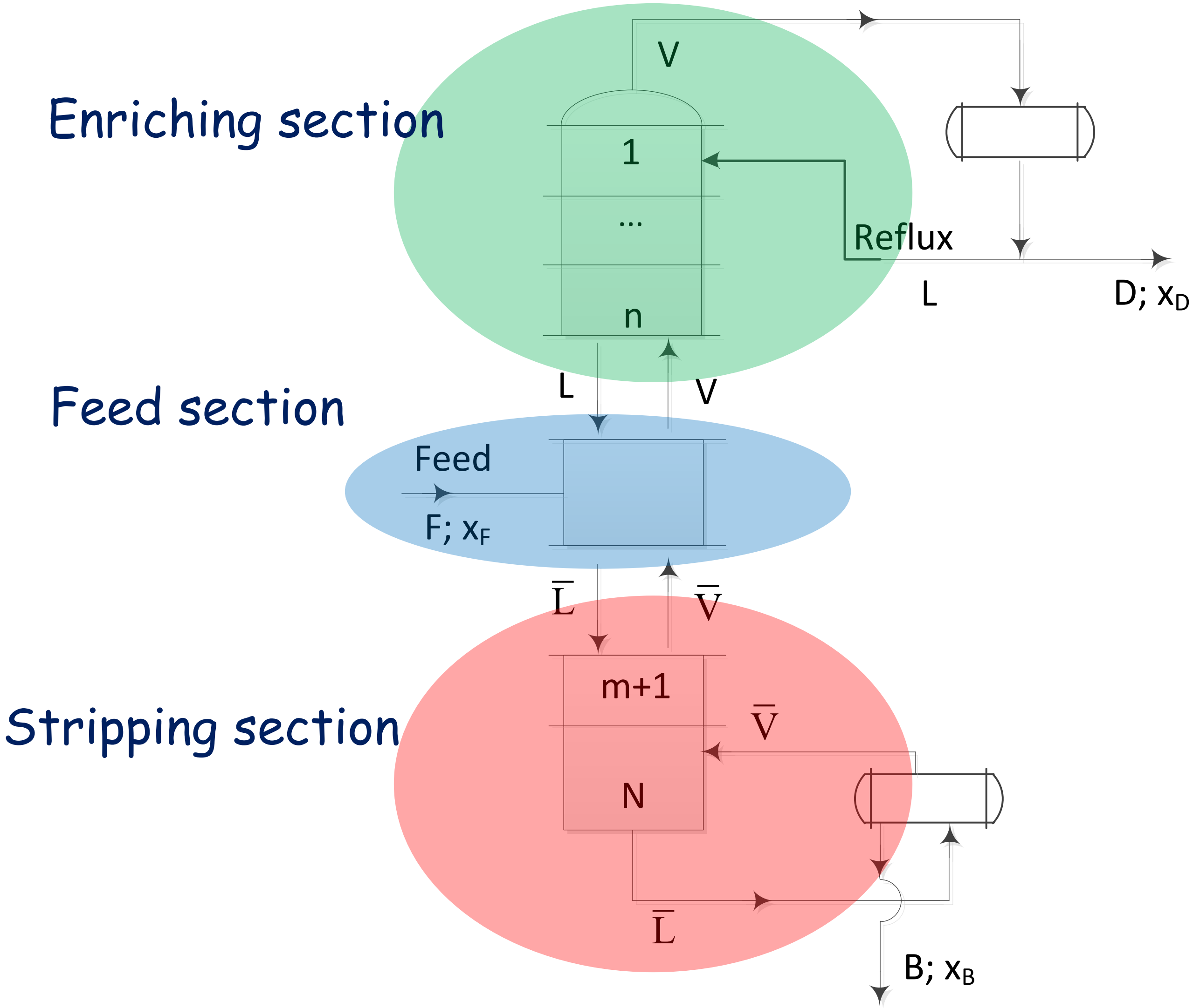
L, V: molar rates in enriching section

$\bar{L}, \bar{V}$: molar rates in stripping section

Problem complexity reduces from

2xN rate variables to just 4!!

McCabe Thiele Method



$$\begin{cases} F = B + D \\ Fx_F = Bx_B + Dx_D \end{cases}$$

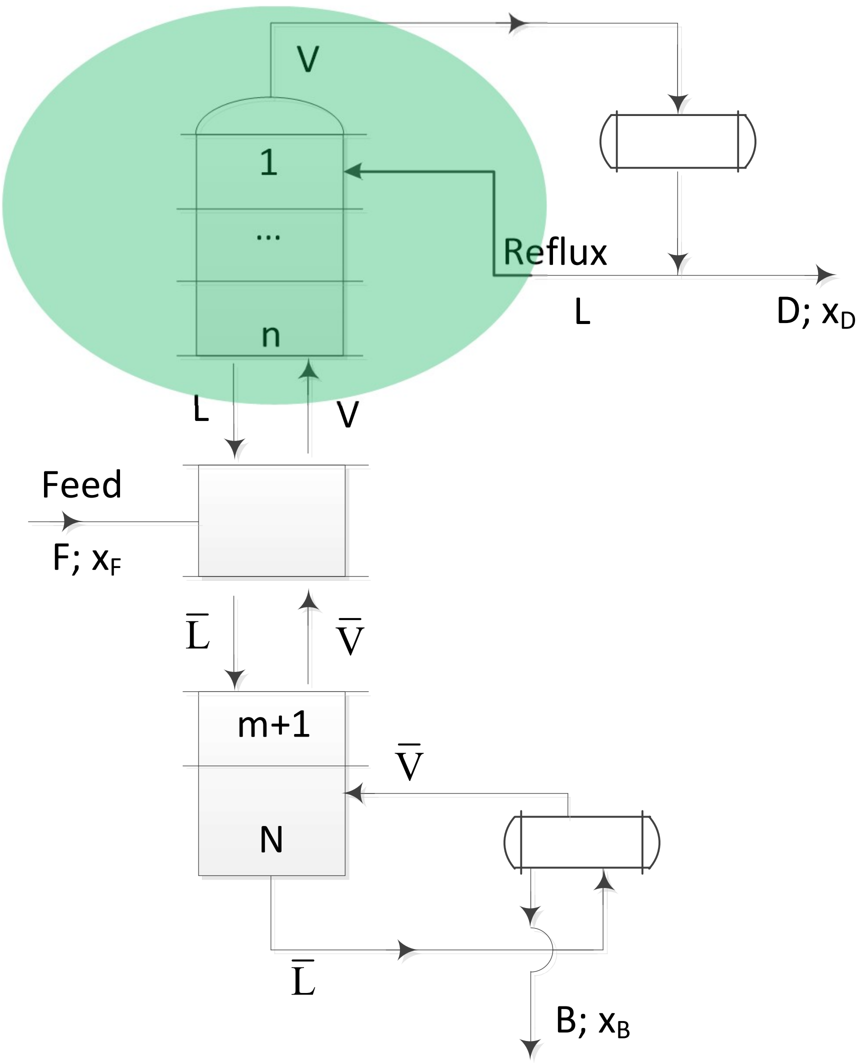
$$V = L + D$$
$$\overline{L} = \overline{V} + B$$

$$R = L/D$$

Reflux rate

Material balances – Operating lines

Enriching section

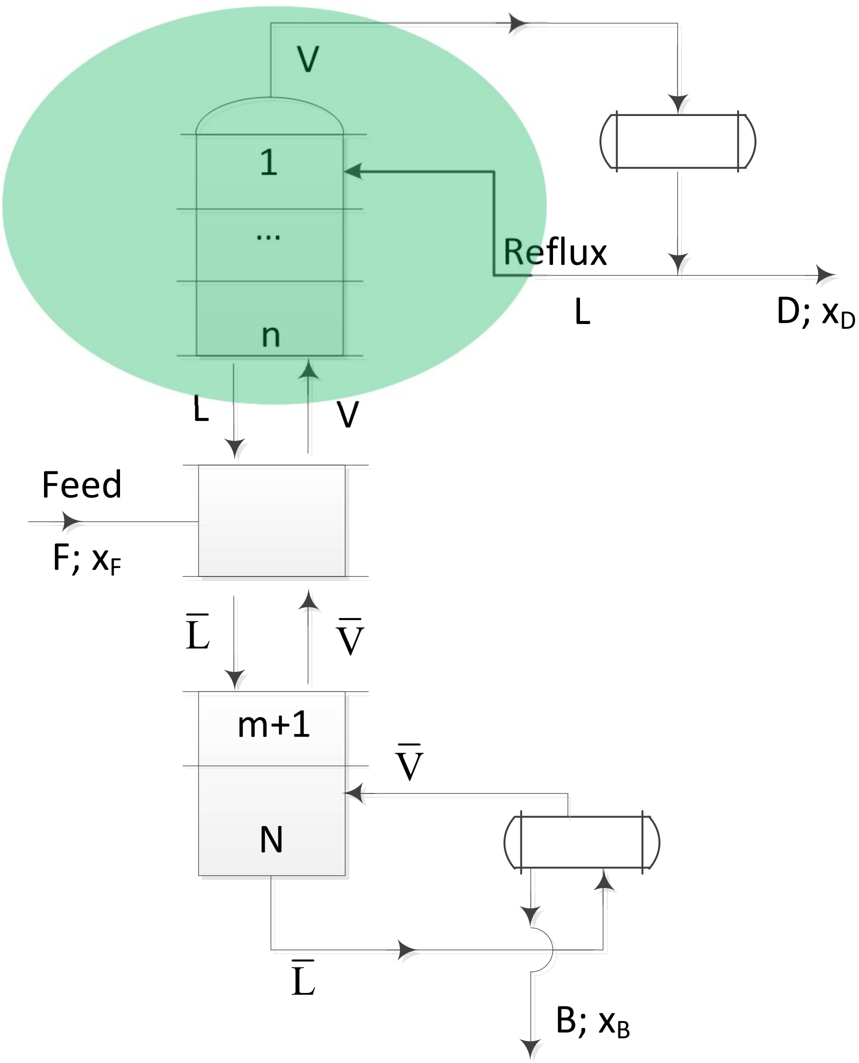


$$y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{Dx_D}{V_{n+1}}$$

$$y_{n+1} = \frac{L}{V} x_n + \frac{Dx_D}{V}$$

Material balances – Operating lines

<u>Enriching section</u>



$$y_{n+1} = \frac{L}{V} x_n + \frac{D x_D}{V}$$

V= L+D

R= L/D

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1}$$

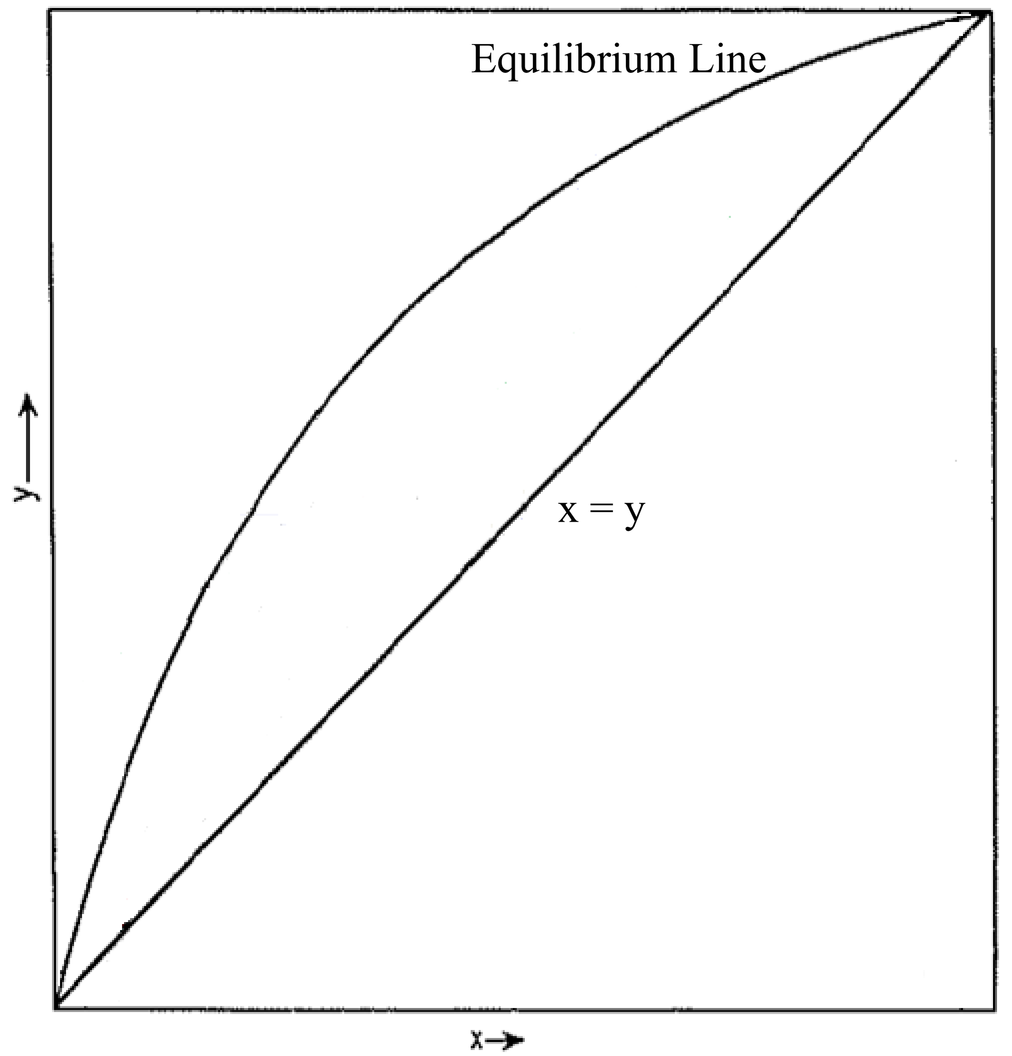
McCabe Thiele Method – graphical resolution

Enriching OL

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1}$$

As said, it is a graphic method of resolution!

So, we need to represent the operating line for the enriching section in the yx diagram

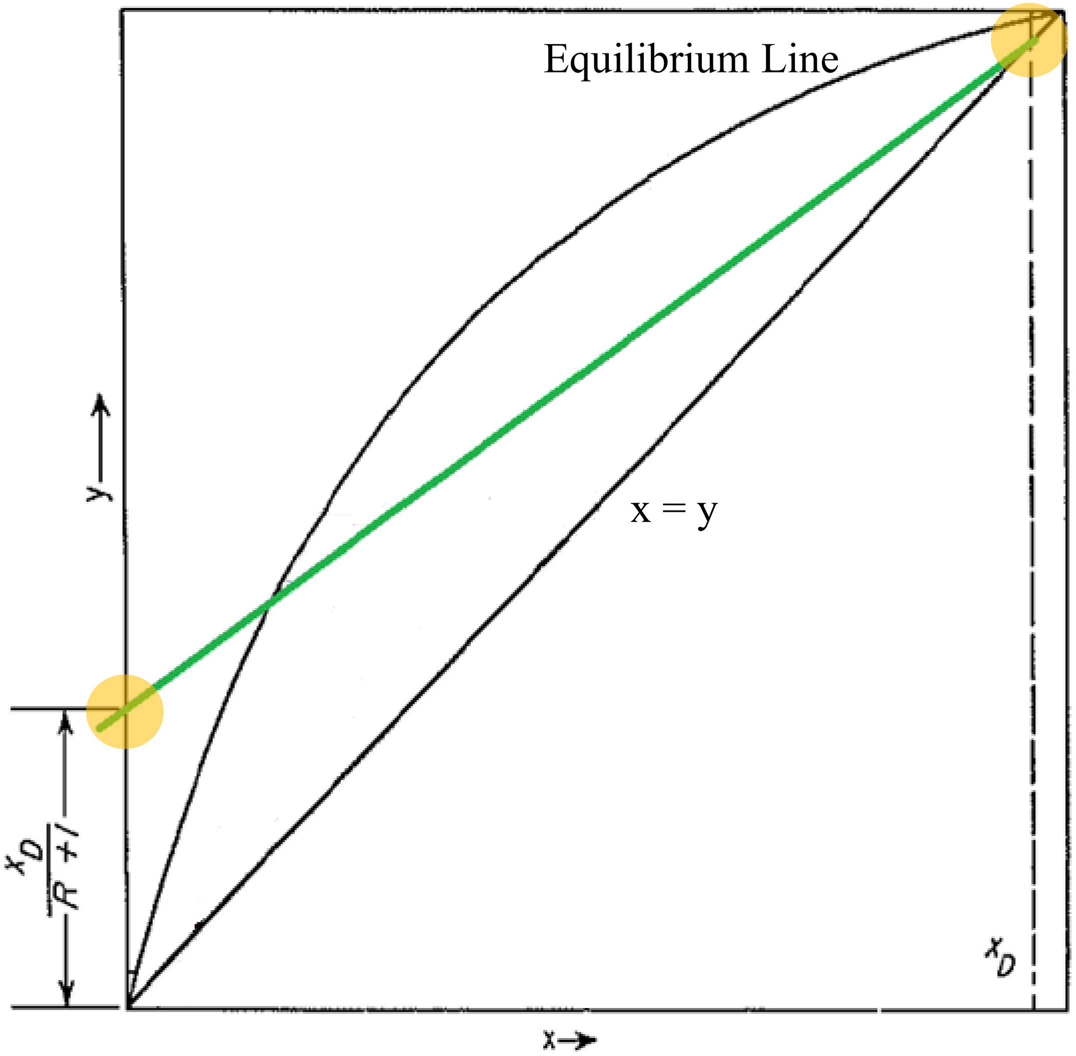


McCabe Thiele Method – graphical resolution

Enriching OL

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1}$$

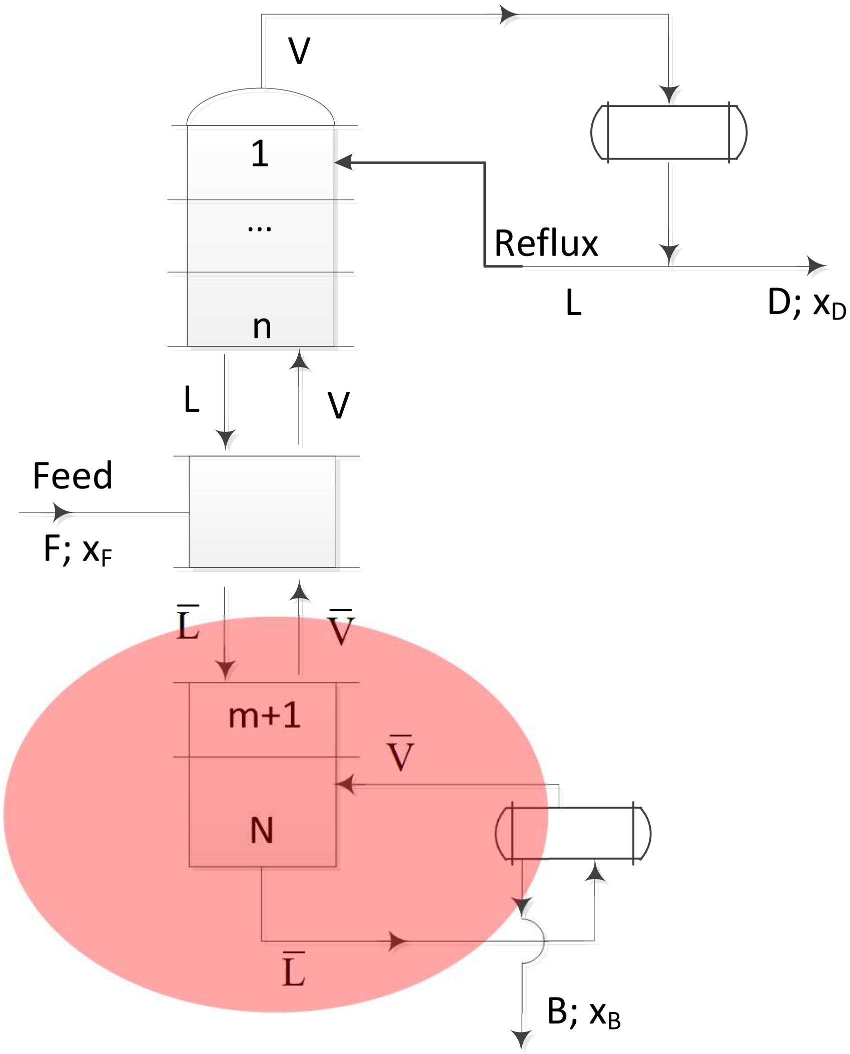
$$\begin{cases} \text{when } x_n = x_D \Rightarrow y_{n+1} = x_D \\ \text{when } x_n = 0 \Rightarrow y_{n+1} = \dfrac{x_D}{R+1} \end{cases}$$



Necessary data: x_D, R

Material balances – Operating lines

<u>Stripping section</u>



$$y_{m+1} = \frac{L_m}{V_{m+1}} x_m - \frac{Bx_B}{V_{m+1}}$$

$$y_{m+1} = \frac{\bar{L}}{\bar{V}} x_m - \frac{Bx_B}{\bar{V}}$$

The slope of the stripping OL is: $\bar{L}/\bar{V}$

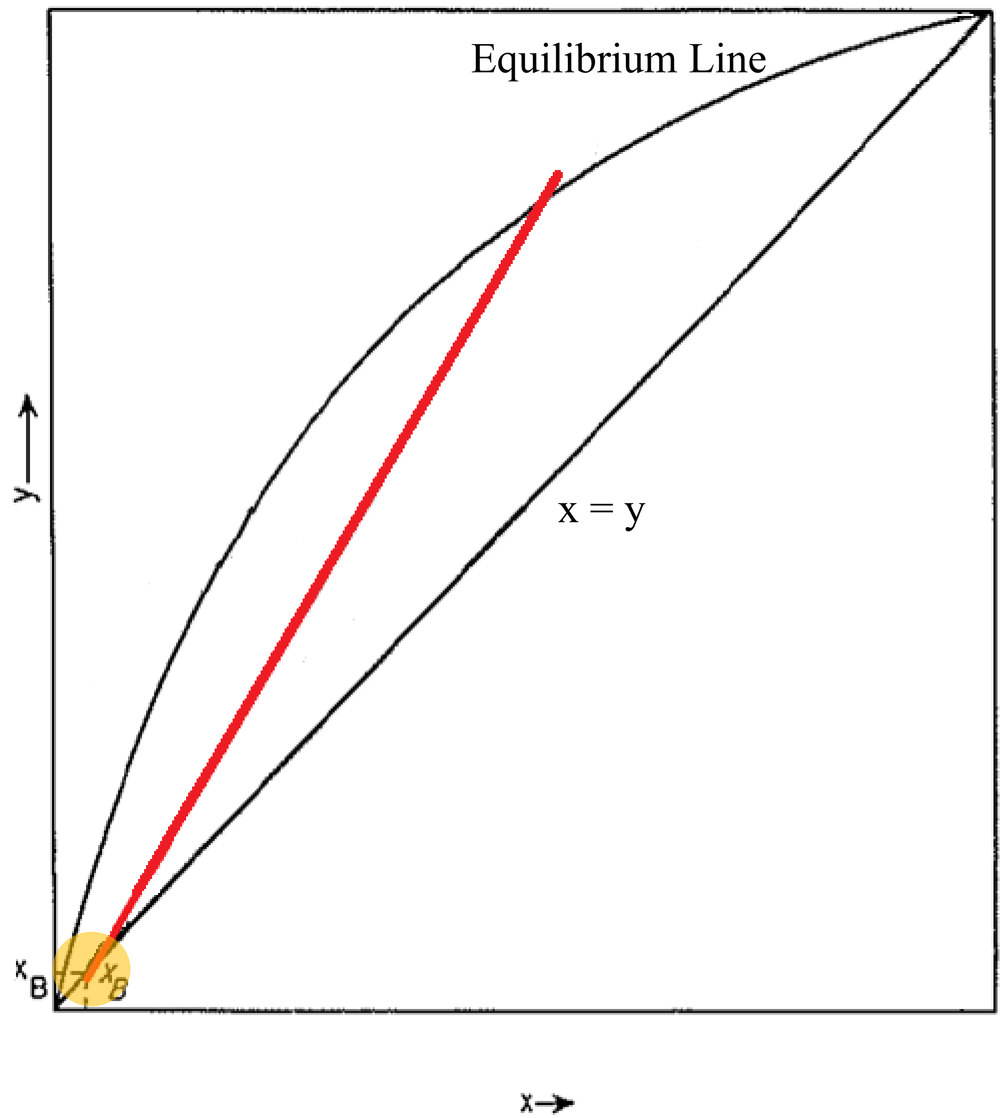
Hard to calculate! No problem…

Stripping OL

$$y_{m+1} = \frac{\bar{L}}{\bar{V}} x_m - \frac{B x_B}{\bar{V}}$$

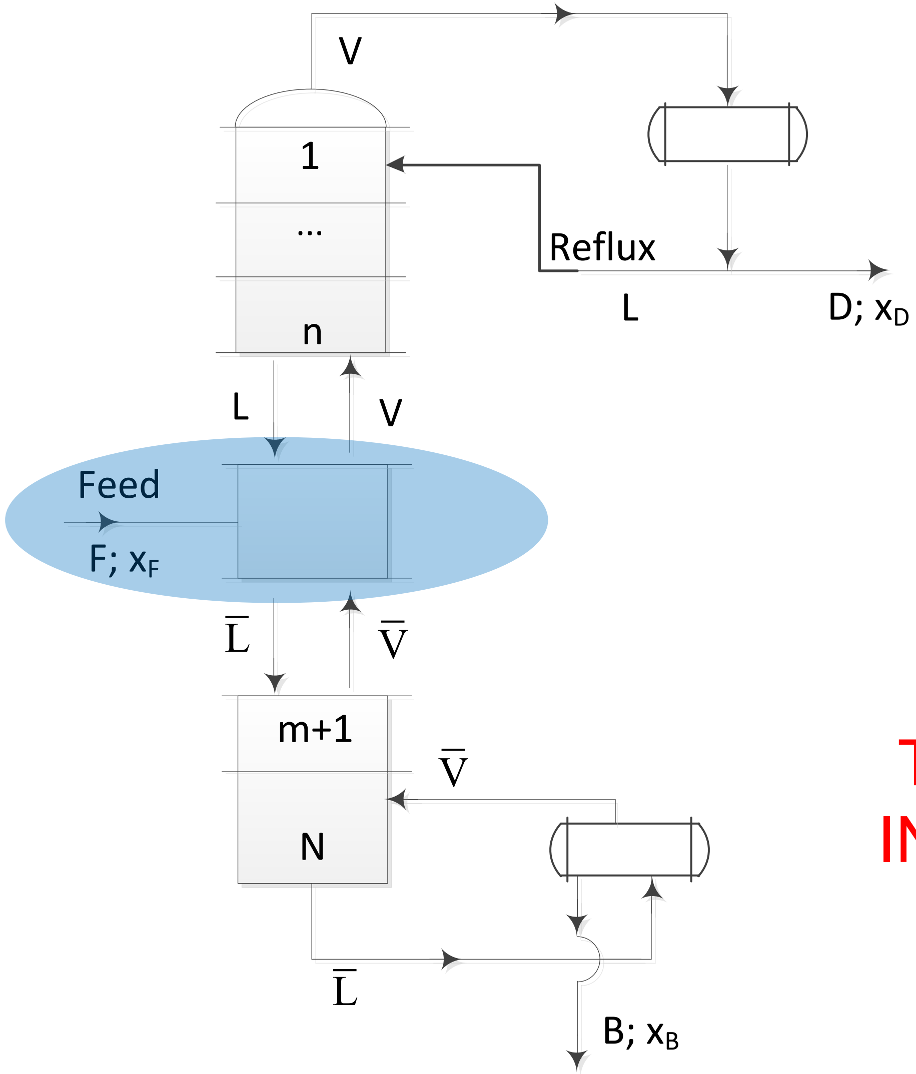
$$\text{when } x_m = x_B \Rightarrow y_{m+1} = x_B$$

$$(\bar{L} = \bar{V} + B)$$



Necessary data: x_B, $\bar{L}/\bar{V}$

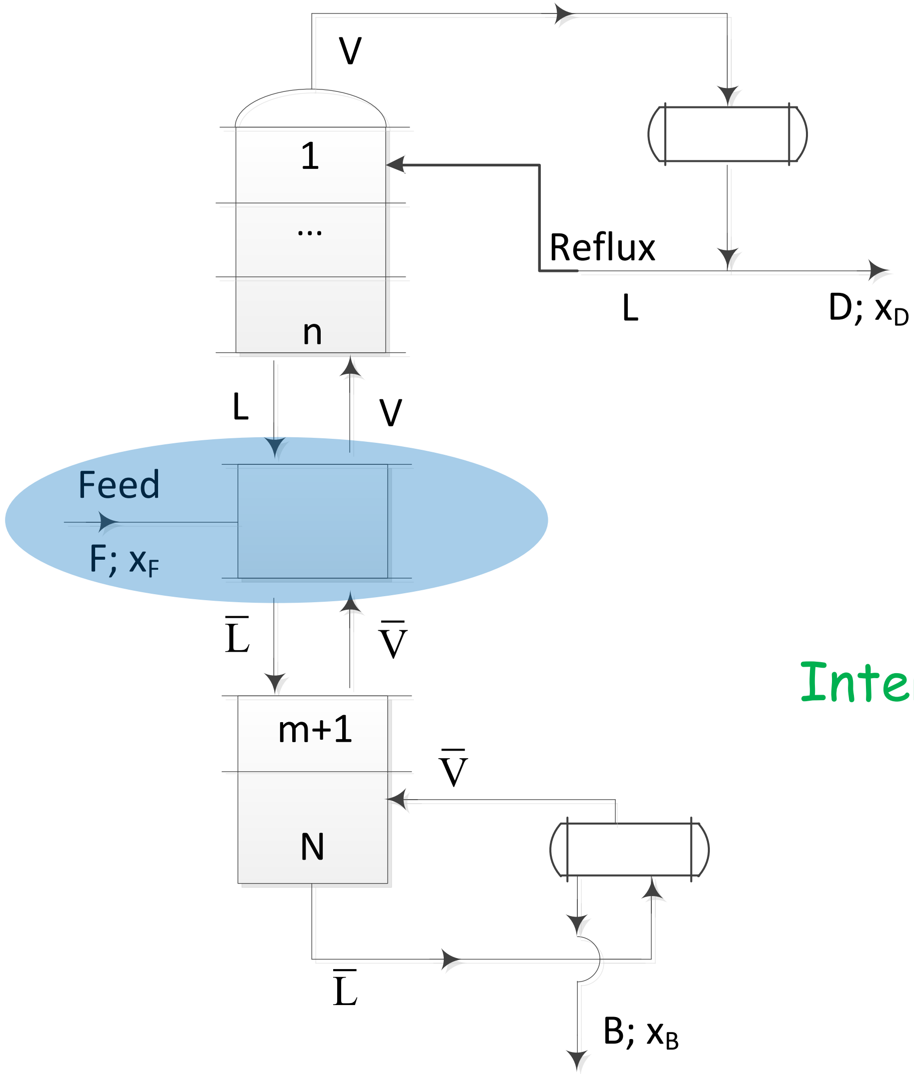
Feed section



Intersection of the enriching and stripping sections

THE **THREE** OLs HAVE TO INTERCEPT IN A GIVEN POINT *x,y* so that the material balance to the column "closes"

Operating line of Feed



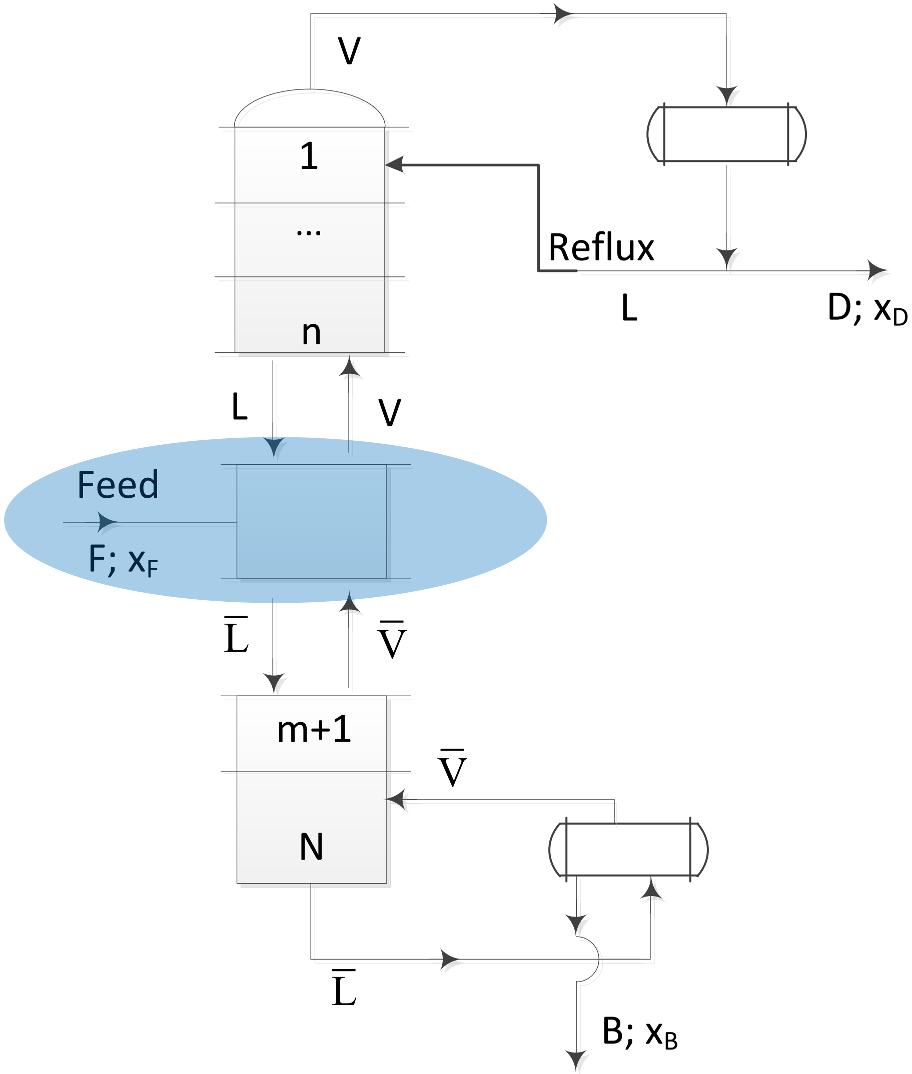
From the former OL's

$$\begin{cases} y_{n+1} = \dfrac{L}{V} x_n + \dfrac{D x_D}{V} \\ y_{m+1} = \dfrac{\bar{L}}{\bar{V}} x_m - \dfrac{B x_B}{\bar{V}} \end{cases}$$

Intersection of enriching and stripping OL's

$$\boxed{y_{n+1} = y_{m+1} = \boldsymbol{y_i} \quad ; \quad x_n = x_m = \boldsymbol{x_i}}$$

Operating line of Feed



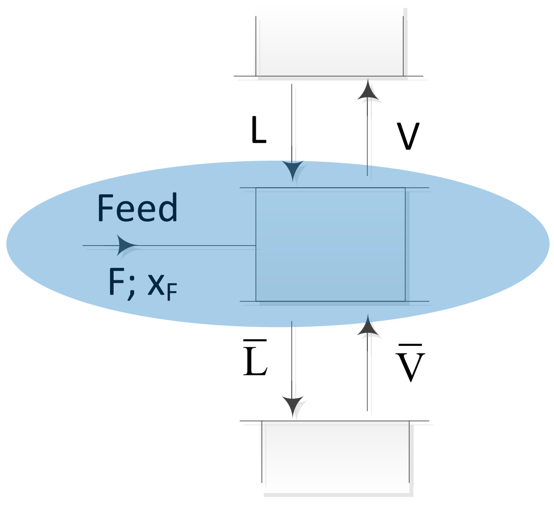
From the former OL's

$$\begin{cases} y_{n+1} = \dfrac{L}{V} x_n + \dfrac{D x_D}{V} \\ y_{m+1} = \dfrac{\bar{L}}{\bar{V}} x_m - \dfrac{B x_B}{\bar{V}} \end{cases}$$

$$\boxed{y_i = \frac{i}{i-1} x_i - \frac{x_F}{i-1}}$$

i : is a parameter that quantifies the physical state of the feed

Physical state of the Feed



a) Subcooled liquid

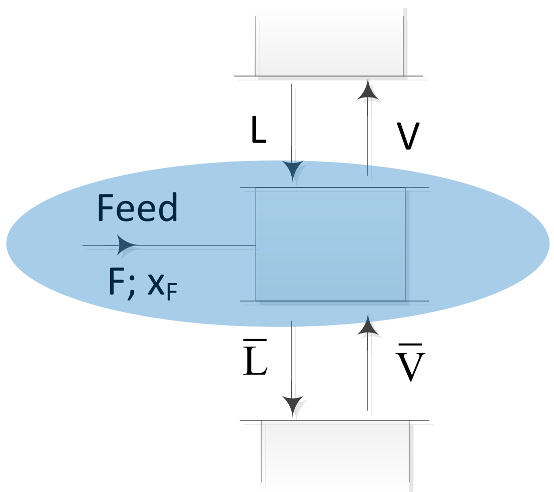
b) Saturated liquid

c) Saturated L+V

d) Saturated vapor

e) Superheated Vapor

Physical state of the Feed – parameter *i*



a) Subcooled liquid

b) Saturated liquid

c) Saturated L+V

d) Saturated vapor

e) Superheated Vapor

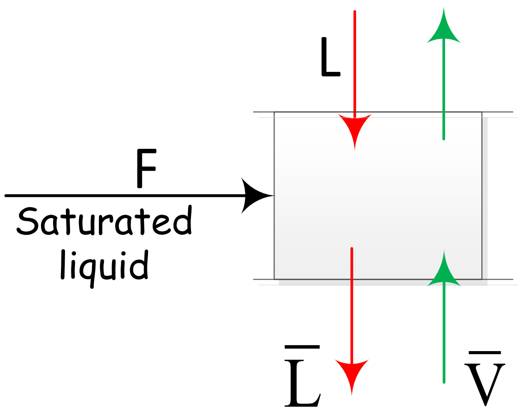
McCabe and Thiele had to find a way to "numerically" quantify the physical state of a given feed mixture

$$\boxed{i = \frac{\bar{L} - L}{F}}$$

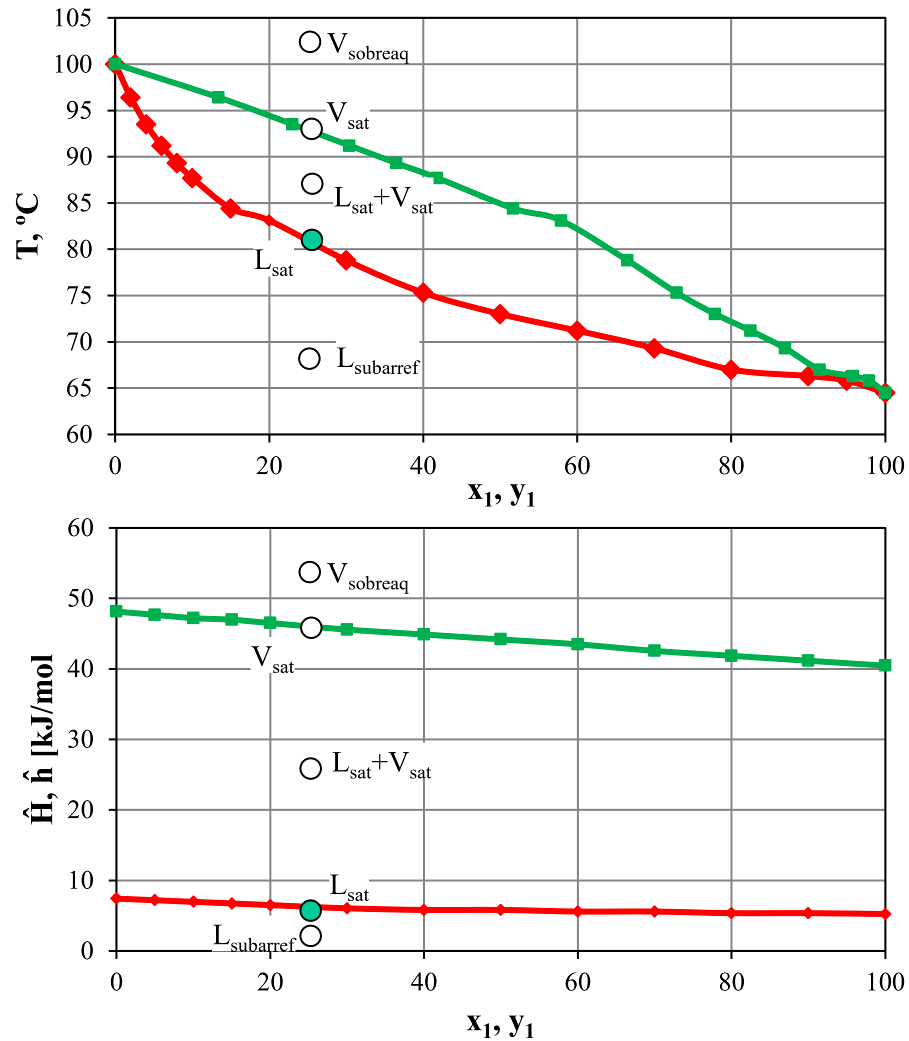
$$i = \frac{moles\ of\ liquid\ flowing\ down}{moles\ of\ feed}$$

Physical state of the Feed – the *i* parameter

b) Saturated liquid

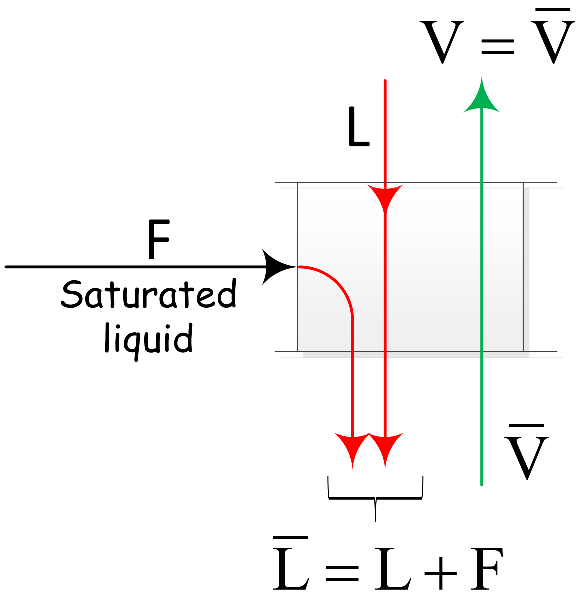


$T_F \cong T_L \cong T_{\bar{L}}$



Physical state of the Feed – the *i* parameter

b) Saturated liquid



$$\boxed{T_F \cong T_L \cong T_{\overline{L}}}$$

$$i = \frac{moles\ of\ liquid\ flowing\ down}{moles\ of\ feed}$$

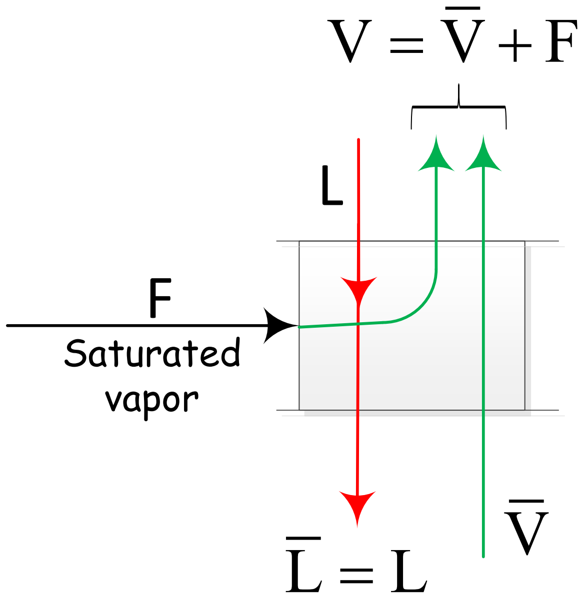
$$\overline{L} = L + F$$

$$\boxed{i = \frac{\overline{L} - L}{F}}$$

$$i = \frac{(L + F) - L}{F} = 1$$

Physical state of the Feed – the *i* parameter

d) Saturated vapor



$\boxed{T_F \cong T_V \cong T_{\overline{V}}}$

$$\overline{L} = L + 0$$

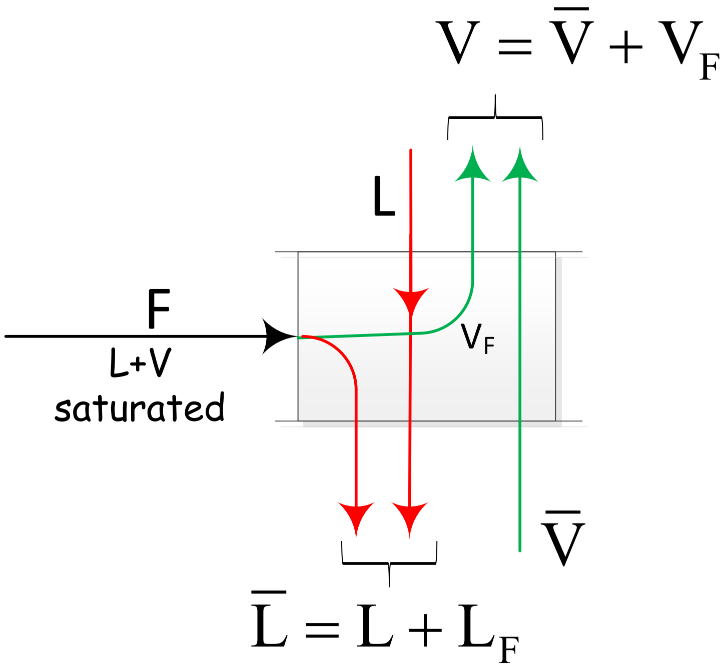
$$\boxed{i = \frac{\overline{L} - L}{F}}$$

$$i = \frac{(L) - L}{F} = 0$$

$$i = \frac{moles\ of\ liquid\ flowing\ down}{moles\ of\ feed}$$

Physical state of the Feed – the *i* parameter

c) L + V saturated



$$i = \frac{\bar{L} - L}{F}$$

$$\bar{L} = L + aF$$

$$i = \frac{(L + aF) - L}{F} = a$$

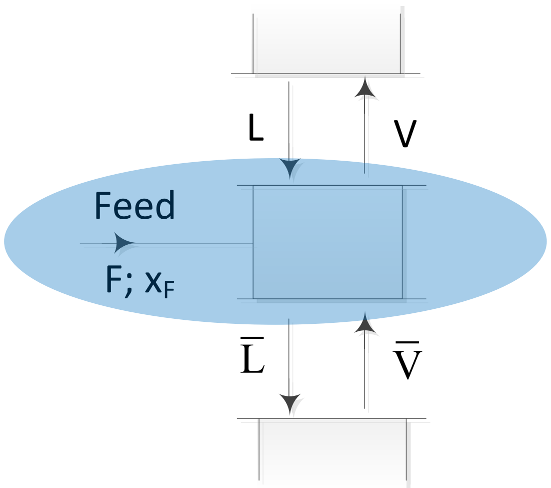
where $L_F = a.F$

(with: $0 < a < 1$)

$$\begin{cases} a = 0 \Rightarrow \text{saturated vapor} \\ a = 1 \Rightarrow \text{saturated liquid} \end{cases}$$

$$i = \frac{moles\ of\ liquid\ flowing\ down}{moles\ of\ feed}$$

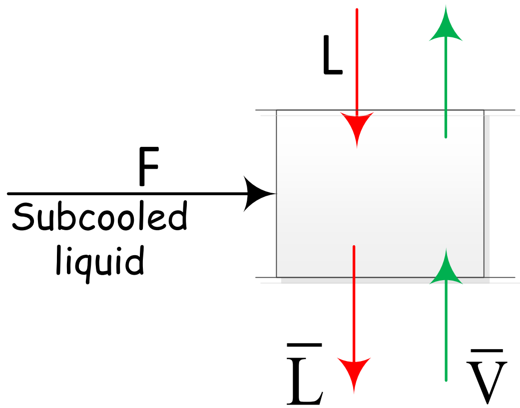
$$\boxed{= \frac{\bar{L} - L}{F}}$$

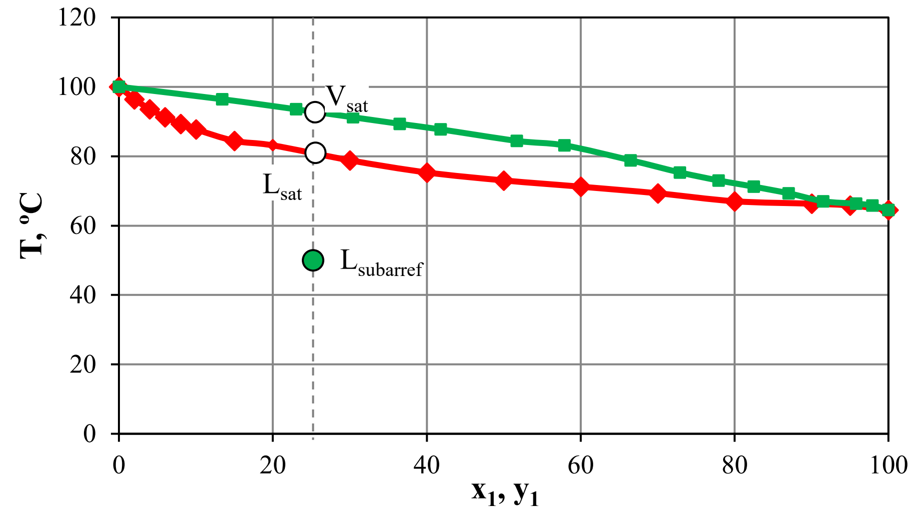


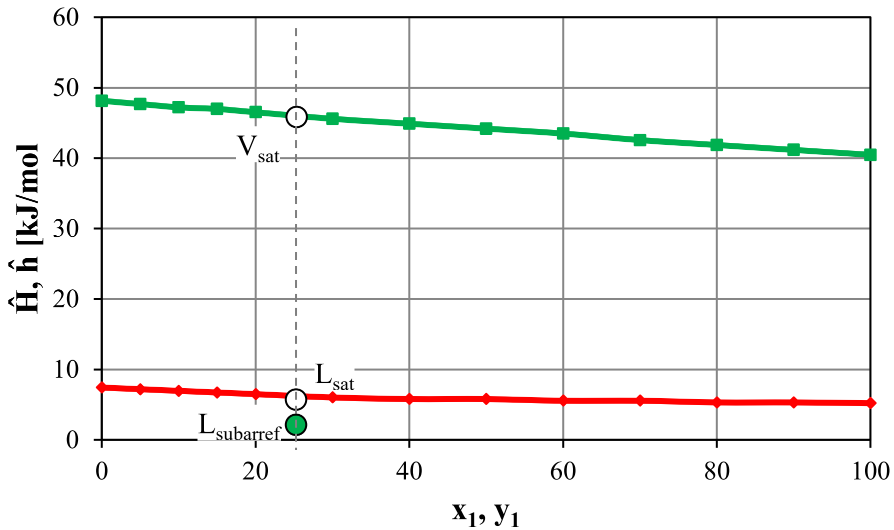
b) Saturated liquid	i = 1
c) Saturated L+V	0 < i < 1
d) Saturated vapor	i = 0

Physical state of the Feed – the *i* parameter

a) Subcooled liquid



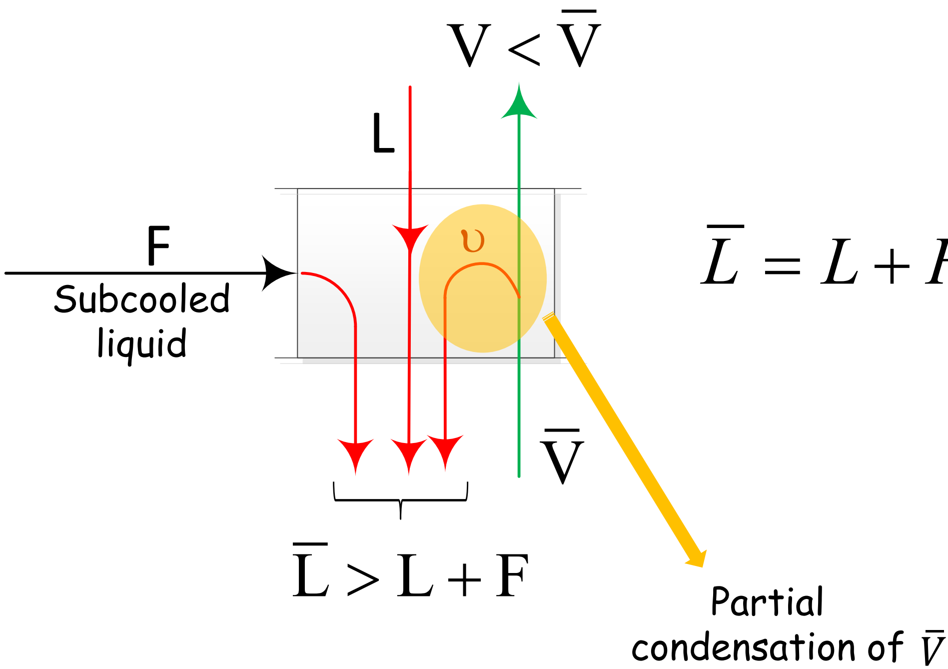




$\boxed{T_F < T_L}$

Physical state of the Feed – the *i* parameter

a) Subcooled liquid



$$\bar{L} = L + F + \upsilon$$

$$\boxed{i = \frac{\bar{L} - L}{F}}$$

$$i = \frac{(L + F + \upsilon) - L}{F}$$

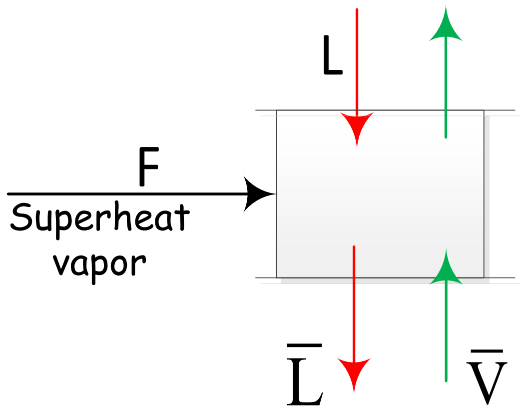
$$i = \frac{F + \upsilon}{F} > 1$$

$\boxed{T_F < T_L}$

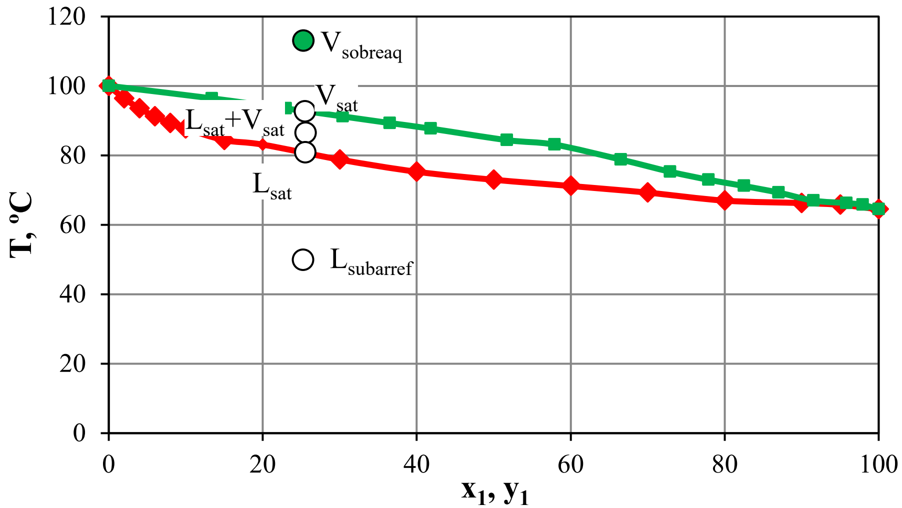
Value of υ: to be determined by an energy balance to feed plate

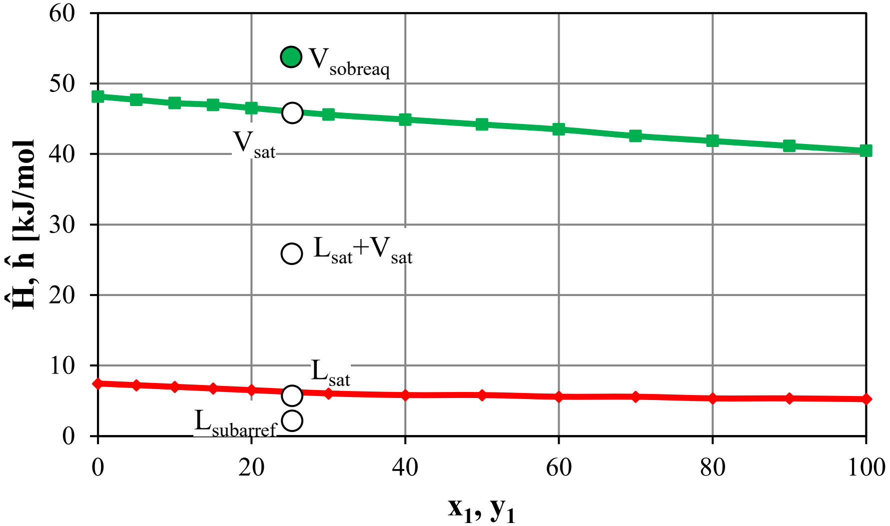
Physical state of the Feed - the *i* parameter

e) Superheated vapor



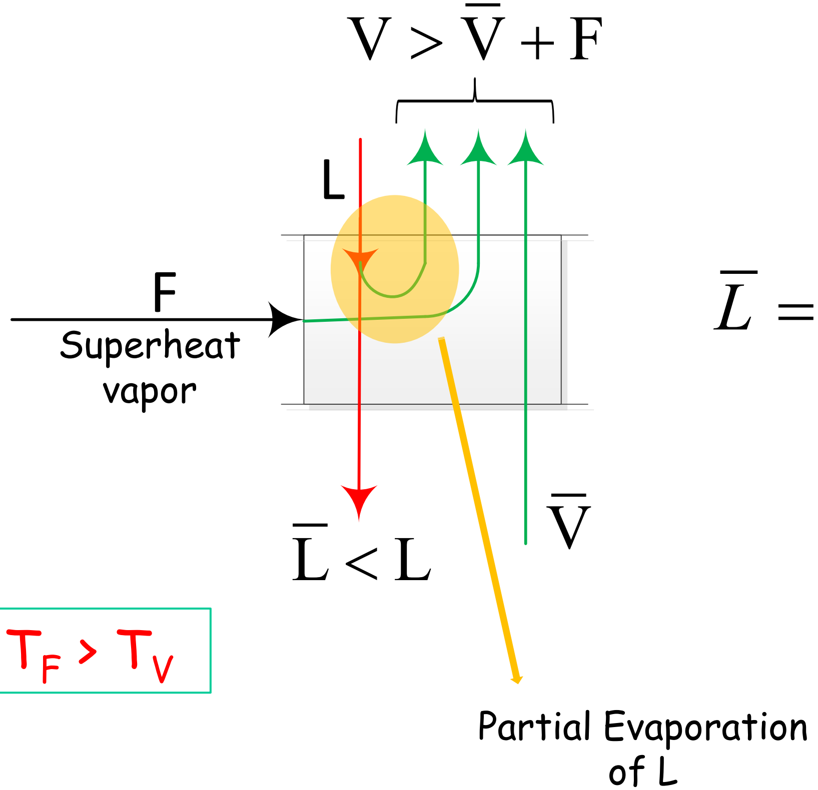
$\boxed{T_F > T_V}$





Physical state of the Feed – the *i* parameter

e) Superheated vapor



$T_F > T_V$

$$\bar{L} = L - \upsilon + 0$$

$$\boxed{i = \frac{\bar{L} - L}{F}}$$

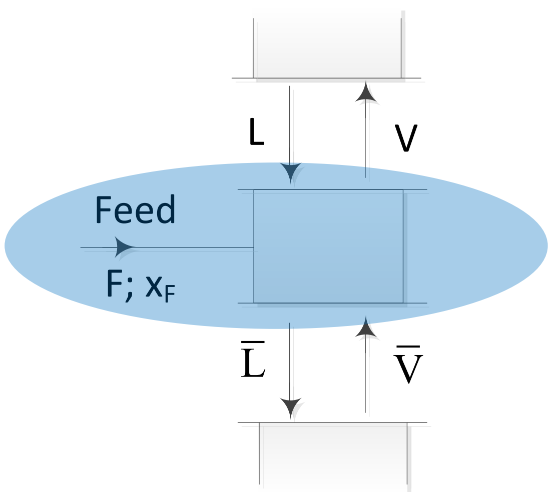
$$i = \frac{(L - \upsilon) - L}{F}$$

$$i = \frac{-\upsilon}{F} < 0$$

Value of υ: to be determined by an energy balance to feed plate

$$\mathrm{i} = \frac{moles\ of\ liquid\ flowing\ down}{moles\ of\ feed}$$

$$\boxed{= \frac{\bar{L} - L}{F}}$$

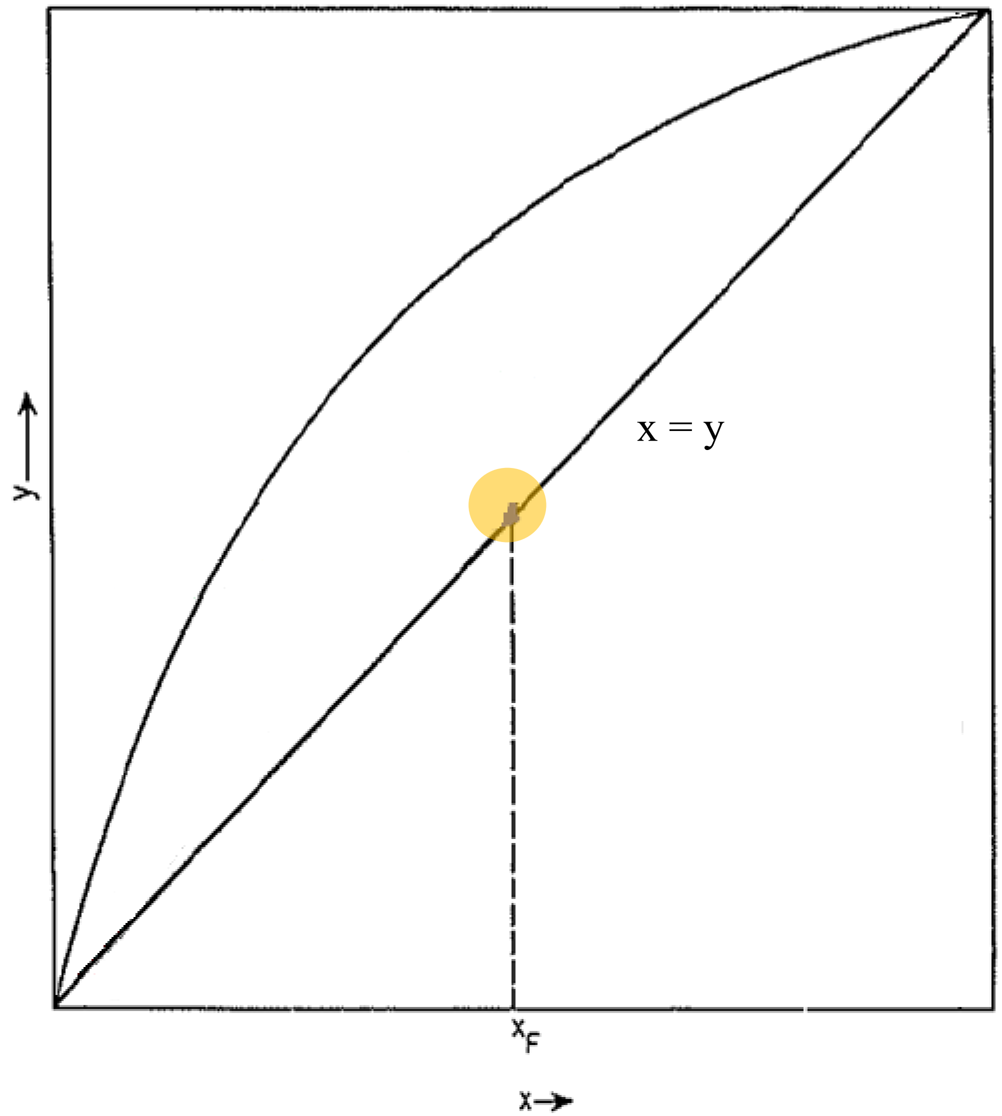


a) Subcooled liquid	i > 1
b) Saturated liquid	i = 1
c) Saturated L+V	0 < i < 1
d) Saturated vapor	i = 0
e) Superheated Vapor	i < 0

Feed OL position

$$\boxed{y_i = \frac{i}{i-1}x_i - \frac{x_F}{i-1}}$$

when $x_i = x_F \Rightarrow y_i = x_F$

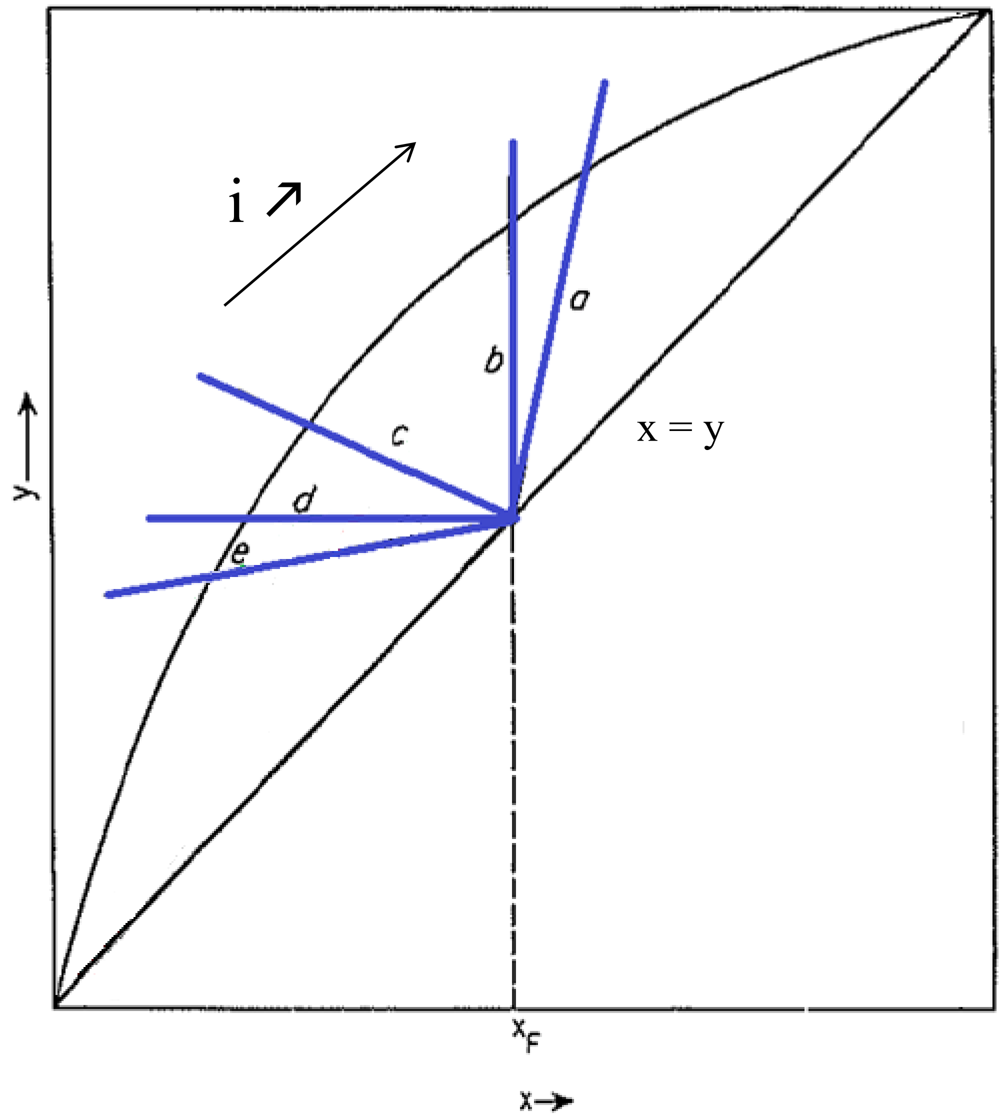


Feed OL position

$$\boxed{y_i = \frac{i}{i-1} x_i - \frac{x_F}{i-1}}$$

$$y_i\Big|_{x_i = x_F} = x_F$$

		$\dfrac{i}{i-1}$
a) Subcooled liquid	i > 1	> 0
b) Saturated liquid	i = 1	∞
c) Saturated L+V	0 < i < 1	< 0
d) Saturated vapor	i = 0	0
e) Superheated vapor	i < 0	> 0



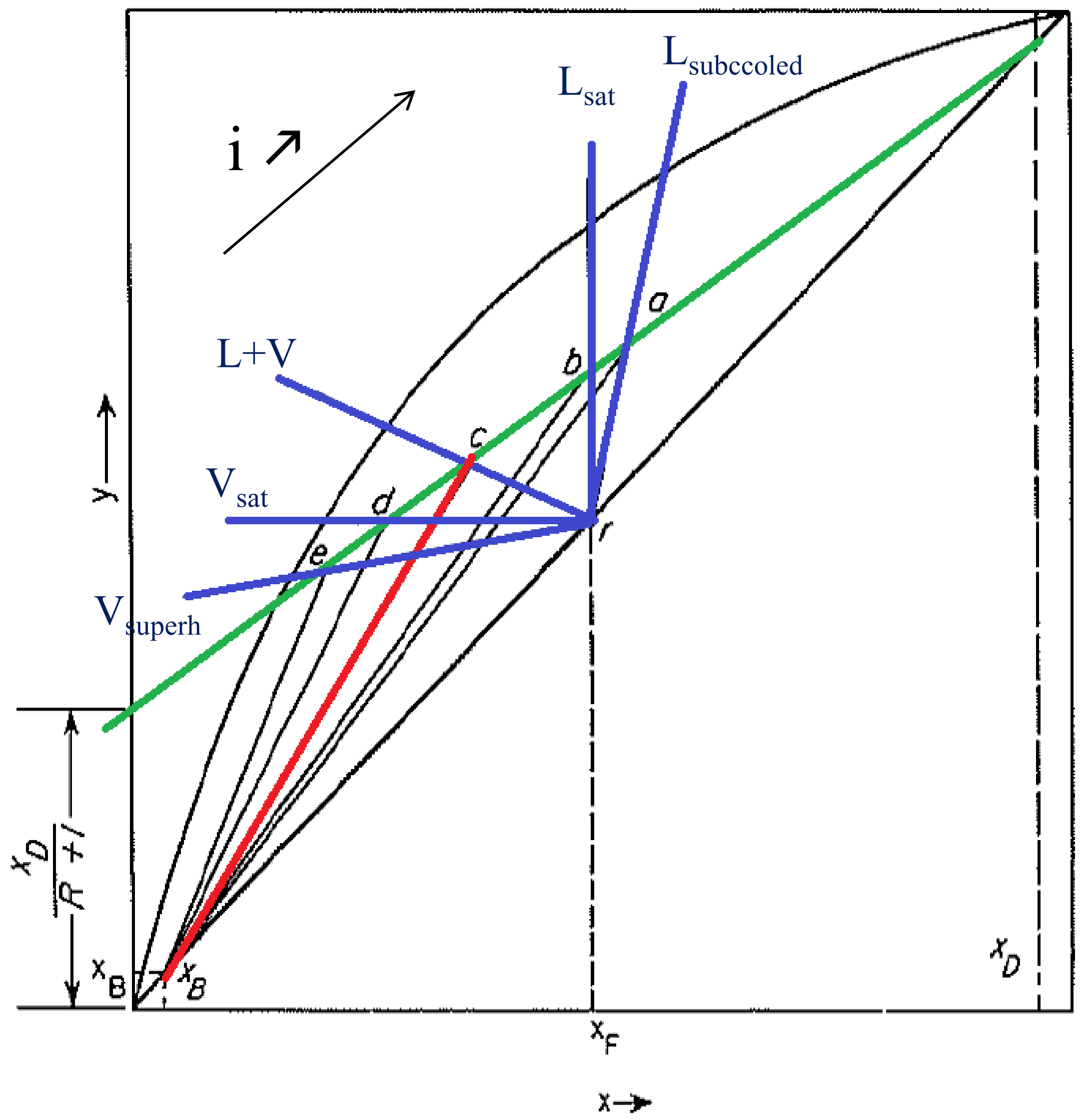
McCabe - Thiele Method

Operating lines

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1}$$

$$y_i = \frac{i}{i-1} x_i - \frac{x_F}{i-1}$$

$$y_{m+1} = \frac{\bar{L}}{\bar{V}} x_m - \frac{B x_B}{\bar{V}}$$



THE **THREE** OLs INTERCEPT IN A GIVEN POINT *x,y*

McCabe – Thiele Method

Operating lines

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1}$$

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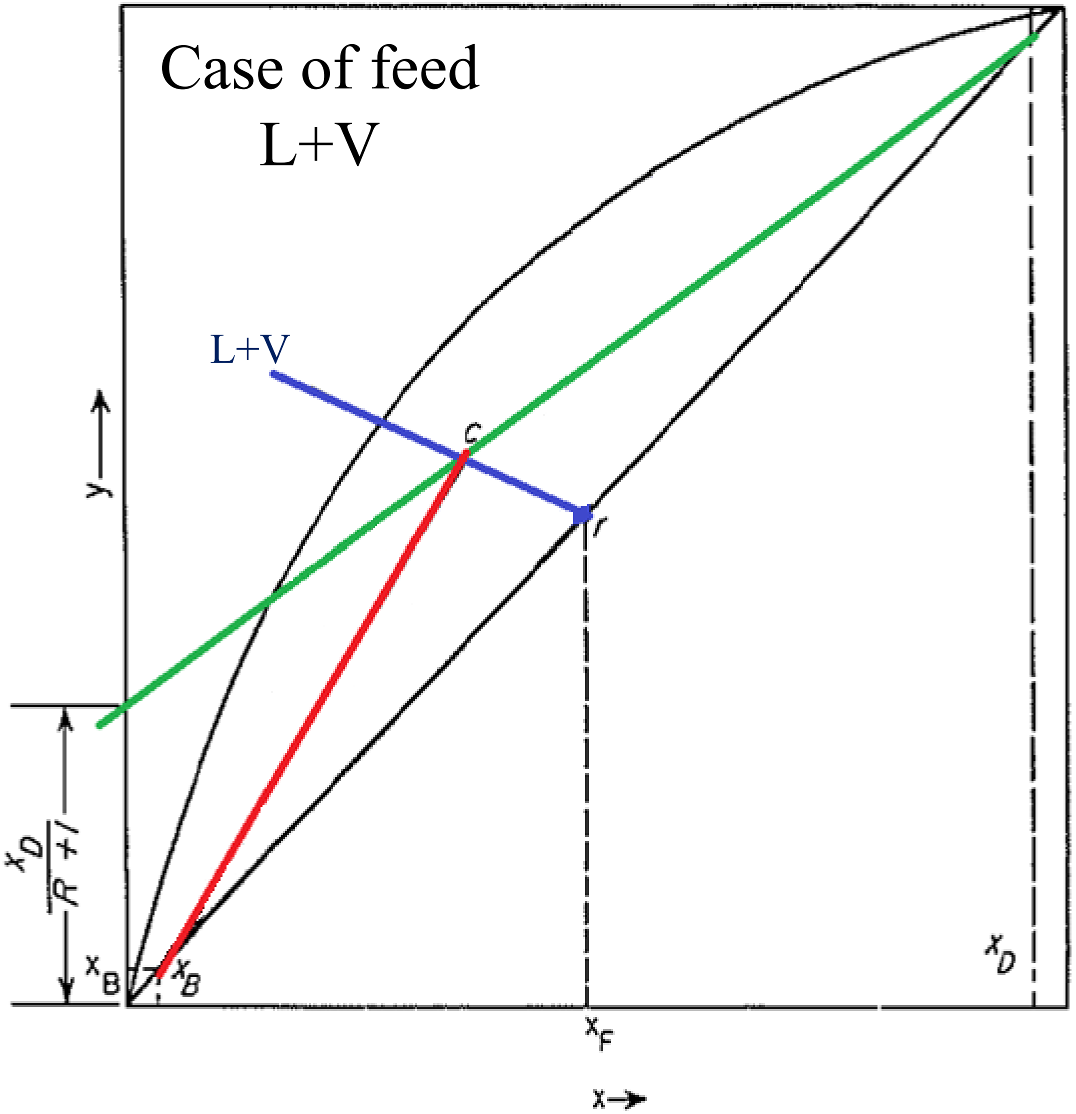
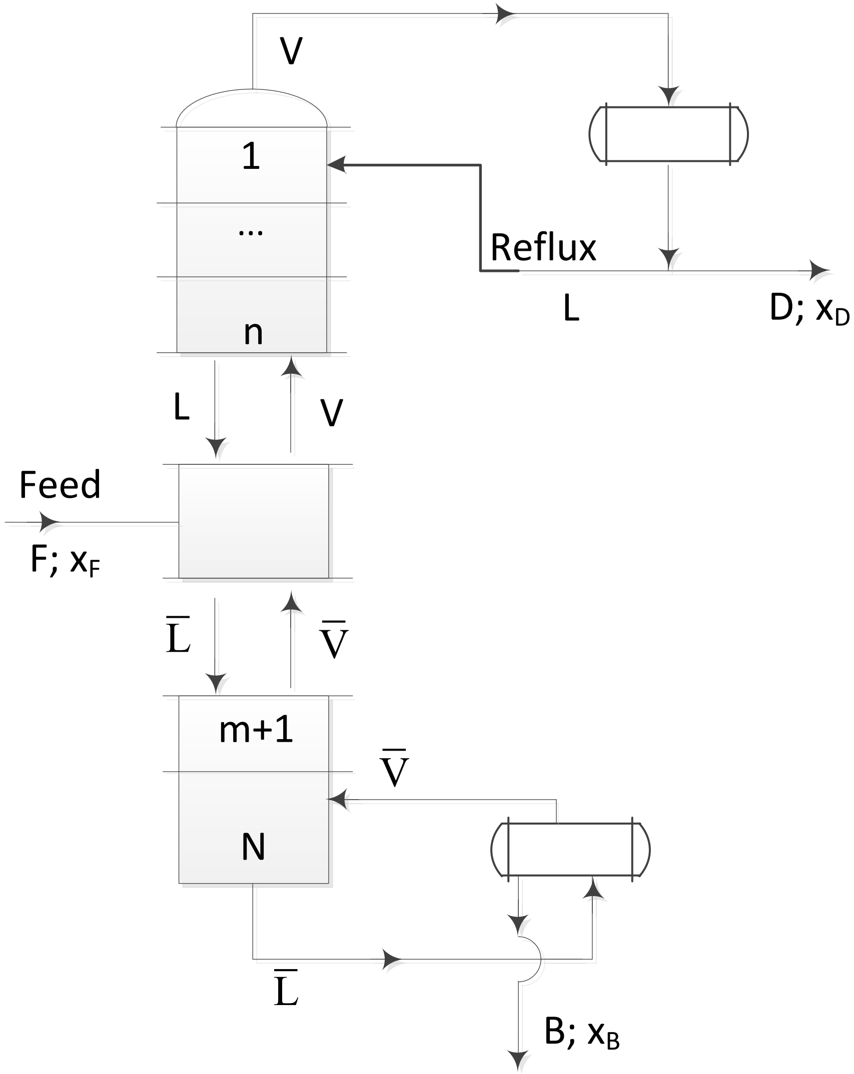
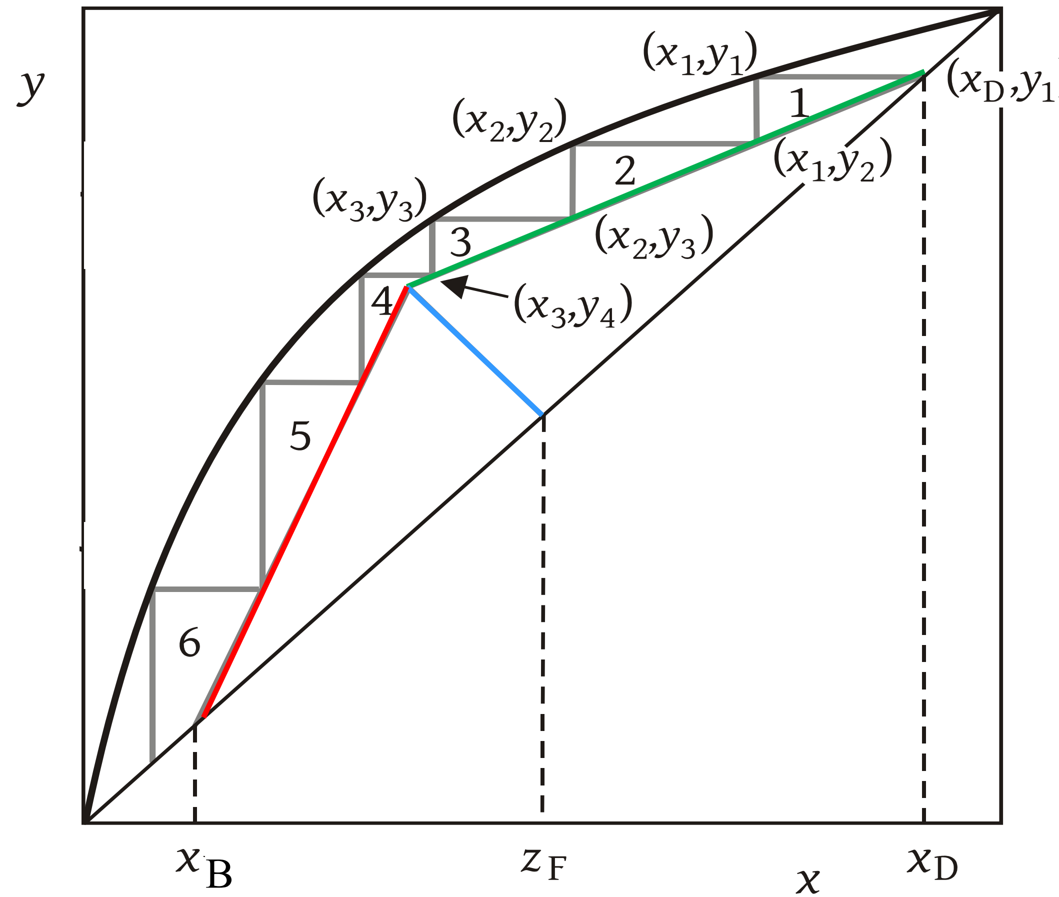


Determination of the number of equilibrium stages





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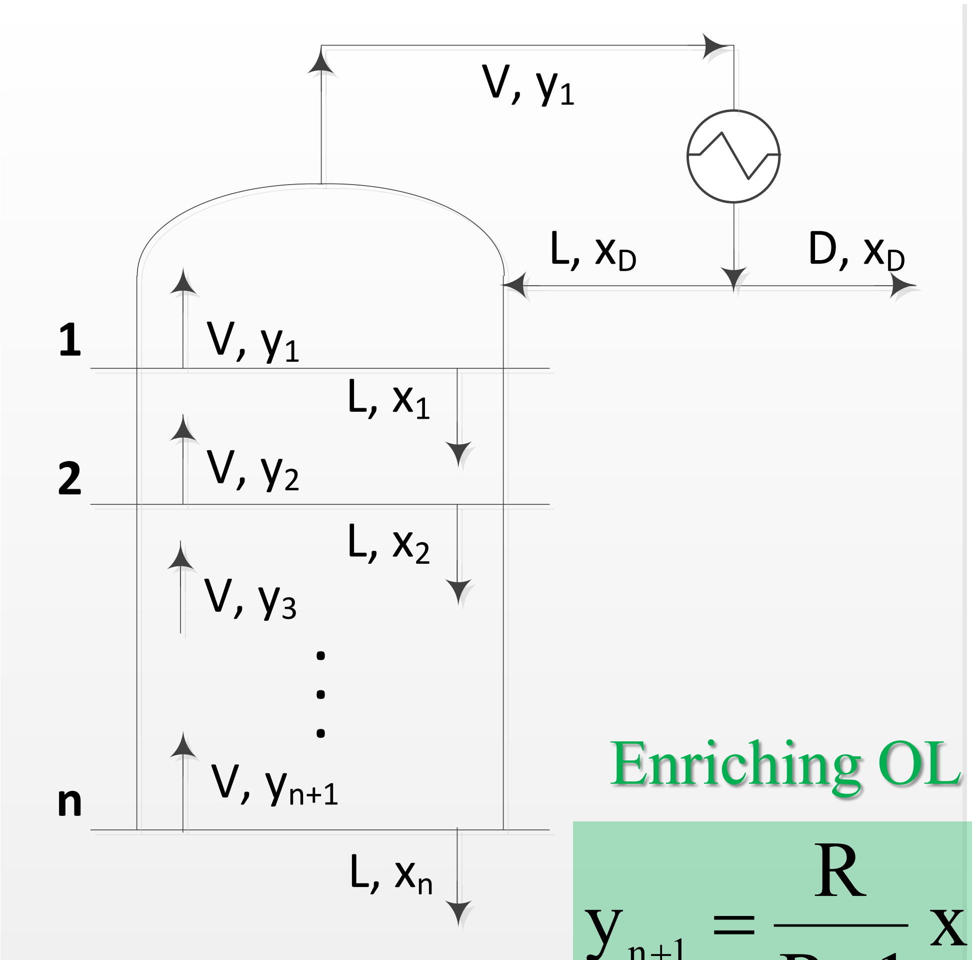
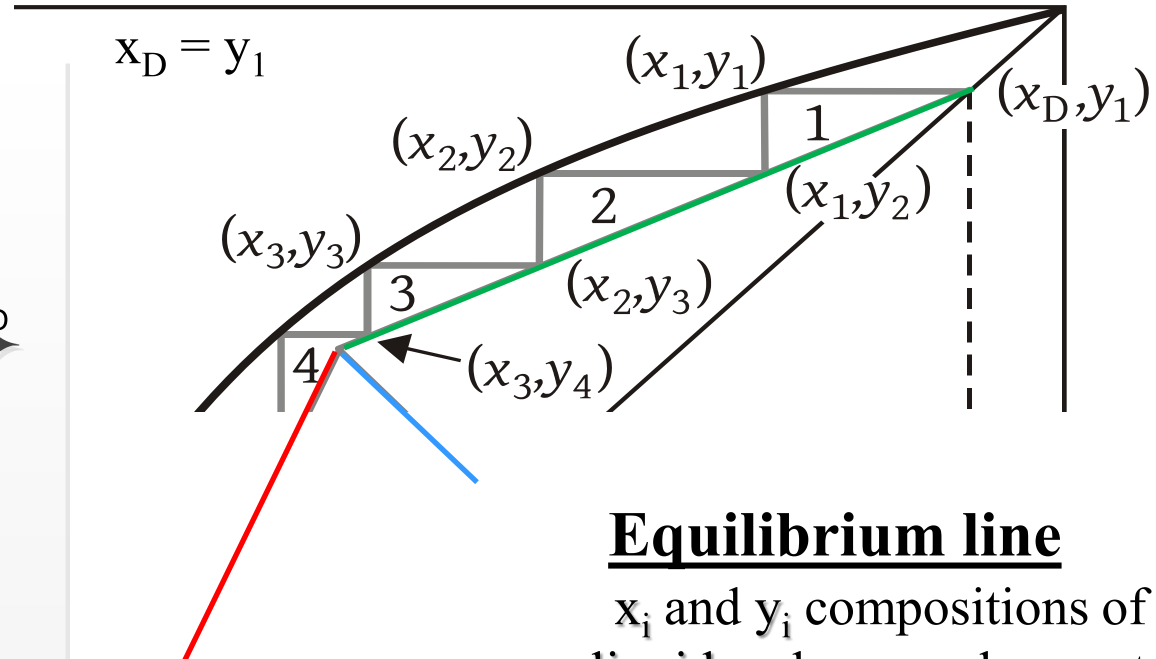




Enriching OL

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1}$$

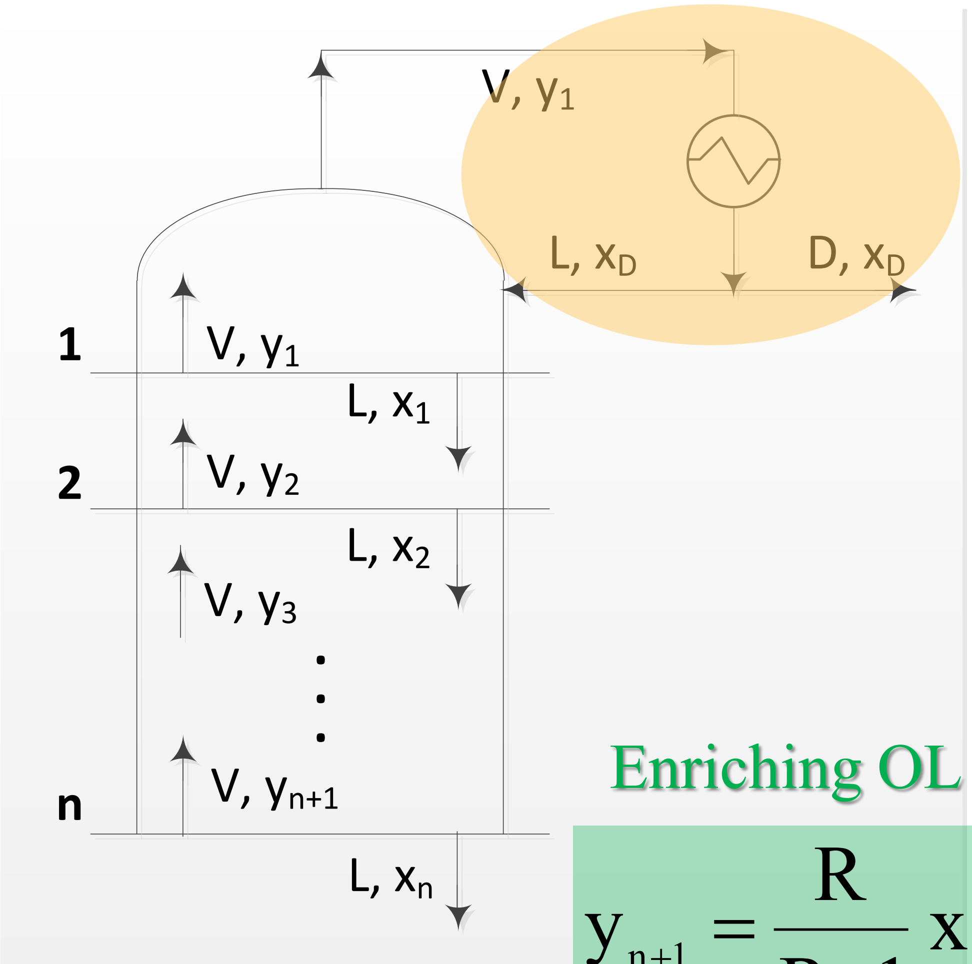
Equilibrium line

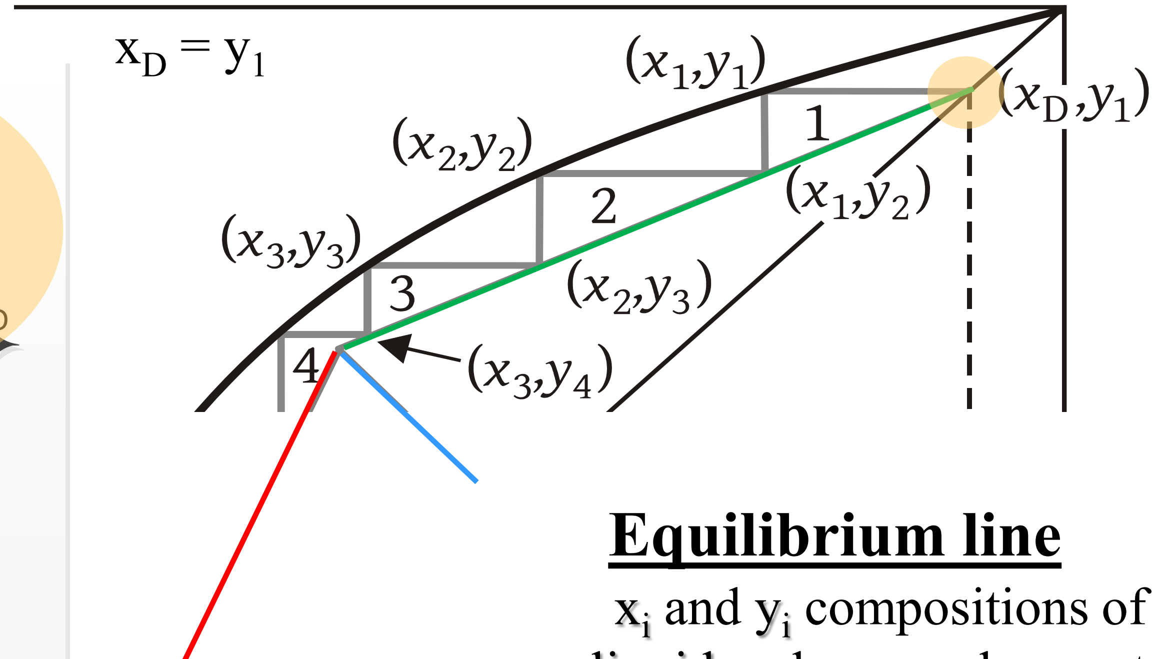
x_i and y_i compositions of liquid and vapor phases at stage *i* at equilibrium

Operating line

x_n and y_{n+1} compositions of liquid and vapor phases in contact with each other

Determination of the number of equilibrium stages





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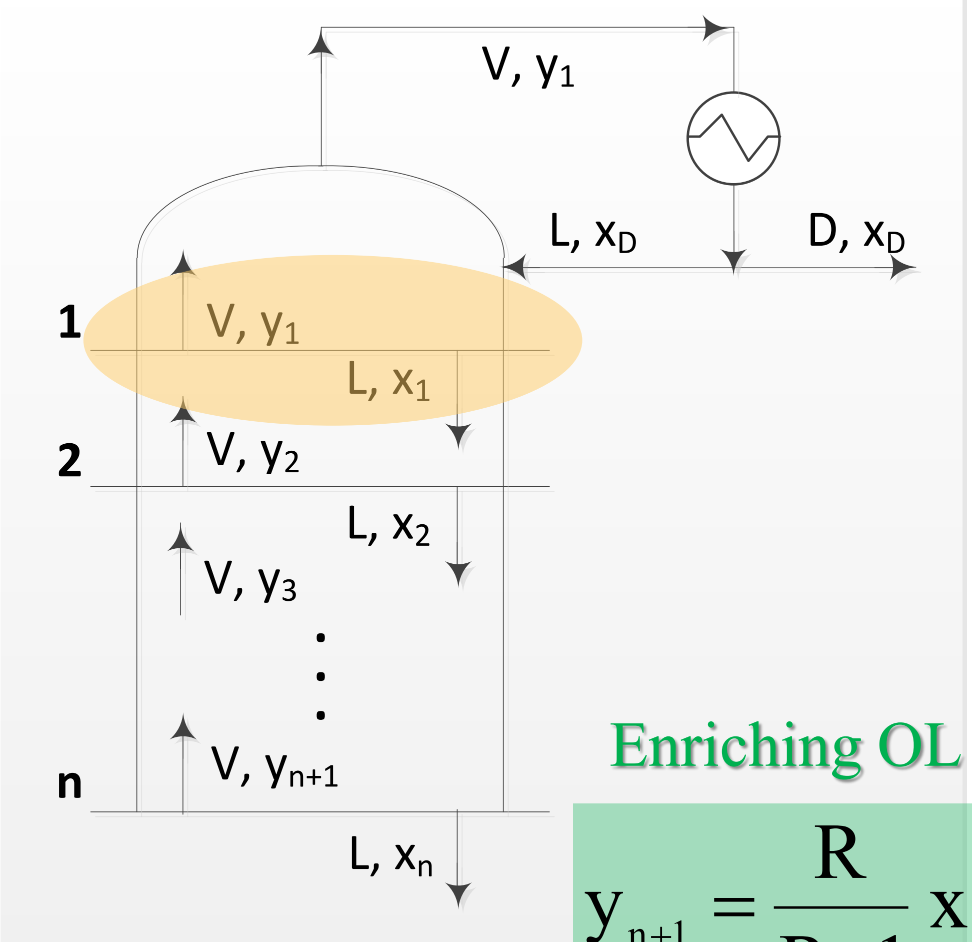

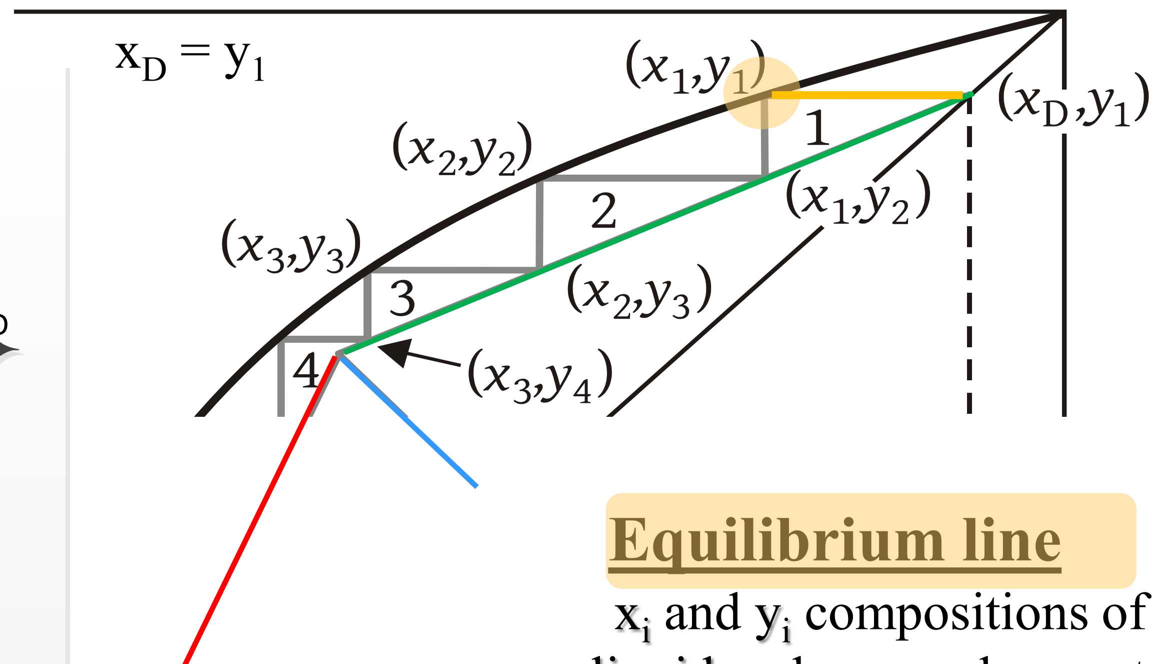

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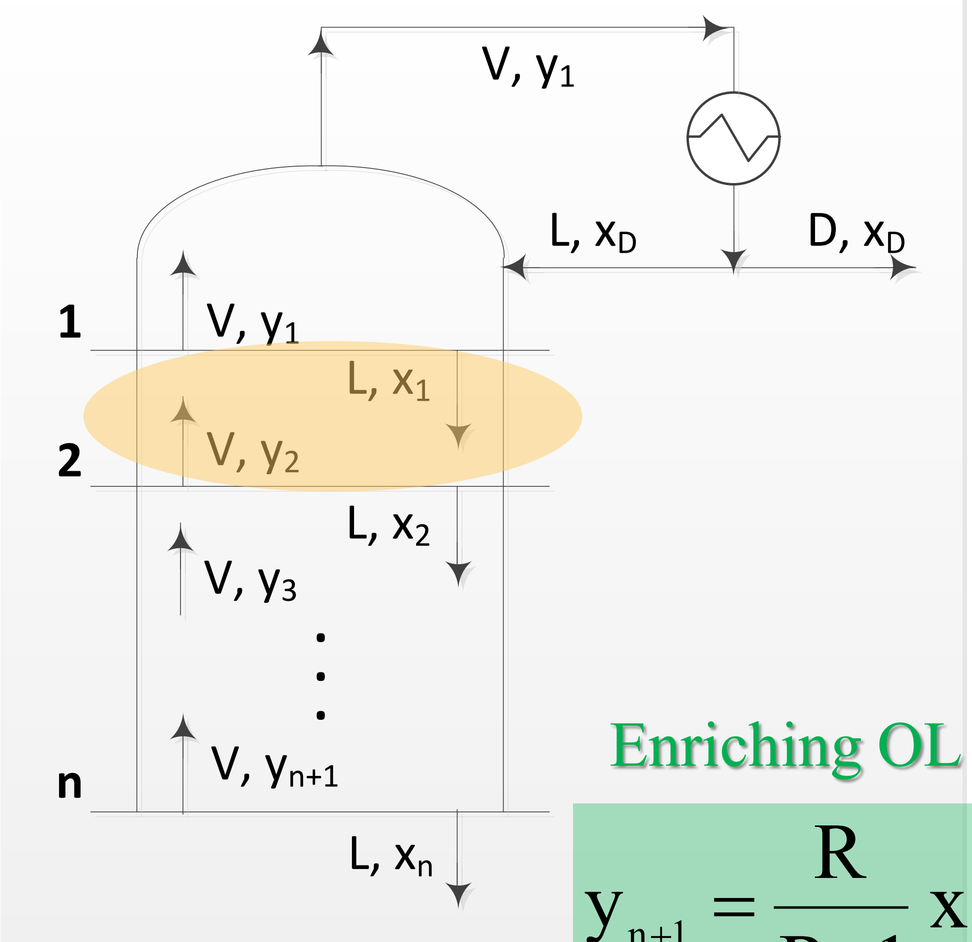

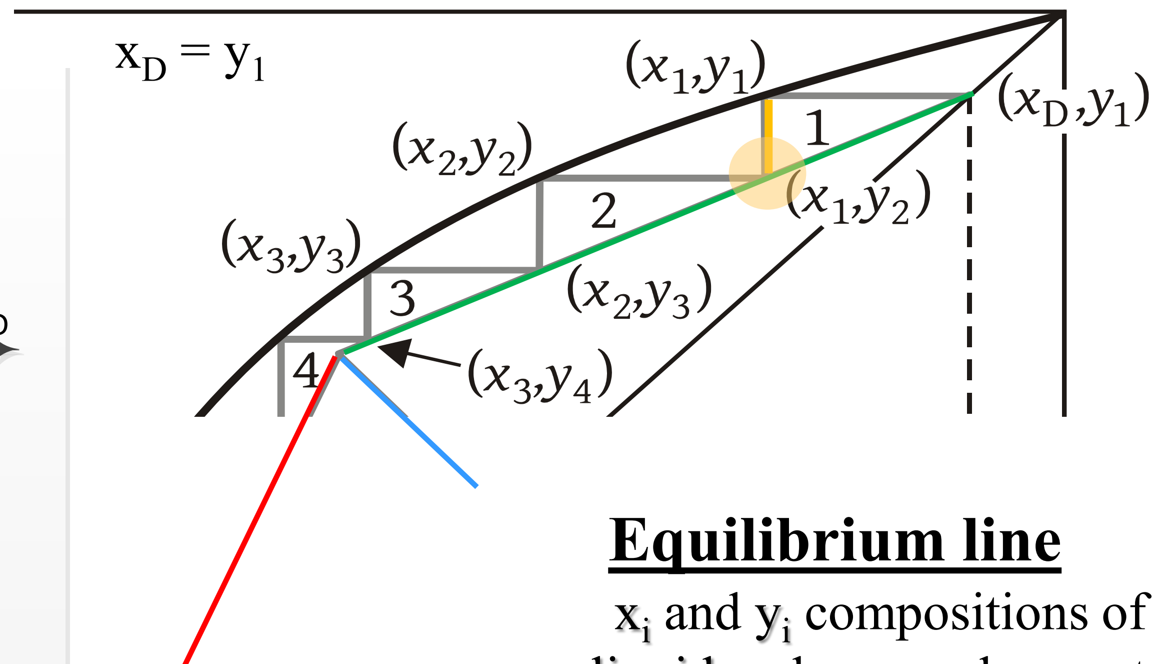

Equilibrium line

x_i and y_i compositions of liquid and vapor phases at <u>stage *i*</u> at equilibrium

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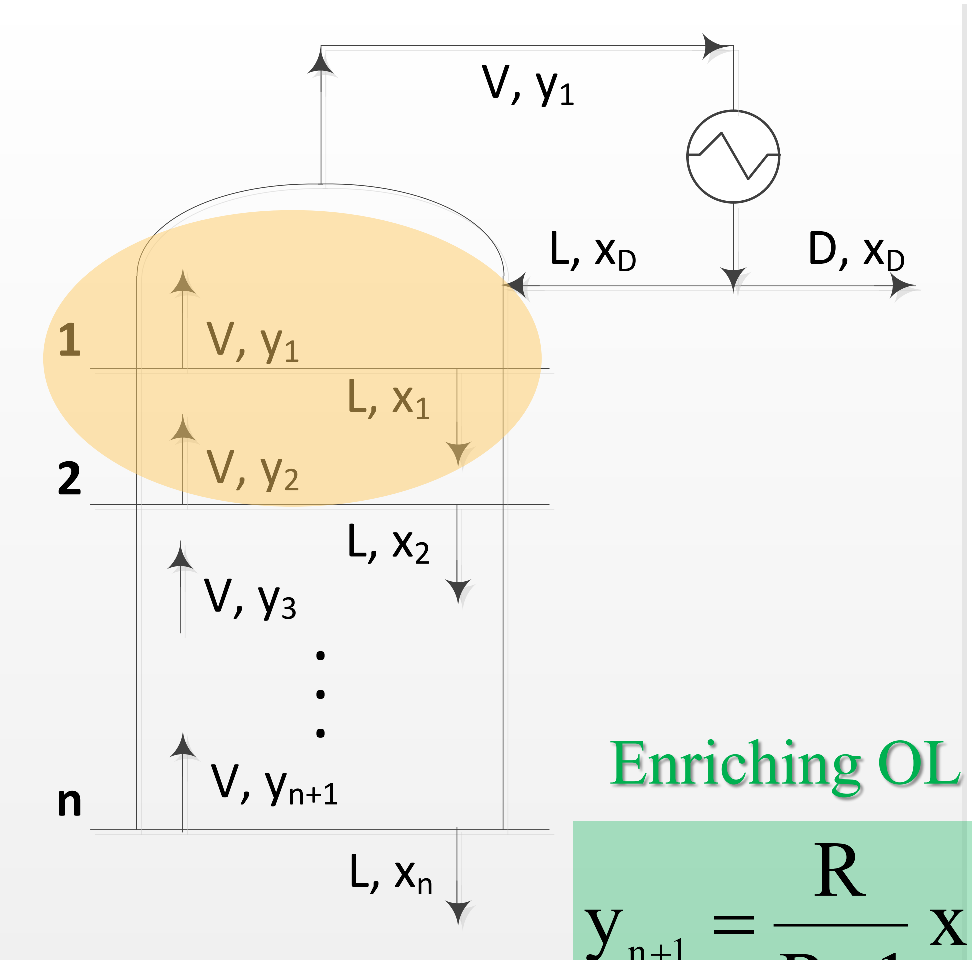
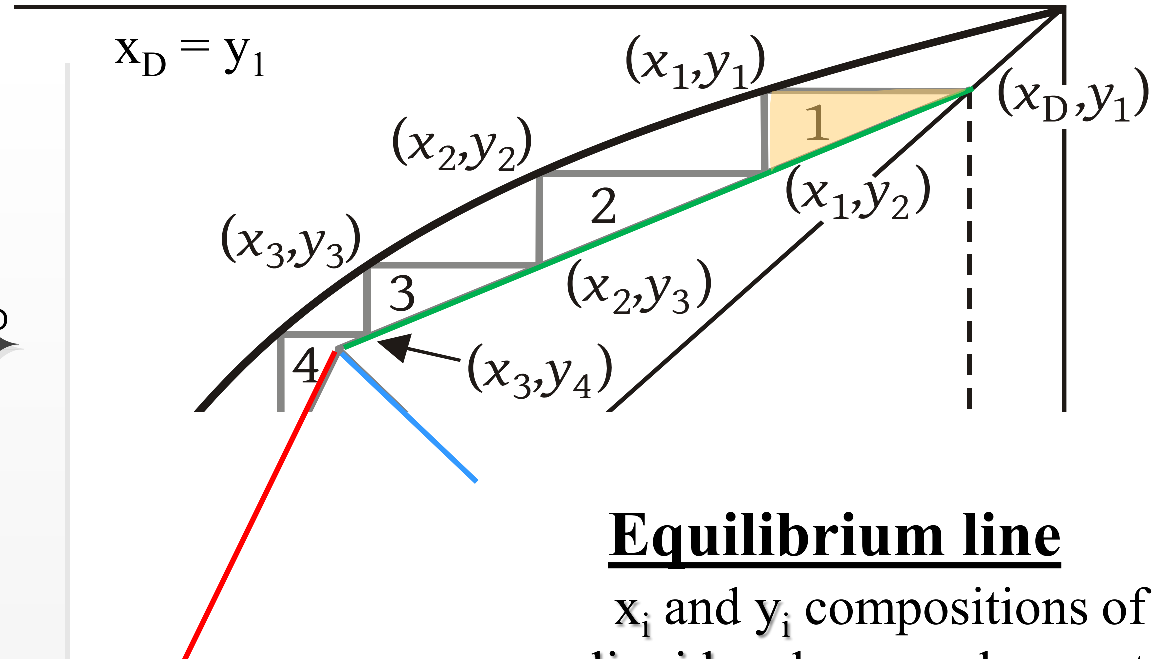




Enriching OL

$$y_{n+1} = \frac{R}{R+1}x_n + \frac{x_D}{R+1}$$

<u>Equilibrium line</u>

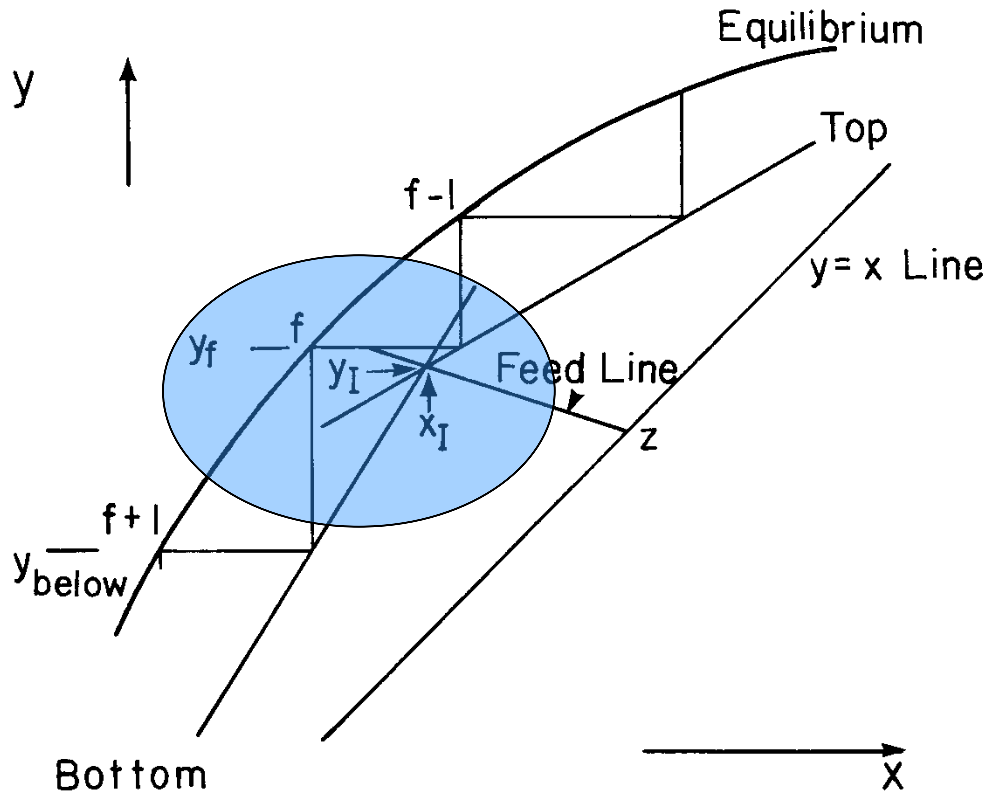
x_i and y_i compositions of liquid and vapor phases at <u>stage *i*</u> at equilibrium

<u>Operating line</u>

x_n and y_{n+1} compositions of liquid and vapor phases in contact with each other

Optimal location of feed stage

The McCabe-Thiele method show that optimal position of the feed stage gives the smallest (optimal) number of total equilibrium stage



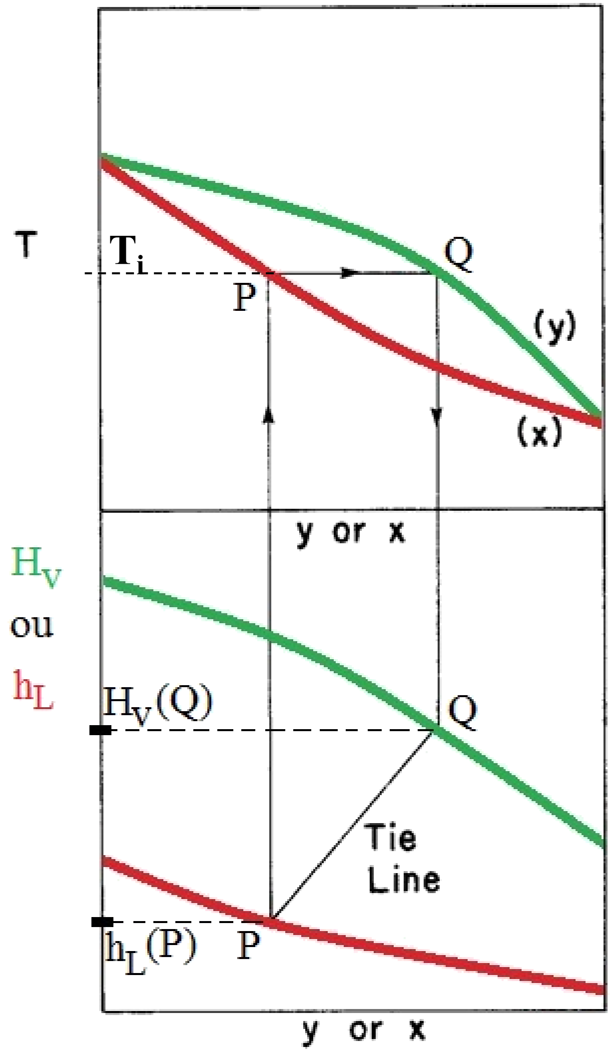
Composition (x,y) – Enthalpy ($\hat{h}$,$\hat{H}$) diagram

$\hat{H}_V$: Enthalpy of vapor phase

$\hat{h}_L$: Enthalpy of liquid phase

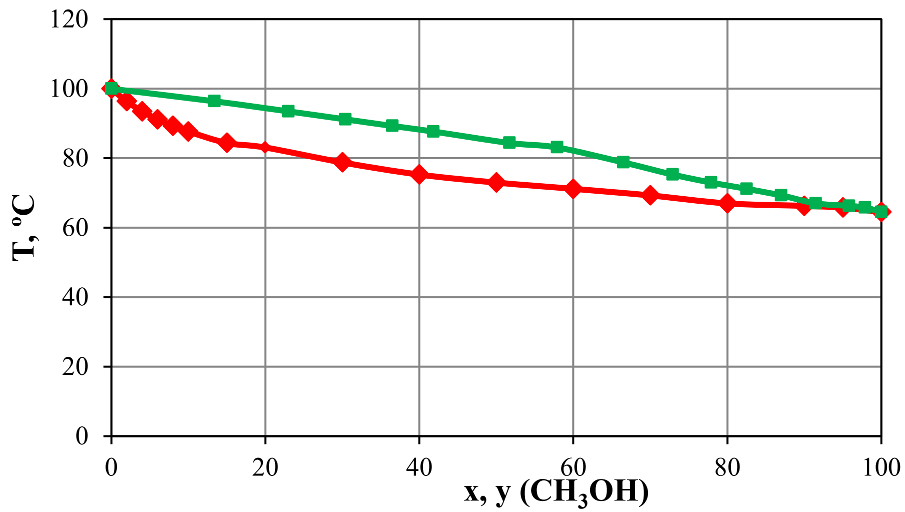
$\hat{H}_V > \hat{h}_L$!

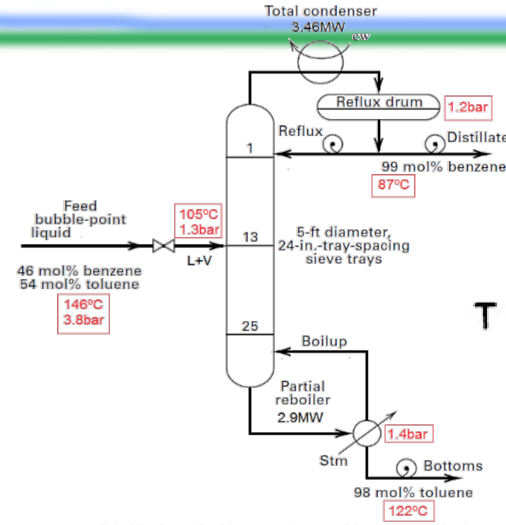
Enthalpy of vaporizarion depends on composition!



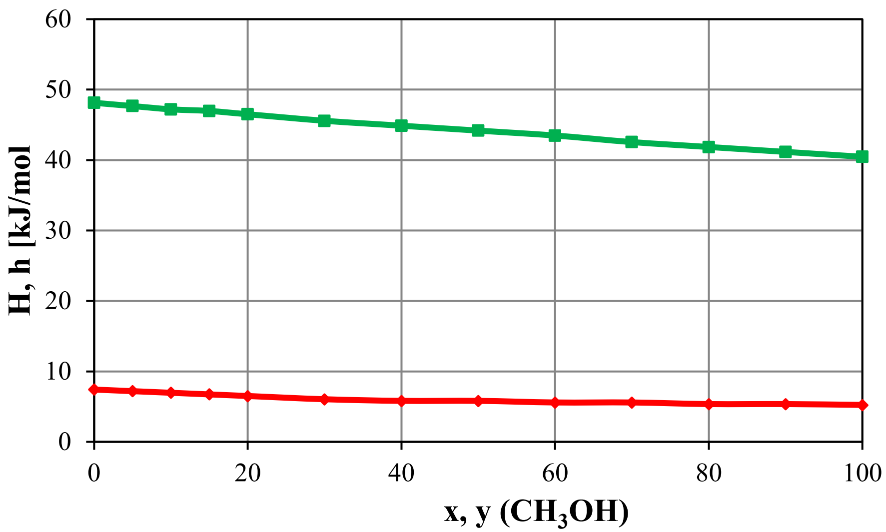
$$\hat{H}_V(Q) - \hat{h}_L(P) = \Delta\hat{H}_{vaporization|T_i}$$

Enthalpy - composition diagram: Methanol + Water



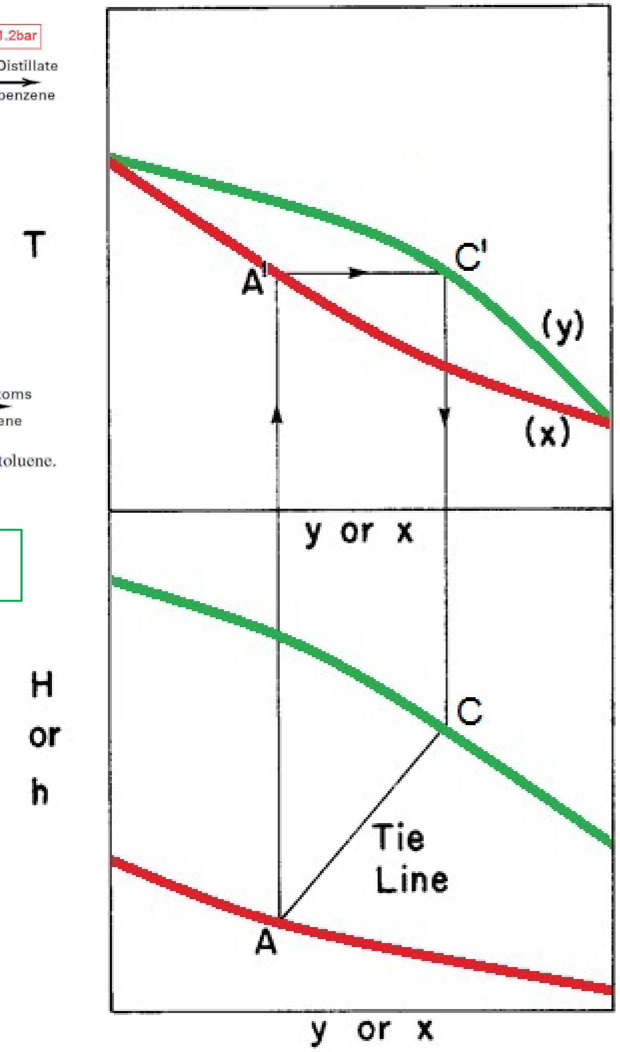


Distillation of a binary mixture of benzene and toluene.



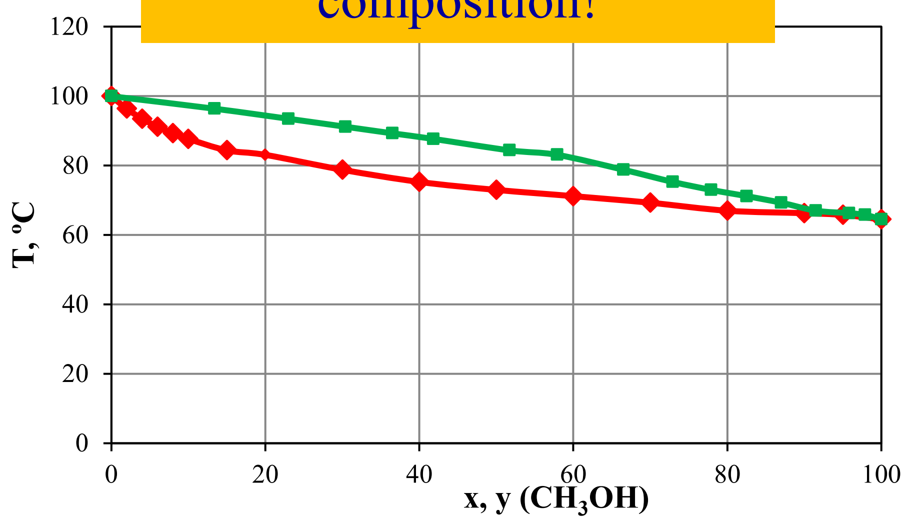
$\Delta H_{vap} = H_{vapor} - h_{líquid}$

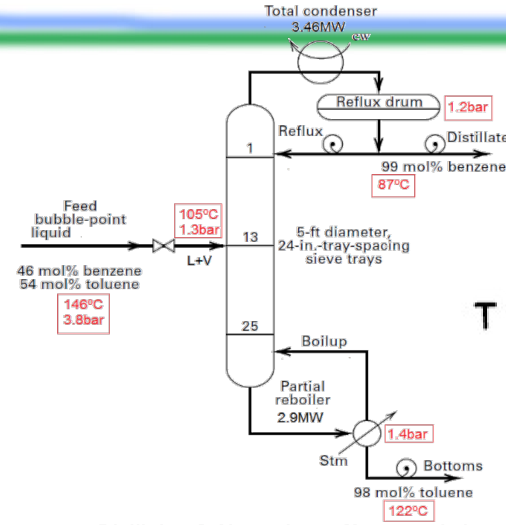
For each mole of liquid vaporized, a mole of vapor is condensed



En... on diagram: Methanol + Water

☛ For this system ΔH_{vap} is reasonably independent of composition!





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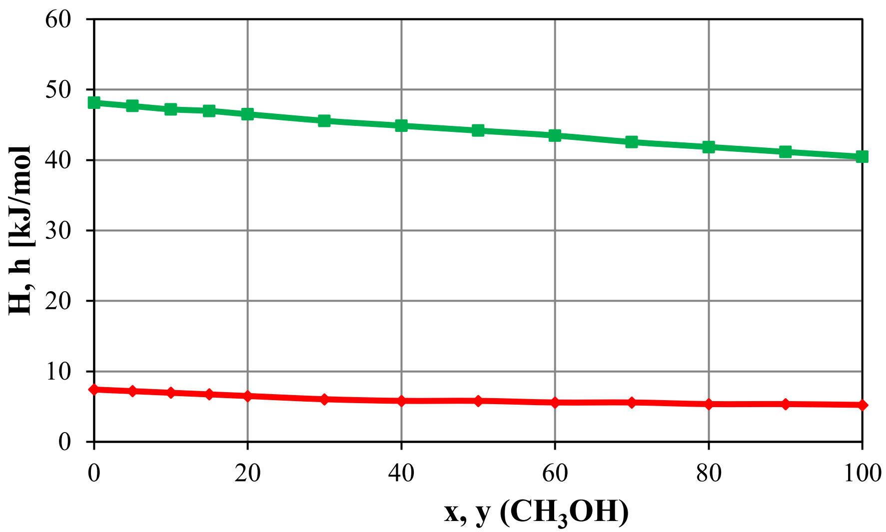

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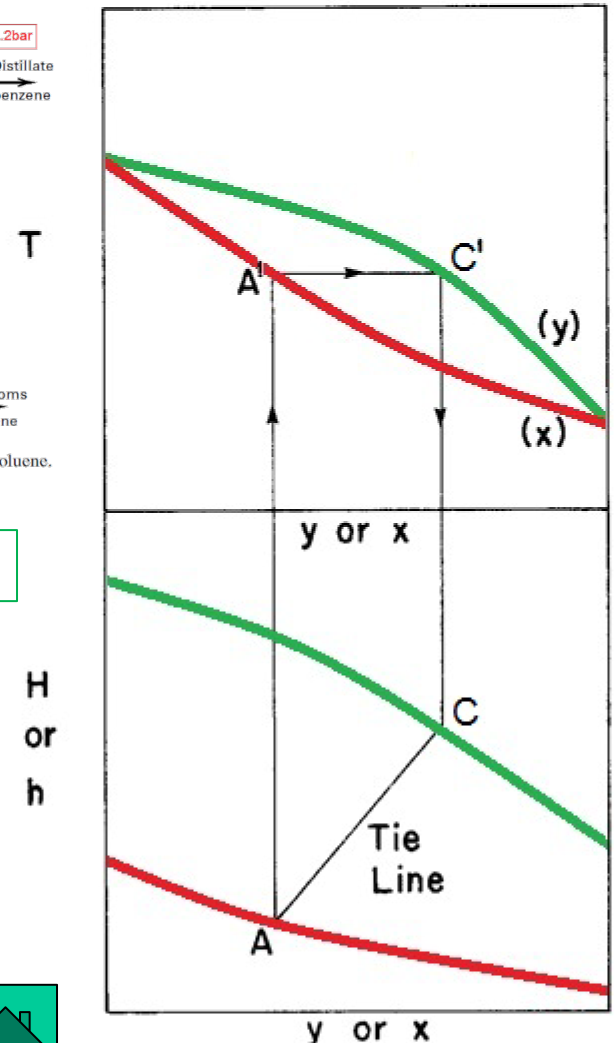


Examples

System Benzene + Toluene

ΔH_{vap} (Benzene) = 30.765 kJ/mol (80.1ºC) = 393.9 kJ/kg

(M = 78 g/mol)

ΔH_{vap} (Toluene) = 37.47 kJ/mol (110.6ºC) = 406.7 kJ/kg

(M = 92 g/mol)

System Methanol + Water

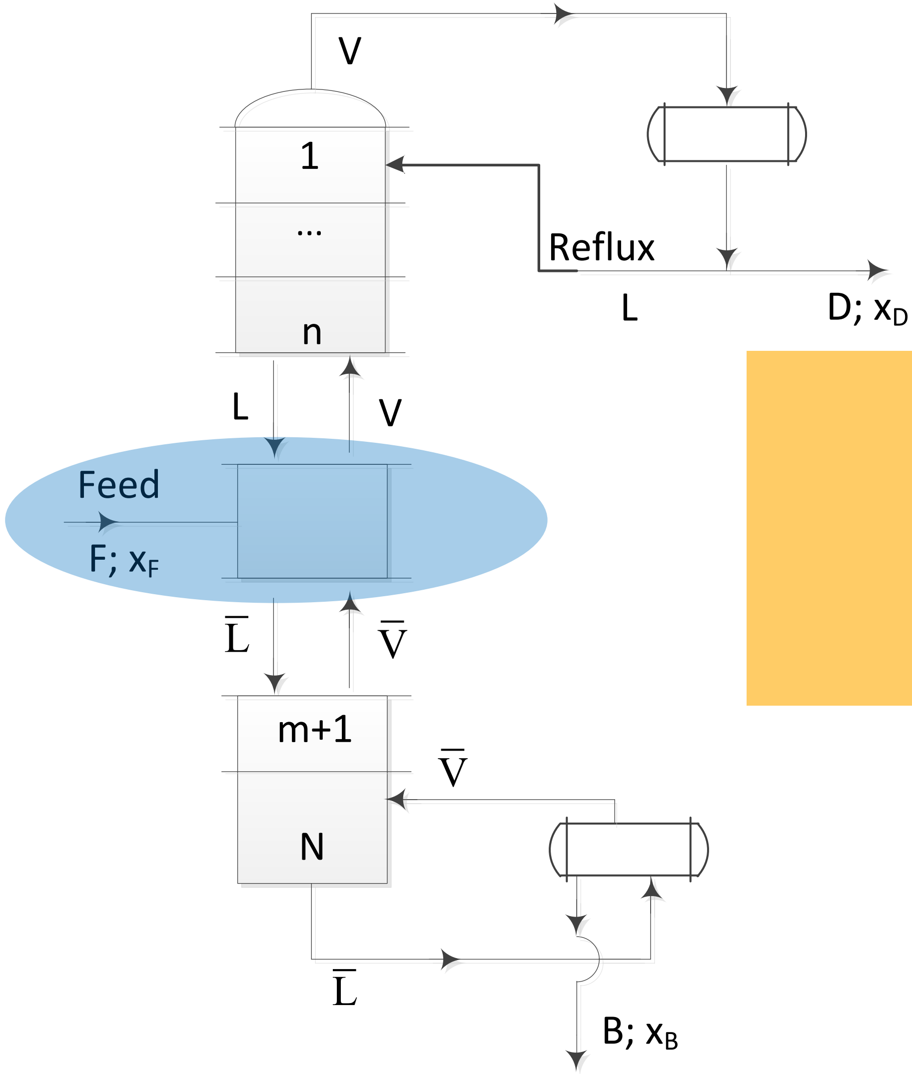
ΔH_{vap} (methanol) = 35.27 kJ/mol (64.7ºC) = 1100.8 kJ/kg

(M = 32 g/mol)

ΔH_{vap} (H_2O) = 40.66 kJ/mol (100ºC) = 2258.9 kJ/kg

(M = 18 g/mol)

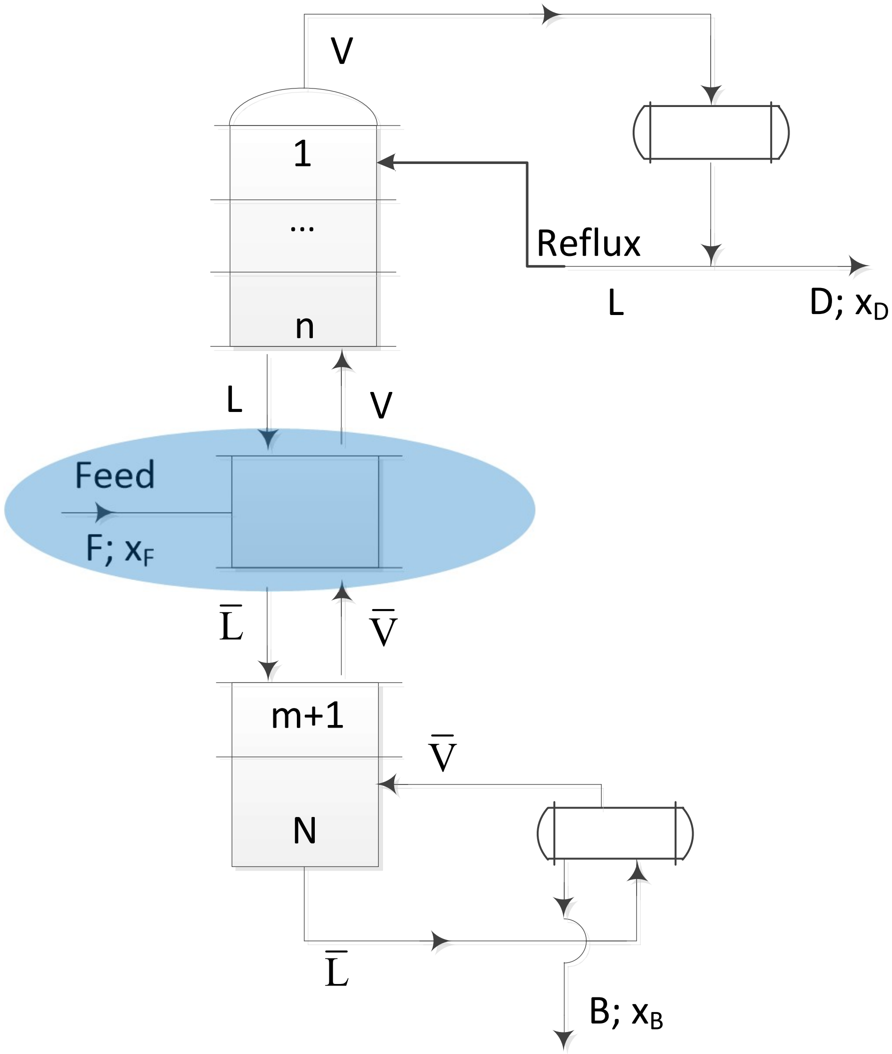
Operating line of Feed



DEDUCTION OF THE FEED

OPERATING LINE

Operating line of Feed

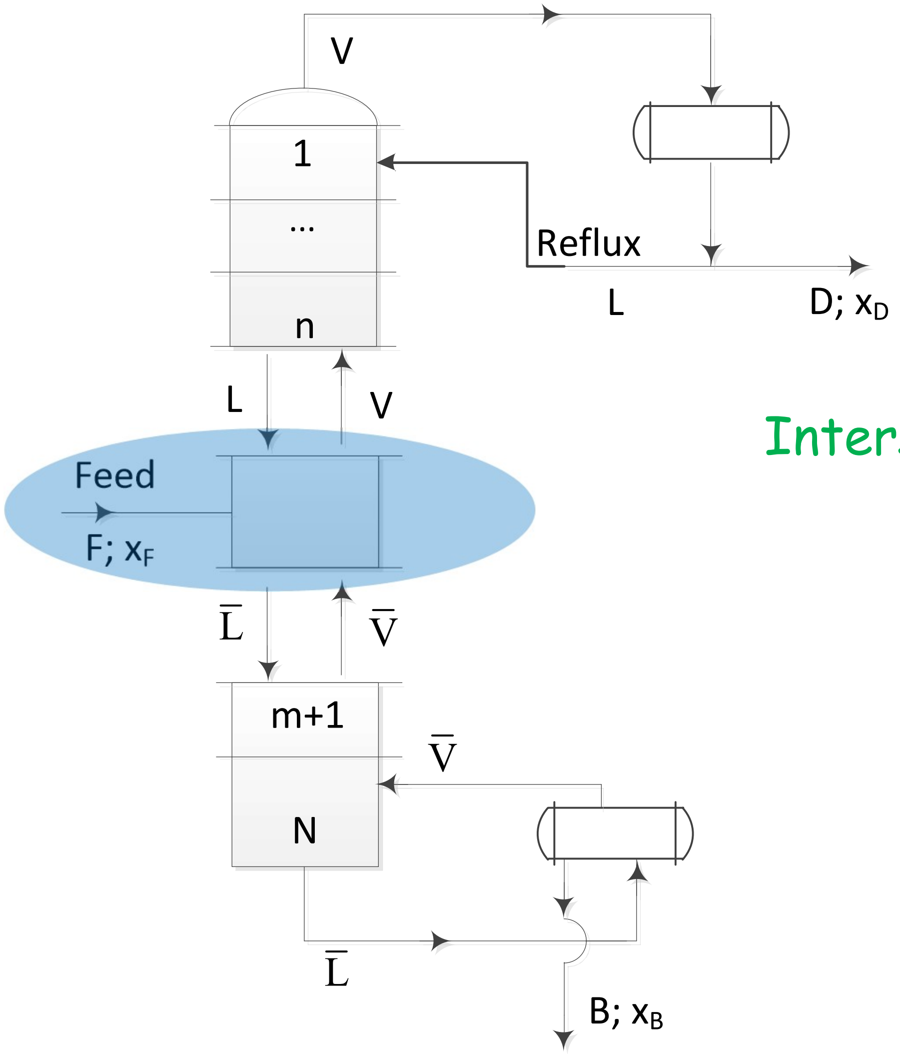


From former OL's

$$\begin{cases} y_{n+1} = \dfrac{L}{V}x_n + \dfrac{Dx_D}{V} \\ y_{m+1} = \dfrac{\bar{L}}{\bar{V}}x_m - \dfrac{Bx_B}{\bar{V}} \end{cases}$$

$$\begin{cases} Vy_{n+1} = Lx_n + Dx_D \\ \bar{V}y_{m+1} = \bar{L}x_m - Bx_B \end{cases}$$

Operating line of Feed



$$\begin{cases} V y_{n+1} = L x_n + D x_D \\ \bar{V} y_{m+1} = \bar{L} x_m - B x_B \end{cases}$$

Intersection of enriching and Stripping OL's

$$\boxed{y_{n+1} = y_{m+1} = \boldsymbol{y_i} \quad ; \quad x_n = x_m = \boldsymbol{x_i}}$$

$$\begin{cases} V y_i = L x_i + D x_D \\ \bar{V} y_i = \bar{L} x_i - B x_B \end{cases}$$

Operating line of Feed

Subtracting the equations

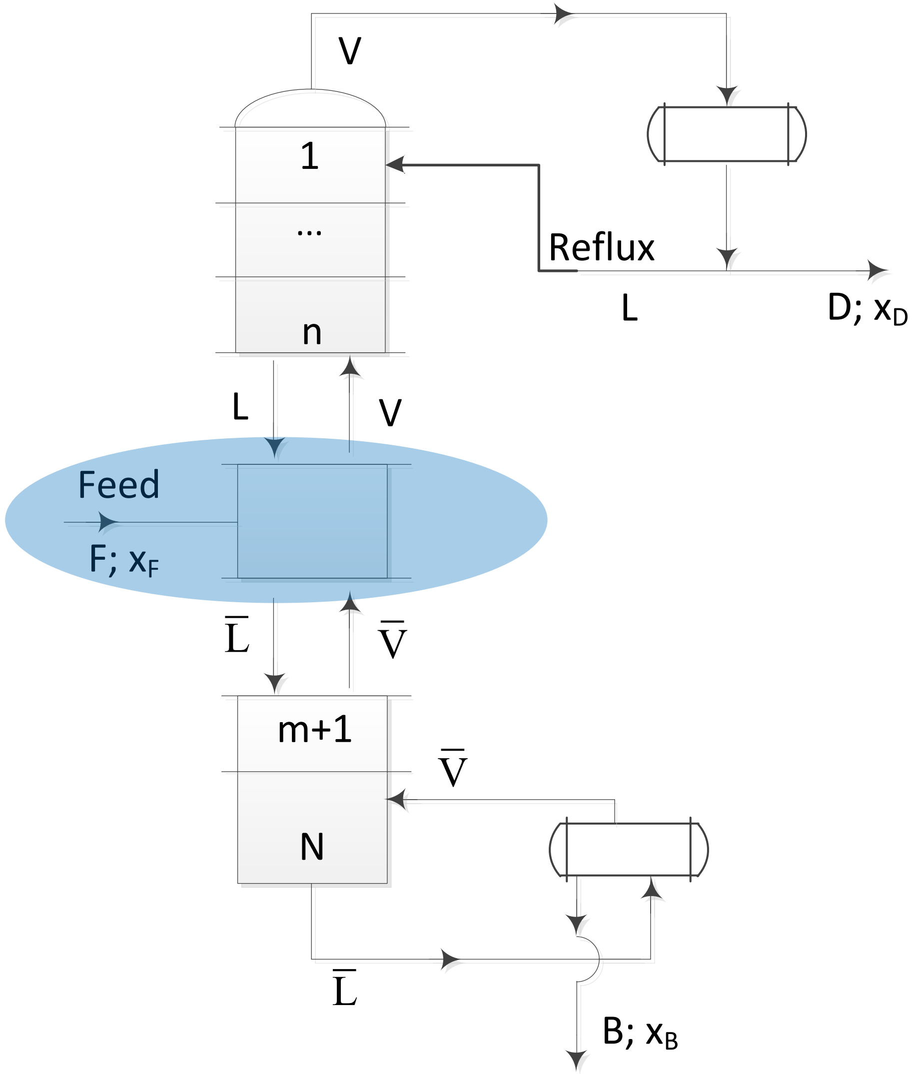
$$\begin{cases} Vy_i = Lx_i + Dx_D \\ \\ \bar{V}y_i = \bar{L}x_i - Bx_B \end{cases}$$

=> $$\left(\bar{V} - V\right) y_i = \left(\bar{L} - L\right) x_i - Dx_D - Bx_B$$

$$\Big\Downarrow \quad (Fx_F = Bx_B + Dx_D)$$

$$\left(\bar{V} - V\right) y_i = \left(\bar{L} - L\right) x_i - Fx_F$$

Operating line of Feed



$$\boxed{i = \frac{\bar{L} - L}{F}}$$

$$\boxed{\bar{L} - L = iF}$$

Material balance to the feed plate:

$$L + \bar{V} + F = V + \bar{L}$$

$$\boxed{\bar{V} - V = (i - 1) F}$$