Binary Column distillation: internal stage by stage balances

Maurizio Fermeglia

Maurizio.fermeglia@units.it

Department of Engineering & Architecture

University of Trieste
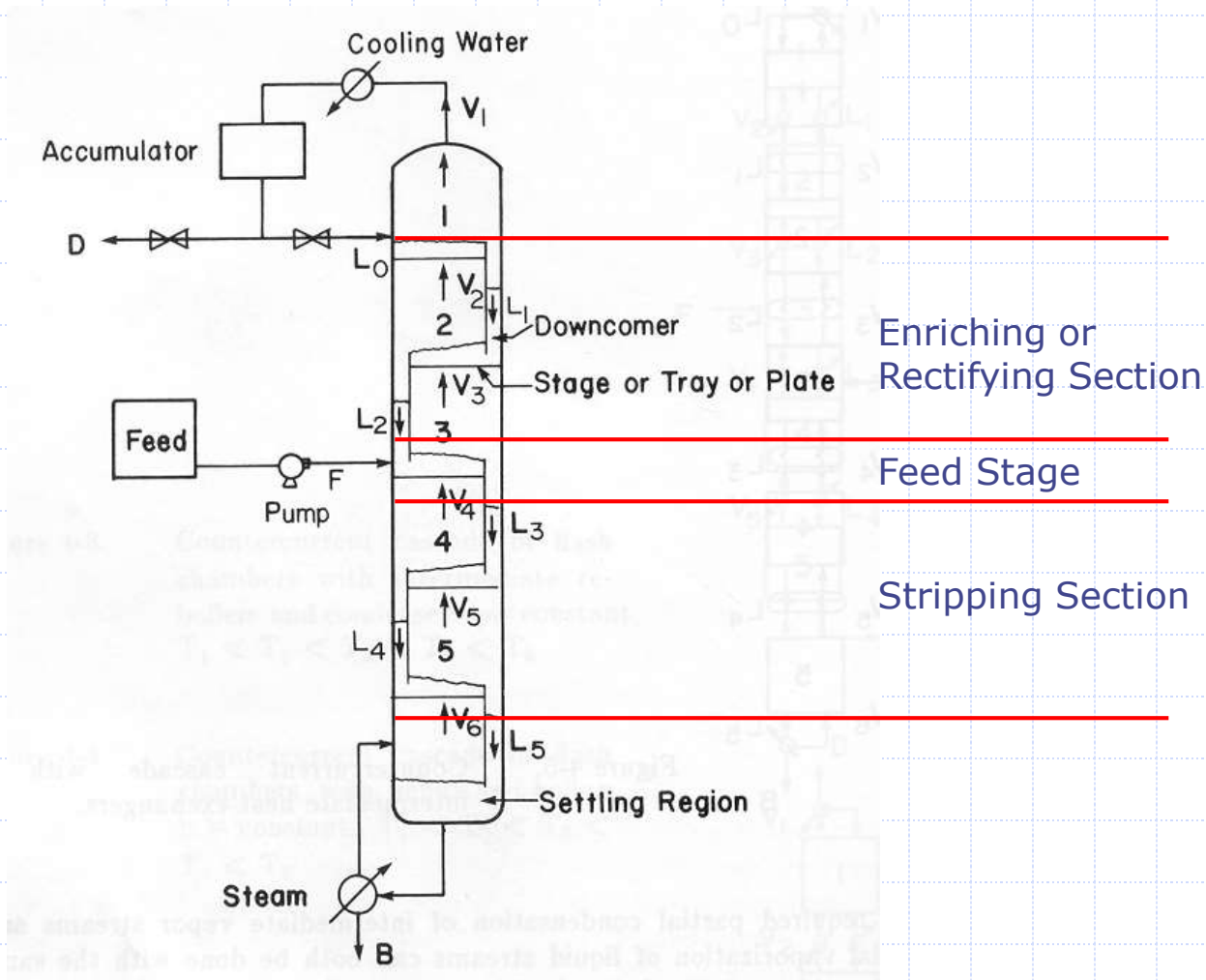
Agenda

◆ Internal balances

◆ Binary stage by stage solution methods

   ▪ Mass and Energy balances enriching session with total condenser
   ▪ Mass and Energy balances stripping session with partial reboiler
   ▪ Mass and Energy balances at the feed stage

◆ Lewis method: constant molar overflow

Internal stage by stage balances

◆ Stage by stage balances starting from the top

◆ Using the output of the first balance as input to the second balance … and so on.

◆ The procedure assumes that

- Each stage is at equilibrium
- (but non equilibrium stage may be dealt with)

◆ Different equations are developed for enriching and stripping sections of the column

Distillation column: enriching and stripping sections

Cooling Water

V_1

Accumulator

D

L_0

V_2 L_1 Downcomer

2

V_3 Stage or Tray or Plate

Feed

L_2 3

F

Pump

V_4

4 L_3

V_5

L_4 5

V_6 L_5

Settling Region

Steam

B

Enriching or Rectifying Section

Feed Stage

Stripping Section

Mass and Energy Balances – Enriching Section and total Condenser

- ◆ Total mass balance
$$V_2 = L_1 + D$$

- ◆ Component mass balance
$$V_2 y_2 = L_1 x_1 + D x_D$$

- ◆ For a well insulated adiabatic column ($Q_{column}=0$), the energy balance:
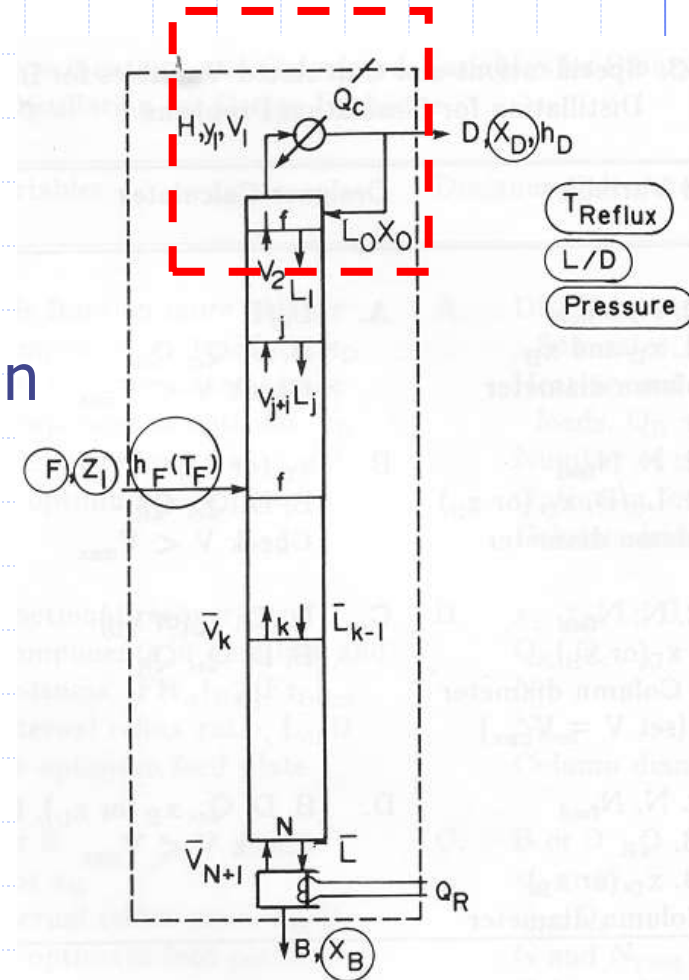$$V_2 H_2 + Q_C = L_1 h_1 + D h_D$$

- ◆ Other three equations are needed
  - ▪ H_1 (x_1); H_2 (y_2) and $x_1(y_1)$

- ◆ The problem may be solved
  - ▪ Distillate is fixed: D, x_D, h_D
  - ▪ Unknowns: L_1, V_2, x_1, y_2, H_2, h_1

Mass and Energy Balances – Enriching Section and total Condenser

◆ For the second stage (same equations)

$$V_3 = L_2 + D$$
$$V_3 y_3 = L_2 x_2 + D x_D$$
$$V_3 H_3 + Q_C = L_2 h_2 + D h_D$$
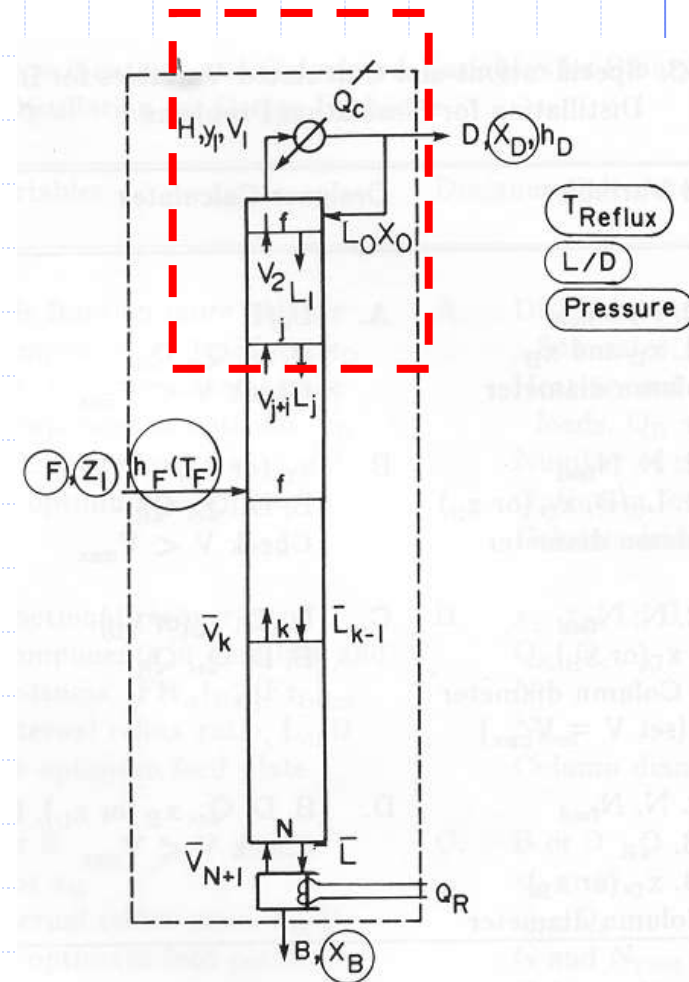
$H_2 (x_2); H_3 (y_3)$ and $x_2(y_2)$

◆ For the j stage

$$V_{j+1} = L_j + D$$
$$V_{j+1} y_{j+1} = L_j x_j + D x_D$$
$$V_{j+1} H_{j+1} + Q_C = L_j h_j + D h_D$$

$H_j (x_j); H_{j+1} (y_{j+1})$ and $x_j(y_j)$

Go on up to the feed stage

Mass and Energy Balances – Stripping Section and Partial Reboiler

- The previous mass and energy balances apply only to the **enriching section**.

- At some point down the column, we will have a feed to one of the equilibrium stages – **the feed stage.**
  - At this feed stage, the enriching section of the column ends.

- At **the feed stage** we have the introduction of **additional liquid and/or vapor** depending upon the nature of the feed stream.
  - Liquid from the feed stream will flow down the column and vapor from the feed stream will rise up the column.
  - Consequently, **the ratio of vapor to liquid in the enriching section above the feed stage is generally different than that in the stripping section** below the feed stage because of the feed between these two sections.

Mass and Energy Balances –
Stripping Section and Partial Reboiler

◆ While we have designated the vapor and liquid streams in the enriching section as L and V, we will designate the vapor and liquid streams in the stripping section using an "underline" or $\underline{V}$ and $\underline{L}$ to delineate them from those in the enriching section.

- L/V < 1 in the enriching section.
- Conversely, $\underline{L}/\underline{V}$ > 1 in the stripping section.

◆ Let's look at the mass and energy balances for the stripping section of the column with a partial reboiler.
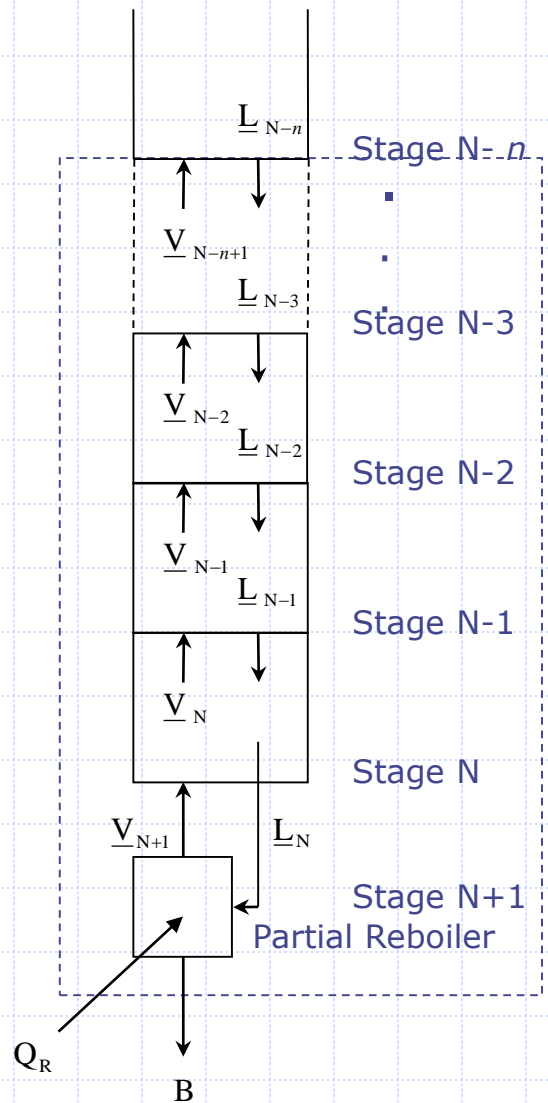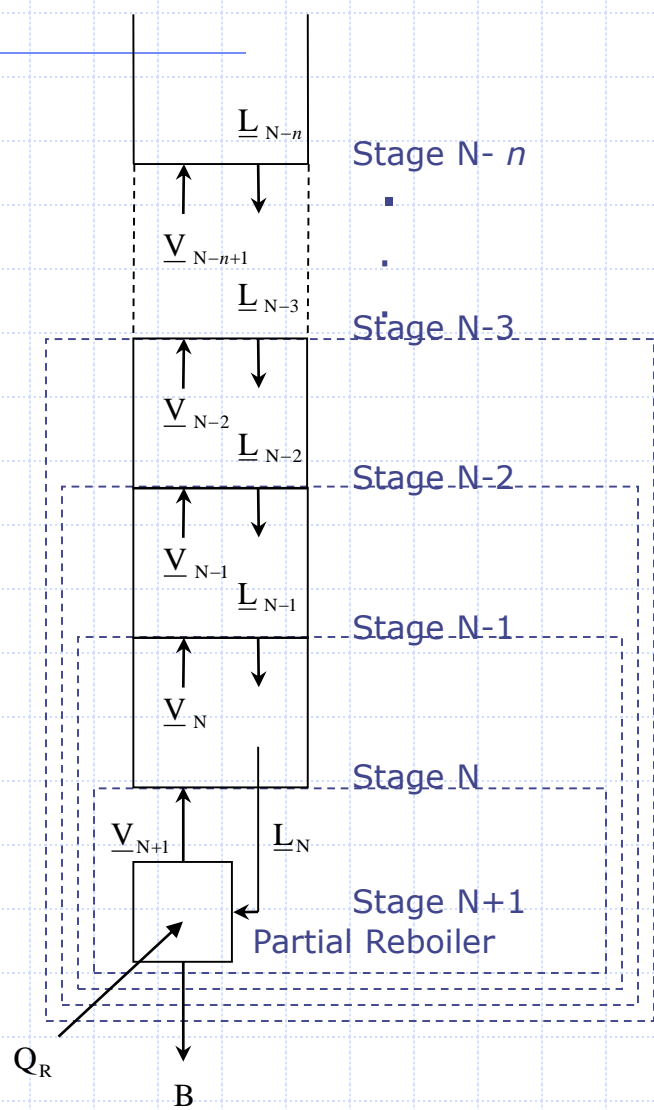
Mass and Energy Balances – Stripping Section and Partial Reboiler

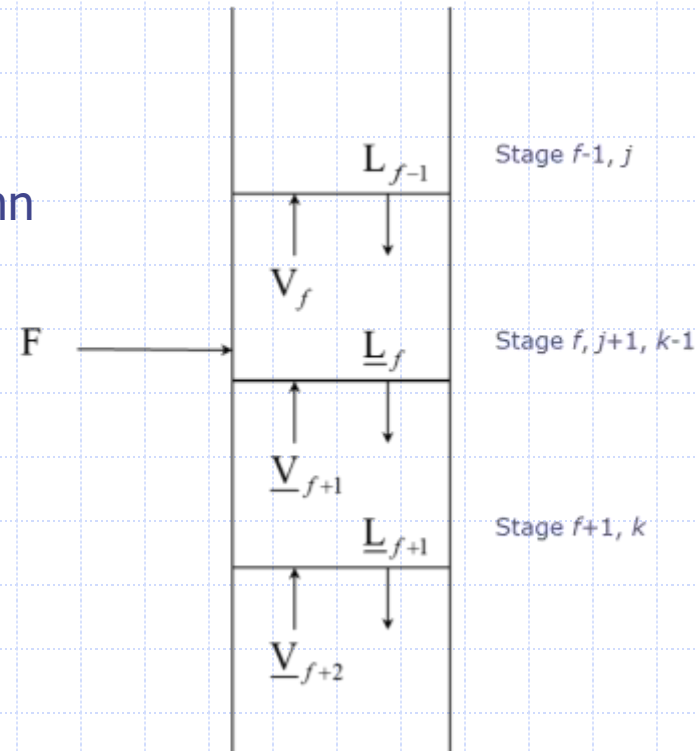| Total Mass Balance	Component Mass Balance	Energy Balance	Stage (Partial Reboiler)
$\underline{V}_{N+1} = \underline{L}_N - B$	$\underline{V}_{N+1} y_{N+1} = \underline{L}_N x_N - B x_B$	$\underline{V}_{N+1} H_{N+1} = \underline{L}_N h_N - B x_B + Q_R$	N+1
$\underline{V}_N = \underline{L}_{N-1} - B$	$\underline{V}_N y_N = \underline{L}_{N-1} x_{N-1} - B x_B$	$\underline{V}_N H_N = \underline{L}_{N-1} h_{N-1} - B x_B + Q_R$	N
$\underline{V}_{N-1} = \underline{L}_{N-2} - B$	$\underline{V}_{N-1} y_{N-1} = \underline{L}_{N-2} x_{N-2} - B x_B$	$\underline{V}_{N-1} H_{N-1} = \underline{L}_{N-2} h_{N-2} - B x_B + Q_R$	N-1
$\underline{V}_{N-2} = \underline{L}_{N-3} - B$	$\underline{V}_{N-2} y_{N-2} = \underline{L}_{N-3} x_{N-3} - B x_B$	$\underline{V}_{N-2} H_{N-2} = \underline{L}_{N-3} h_{N-3} - B x_B + Q_R$	N-2
.	.	.	.
.	.	.	.
.	.	.	.
$\underline{V}_{N-n+1} = \underline{L}_{N-n} - B$	.	.	.
	.	.	.
	$\underline{V}_{N-n+1} y_{N-n+1} = \underline{L}_{N-n} x_{N-n} - B x_B$	.	.
		.	.
		$\underline{V}_{N-n+1} H_{N-n+1} = \underline{L}_{N-n} h_{N-n} - B x_B + Q_R$	N- n

$$n = 0, 1, 2, \dots$$

Feed Stage

◆ **At the feed stage.**

- The phase and temperature of the feed affects the vapor and liquid flow rates in the column.
- If the feed is a liquid, then $\underline{L} > L$.
- If the feed is a vapor, then $V > \underline{V}$.
- The feed may also be flashed into the column yielding both vapor and liquid – remember flash distillation!

◆ **Remember that**

- $L/V < 1$ in the enriching section
- $\underline{L}/\underline{V} > 1$ in the stripping section

◆ **Let's look at the feed stream and how we handle it...**

Mass and Energy Balances – Feed Stage

Total Mass Balance

$$F + L_{f-1} + \underline{V}_{f+1} = \underline{L}_f + V_f$$

Component Mass Balance

$$Fz_F + L_{f-1}x_{f-1} + \underline{V}_{f+1}y_{f+1} = \underline{L}_f x_f + V_f y_f$$

Energy Balance

$$Fh_F + L_{f-1}h_{f-1} + \underline{V}_{f+1}H_{f+1} = \underline{L}_f h_f + V_f H_f$$

Sorel and Ponchon-Savarit methods of solution

- The challenge for any stage-by-stage solution method is to solve the three balance equations and the three equilibrium relationships simultaneously in an efficient manner.
- This problem was first solved by Sorel (1893), and graphical solutions of Sorel's method were developed independently by Ponchon (1921) and Savarit (1922).
  - These methods all solve the complete mass and energy balance and equilibrium relationships stage by stage.
- Starting at the top of the column we can find:
  - liquid composition, x_1, in equilibrium with the leaving vapor composition, y_1, and liquid enthalpy, h_1, is easily found from Eqs.
  - The remaining four Eqs. for stage 1 are coupled and must be solved simultaneously.
- Ponchon-Savarit method does this graphically.
- Sorel method uses a trial-and-error procedure on each stage.
  - The trial-and-error calculations on every stage of the Sorel method are obviously slow and laborious.

Historical Review of Calculation Methods

- **until 1970s:**
  - simplified, partially graphical design procedures for tray columns separating binary mixtures: Ponchon-Savarit (1921/22), McCabe-Thiele (1925)
  - approximate calculation methods for the solution of multicomponent, multistage sepa-ration problems (Shortcut methods): Fenske (1932), Gilliland (1940), Underwood (1946)
  - design of packed columns based on NTU/HTU concepts: Chilton, Colburn (1935)

- **in the present:**
  - complex mathematical matrix methods allow to find exact solutions of nonlinear equation systems: Wang-Henke (1966), Naphtali-Sandholm (1971)
  - commercial process simulation software allowing design and rating calculations of tray and packed columns operating at steady or unsteady state conditions (ASPEN®, CHEMCAD®)

Lewis method: constant molal overflow

◆ **Lewis** (1922) noted that in many cases the **molar vapor and liquid flow** rates in each section (a region between input and output ports) were constant.

- Related to the energy balance for an equilibrium stage and nearly constant heat of vaporization

◆ For the **enriching section**

- $L_1 = L_2 = \ldots = L_n = L$
- $V_1 = V_2 = \ldots = V_n = V$

◆ And the same for the **stripping section**

Lewis method: constant molal overflow

- ◆ For each additional column section there will be another set of equations for constant flow rates.
  - Valid if every time a mole of vapor is condensed a mole of liquid is vaporized.
- ◆ This will occur if:
  1. The column is adiabatic.
  2. The specific heat changes are small compared to latent heat changes.
  3. The heat of vaporization per mole, λ, is constant; that is, λ does not depend on concentration.
     - ◆ Condition 3 is the most important criterion. Lewis called this set of conditions *constant molal overflow* (CMO). Molal: m = moles solute / kilograms solvent
  4. An alternative to conditions 2 and 3 is that the saturated liquid and vapor lines on an enthalpy-composition diagram (in molar units) are parallel.

Lewis method: constant molal overflow

◆ For some systems, such as hydrocarbons, the latent heat of vaporization per kilogram is approximately constant.

  ▪ Then the mass flow rates are constant, and constant *mass* overflow should be used.
  ▪ The Lewis method assumes CMO is valid → energy balances are will be automatically satisfied.

◆ With CMO the 2 eq. can be combined:

$$V_{j+1} = Lj + D$$
$$V_{j+1}y_{j+1} = L_j x_j + D x_D$$

◆ Resulting in:

$$V_{j+1}y_{j+1} = L_j x_j + (V_{j+1} - L_j)x_D$$
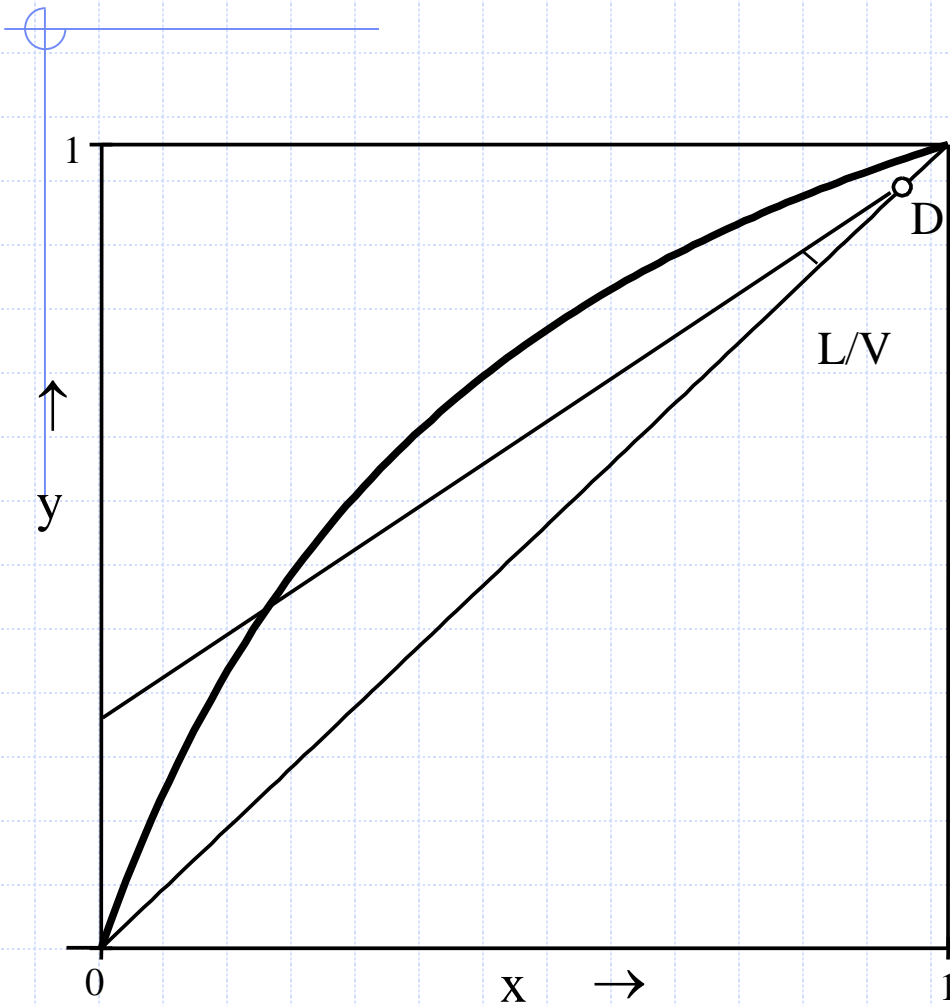
◆ Solving for y_{J+1}:

$$y_{j+1} = \frac{L_j}{V_{j+1}} x_j + \left(1 - \frac{L_j}{V_{j+1}}\right) x_D$$

◆ Since CMO:

$$y_{j+1} = \frac{L}{V} x_j + \left(1 - \frac{L}{V}\right) x_D$$

◆ This is the operating equation in the **enriching section** (represent mass balance) with slope L/V and a y intercept (1-L/V) x_D.

◆ Equations may be solved iteratively starting from the column balances to calculate D and B, then L_0 and V_1 and x_1 from y_1 (=x_D) and then using the above equation to go on down the column.

Graphical representation

$$y = \frac{L}{V}x + \frac{D}{V}y_D$$

$$0 < \frac{L}{V} < 1$$

Operating lines goes through point D (y_D, y_D)

Lewis method: constant molal overflow

- In the **stripping section** following the same procedure (CMO)

- Solving for y_{J+1}:

$$y_k = \frac{\underline{L_{k-1}}}{\underline{V_k}} x_{k-1} - \left(\frac{\underline{L_{k-1}}}{\underline{V_k}} - 1 \right) x_B$$
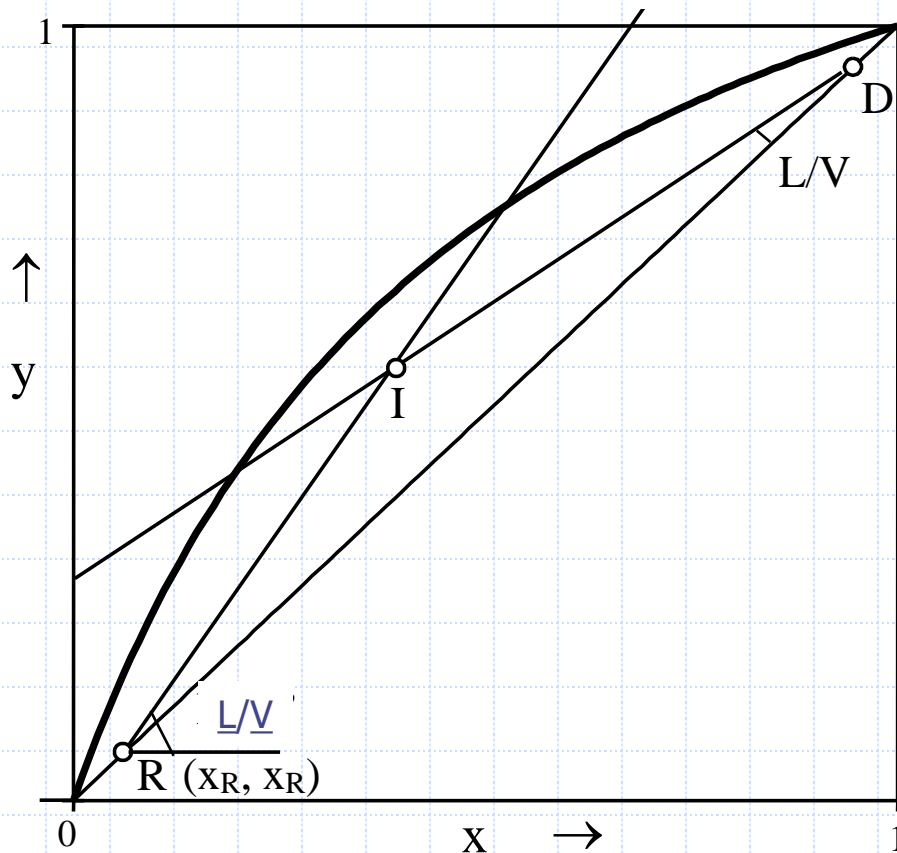
- Since CMO:

$$y_k = \frac{\underline{L}}{\underline{V}} x_{k-1} + \left(\frac{\underline{L}}{\underline{V}} - 1 \right) x_B$$

- This is the operating equation in the **stripping section** (mass balance)

  - with slope $\underline{L}/\underline{V}$ and an y intercept $-(\underline{L}/\underline{V} - 1)\ x_B$.

Graphical representation

$$y = \frac{L}{V} x - \frac{R}{V} x_R$$

$$\frac{L}{V} > 1$$

Operating lines goes through point R (x_R, x_R)

Lewis method: constant molal overflow

◈ The phase and temperature of the feed obviously affect the vapor and liquid flow rates in the column.

◈ Mass and energy balances **around the feed**:
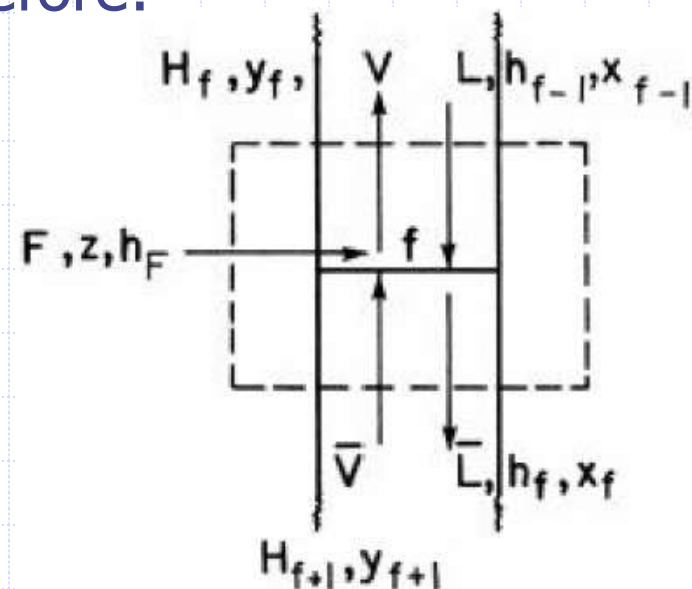
$$F + \underline{V} + L = \underline{L} + V$$

$$Fh_f + \underline{V}H_{f+1} + Lh_{f+1} = \underline{L}h_f + VH_f$$

◈ If we assume CMO, enthalpies do not vary very much, therefore $H_{f+1} \approx H_f$ and $h_{f-1} \approx h_f$. Therefore:

$$Fh_f + (\underline{V} - V)H - (\underline{L} - L)h = 0$$

◈ Combining with mass balance and defining q as:

$$q = (\underline{L} - L)/F \approx (H - h_f)/(H - h)$$

Lewis method: constant molal overflow

◈ Combining mass and energy balance equation with the definition of q one gests:

$$q = 1 + \frac{\overline{V} - V}{F} = \frac{H_V - h_F}{H_V - h_L}$$

◈ The quality q is:

$$q = \frac{\text{liquid flow rate below the feed} - \text{liquid flow rate above the feed}}{\text{feed rate}}$$

$$q = \frac{\text{vapor enthalpy on the feed plate} - \text{feed enthalpy}}{\text{vapor enthalpy on the feed plate} - \text{liquid enthalpy on the feed plate}}$$

◈ The quality, q, is the fraction of feed that is liquid.

  ▪ This is analogous to the q that we saw defined for flash distillation.
  ▪ WE assume that the feed is adiabatically flashed to the column pressure!

OL Intersection

- Straight line y=x
- Equilibrium curve
- Enriching section OL
  - slope L/V
  - y intercept $(1-L/V) x_D$.
- Stripping section OL
  - slope $\underline{L}/\underline{V}$
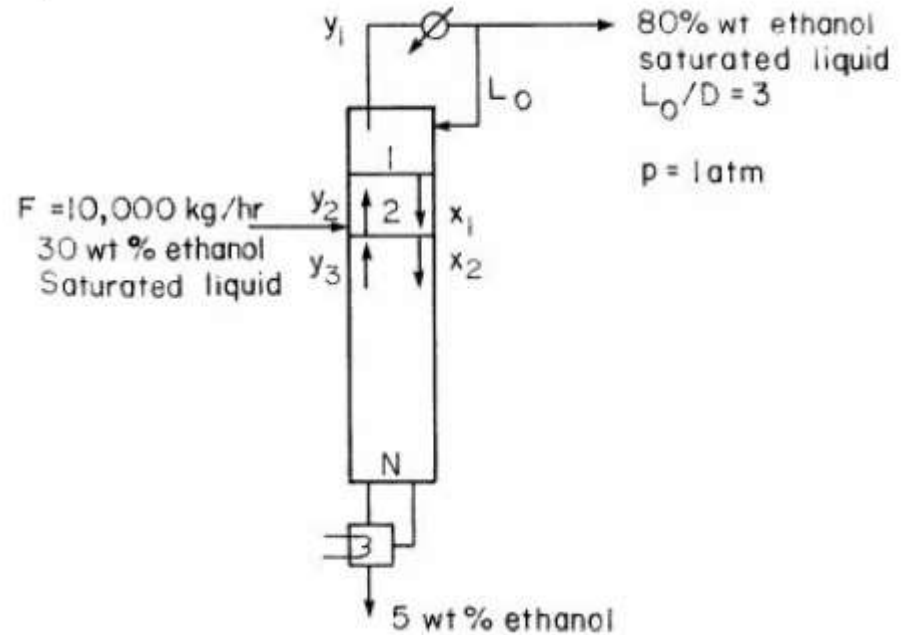 - y intercept $-(\underline{L}/\underline{V} - 1) x_B$.
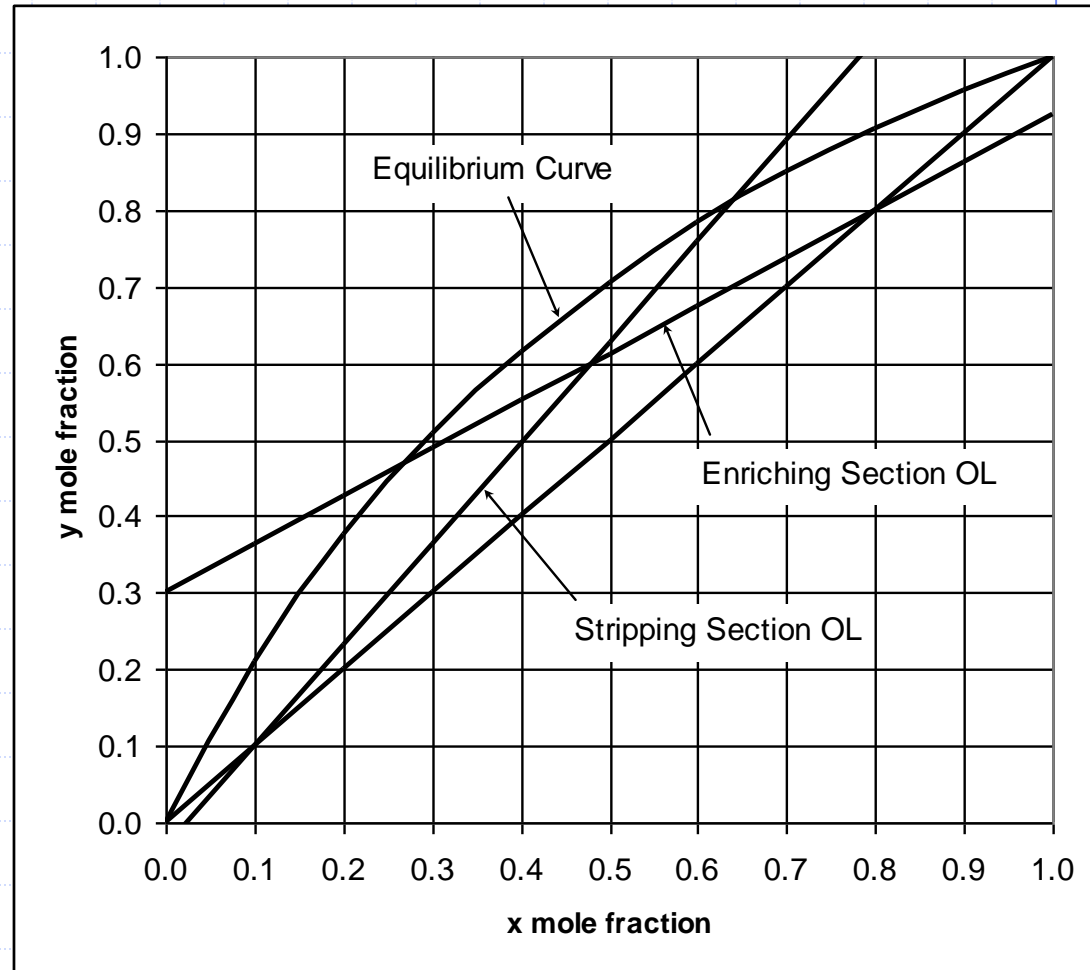
Lewis method: example

◆ A steady-state countercurrent, staged distillation column is to be used to separate ethanol from water.

- The feed is a 30 wt % ethanol, 70 wt % water mixture that is a saturated liquid at 1 atm pressure. Flow rate of feed is 10,000 kg/h.

- The column operates at a pressure of 1 atm.

- The reflux is returned as a saturated liquid. A reflux ratio of L/D = 3.0 is being used.

- We desire a bottoms composition of xB =0.05 (weight fraction ethanol) and a distillate composition of xD = 0.80 (weight fraction ethanol).

- The system has a total condenser and a partial reboiler.

- The column is well insulated.

- Use the Lewis method to find the number of equilibrium contacts required if the feed is input on the second stage from the top.

Lewis method: example

- ◆ hxx

The diagram shows a distillation column with the following labels:

- Top: y_i with condenser, output: 80% wt ethanol, saturated liquid, $L_0/D = 3$
- L_0 (reflux)
- $p = 1\ atm$
- Stage 1
- Feed: $F = 10,000\ kg/hr$, 30 wt % ethanol, Saturated liquid, with y_2, x_i, stage 2, y_3, x_2
- Stage N
- Reboiler (stage 3)
- Bottom output: 5 wt % ethanol

Preliminary calculations: convert to molar units

$$MW_W = 18, \qquad MW_E = 46, \qquad z_E = \frac{0.3/46}{0.3/46 + 0.7/18} = 0.144$$

Average molecular weight of feed is

$$\overline{MW}_F = (0.144)(46) + (0.856)(18) = 22.03$$

Feed rate = (10,000 kg/h)/(22.03 kg/kmol) = 453.9 kmol/h

$$x_{D.E} = \frac{0.8/46}{0.8/46 + 0.2/18} = 0.61, \qquad x_{BE} = 0.02$$

For distillate, the average molecular weight is

$$\overline{MW}_{dist} = (0.61)(46) + (0.39)(18) = 35.08$$

which is also the average for the reflux liquid and vapor stream V since they are all the same composition.

Then D = (3333 kg/h)/35.08 = 95.2 kmol/h and

$$L = (\frac{L}{D})D = (3)(95.23) = 285.7 \text{ kmol/h}$$

while

V = L + D = 380.9. Thus,

$$\frac{L}{V} = \frac{285.7}{380.9} = 0.75$$

Because of CMO, L/V is constant in the rectifying section.

Since the feed is a saturated liquid,

$$\overline{L} = L + F = 285.7 + 453.9 = 739.6 \text{ kmol/h}$$

where we have converted F to kmol/h. Since a saturated liquid feed does not affect the vapor, $\overline{V} = V = 380.9$. Thus,

$$\frac{\overline{L}}{\overline{V}} = \frac{739.6}{380.9} = 1.94$$

An internal check on consistency is L/V < 1 and $\overline{L}/\overline{V} > 1$.

Stage by stage calculations

- At the top of the column, y1 = xD = 0.61.
  - Liquid stream L1 of concentration x1 is in equilibrium with the vapor stream y1.
  - From eq. data (x-y), x1 = 0.4. (Note that y1>x1 since ethanol is the more volatile component).
- Vapor stream y2 is a passing stream relative to x1 and can be determined from the operating line

$$y_2 = \frac{L}{V} x_1 + (1 - \frac{L}{V})x_D = (0.75)(0.4) + (0.25)(0.61) = 0.453$$

  - Stream x2 is in equilibrium with y2: we obtain x2 = 0.11.
- Since stage 2 is the feed stage, use bottom operating line for y3.

$$y_3 = \frac{\overline{L}}{\overline{V}} x_2 + (1 - \frac{\overline{L}}{\overline{V}})x_B = (1.942)(0.11) + (-0.942)(0.02) = 0.195$$

  - Stream x3 is in equilibrium with y3: therefore x3 = 0.02.
  - Since x3 = xB (in mole fraction), we are finished.
- The third equilibrium contact would be the partial reboiler.
- Thus the column has two equilibrium stages plus the partial reboiler.