Binary distillation: McCabe Thiele method

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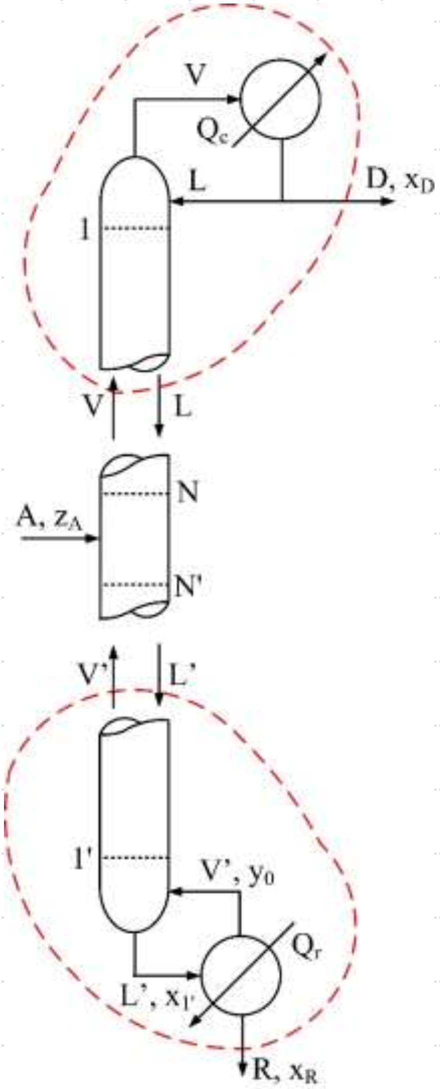
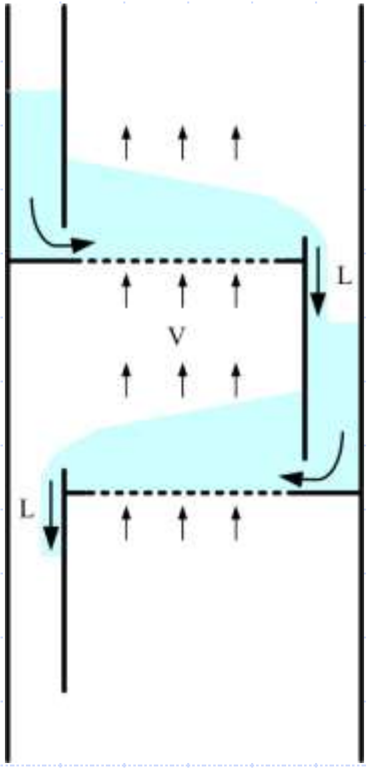
Agenda

- Introduction to McCabe Thiele method
- Enriching and stripping sections
- Feed line
- Methodology of McCabe Thiele method
- McCabe-Thiele graphical construction
  - Determination of N and X_B
  - Minimum number of stages N
  - Minimum reflux
  - Example
- Other distillation column situations
  - Subcooled Reflux
  - Partial condensers
  - Multiple Feeds
  - Side stream products
  - Open steam
  - Non-ideal distillation: Murphree efficiency
- McCabe Thiele: algebraic method
- Fractional stage at top and bottom
- Limiting operating conditions
  - Total reflux, minimum reflux, punch points
- Examples

The conventional distillation column

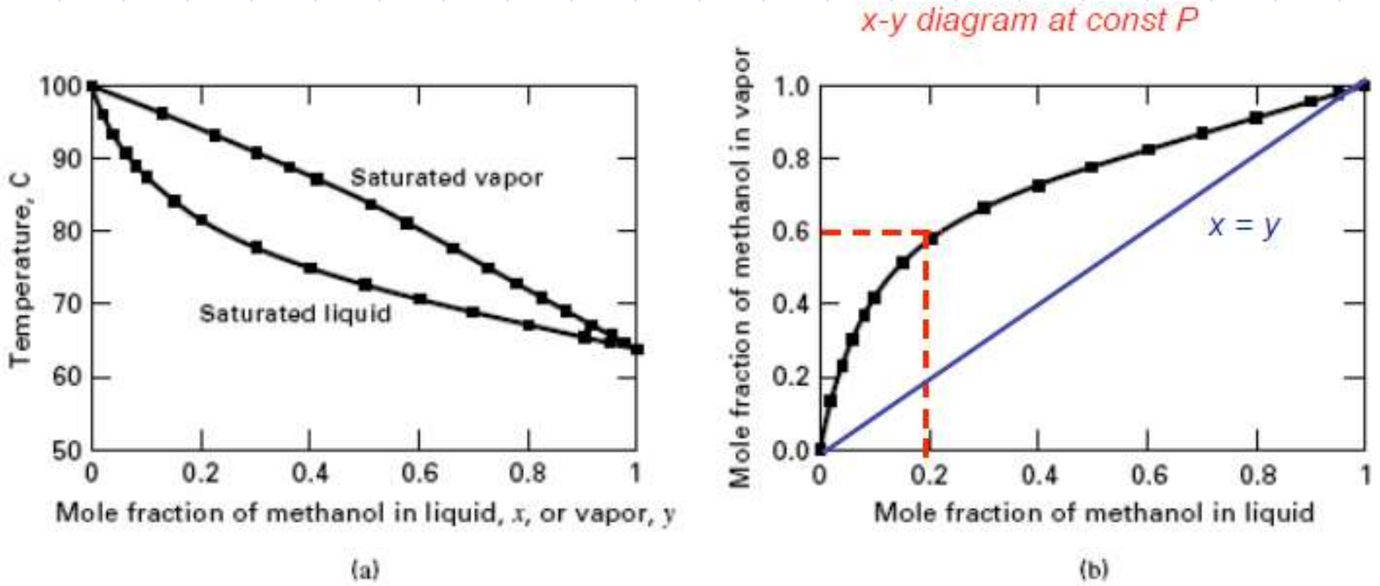
- A cylindrical tower filled with plates or packing
- A reboiler to produce the vapor flow V’ at the bottom
- A condenser to produce the liquid flow L at the top
- Two products: a distillate D and a residue R
- A feed which cuts the column in two parts:
    - Enrichment section (upper)
    - Stripping section (lower)





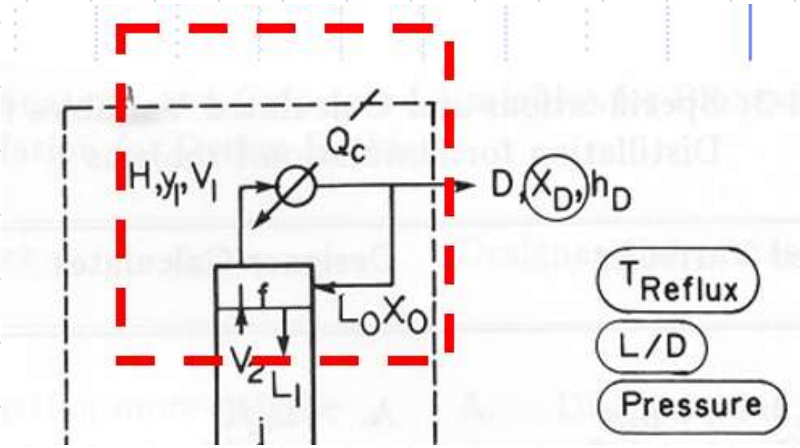
Introduction to McCabe Thiele method

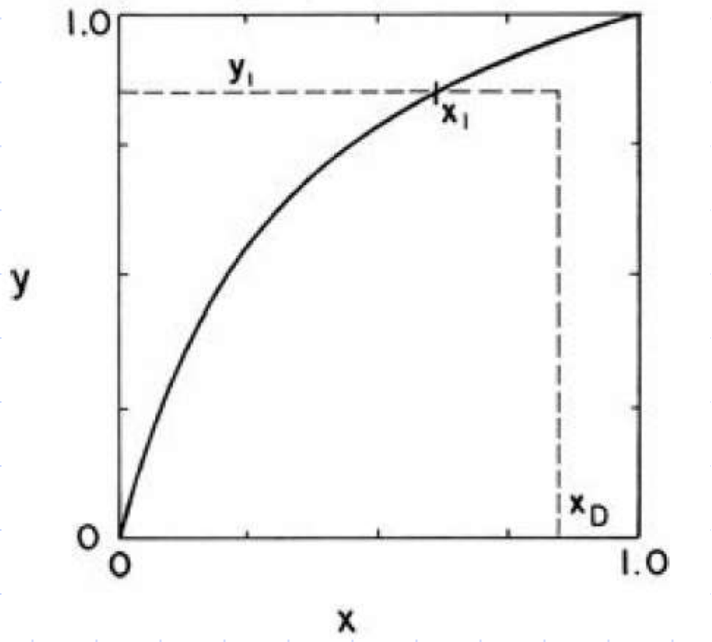
- McCabe and Thiele (1925) developed a graphical solution method
  - based on Lewis' method
  - and the observation that the operating Eqs. plot as straight lines (the *operating lines*) on a y-x diagram.
  - On this graph the equilibrium relationship can be solved from the y-x equilibrium curve and the mass balances from the operating lines.



Introduction to McCabe Thiele method

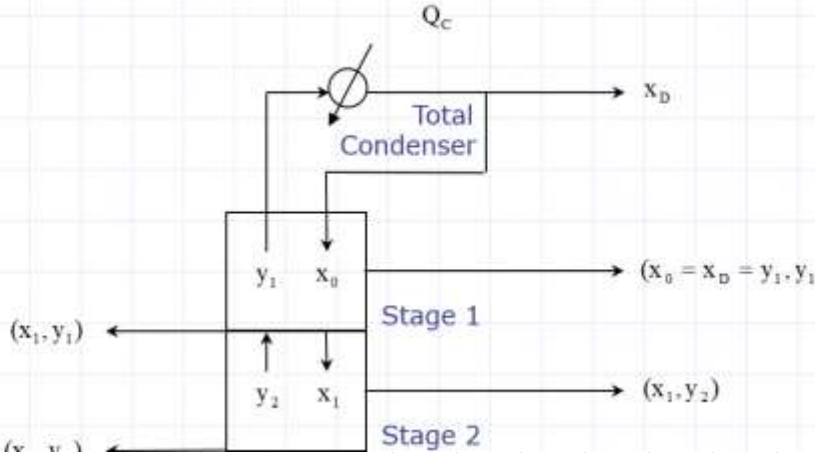
- Assumptions
  - Equilibrium data are available at the operating pressure of the column
  - Pressure is constant
  - At the top of the column is a total condenser: this means that $y_1=x_D= x_0$.

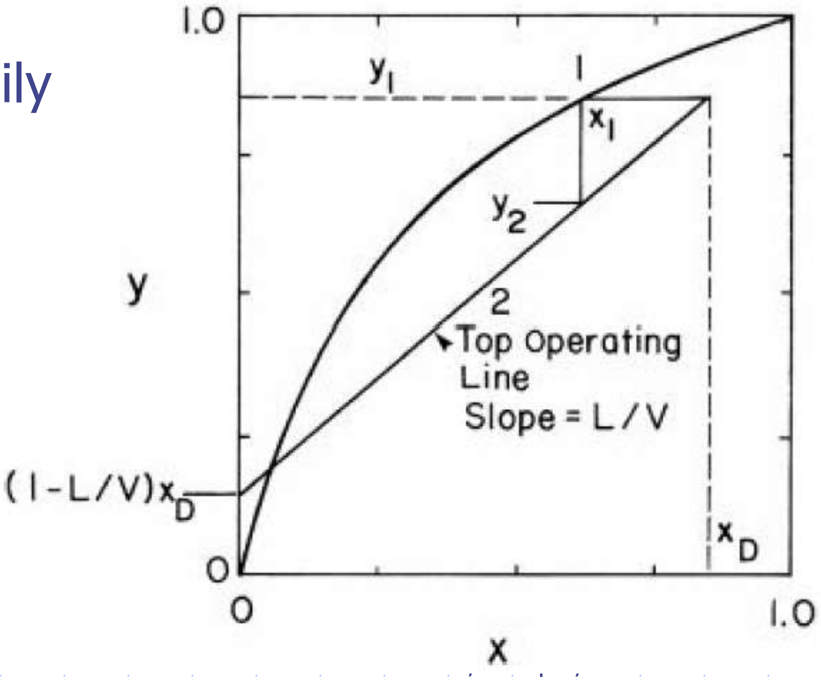




Introduction to McCabe Thiele method: enriching section

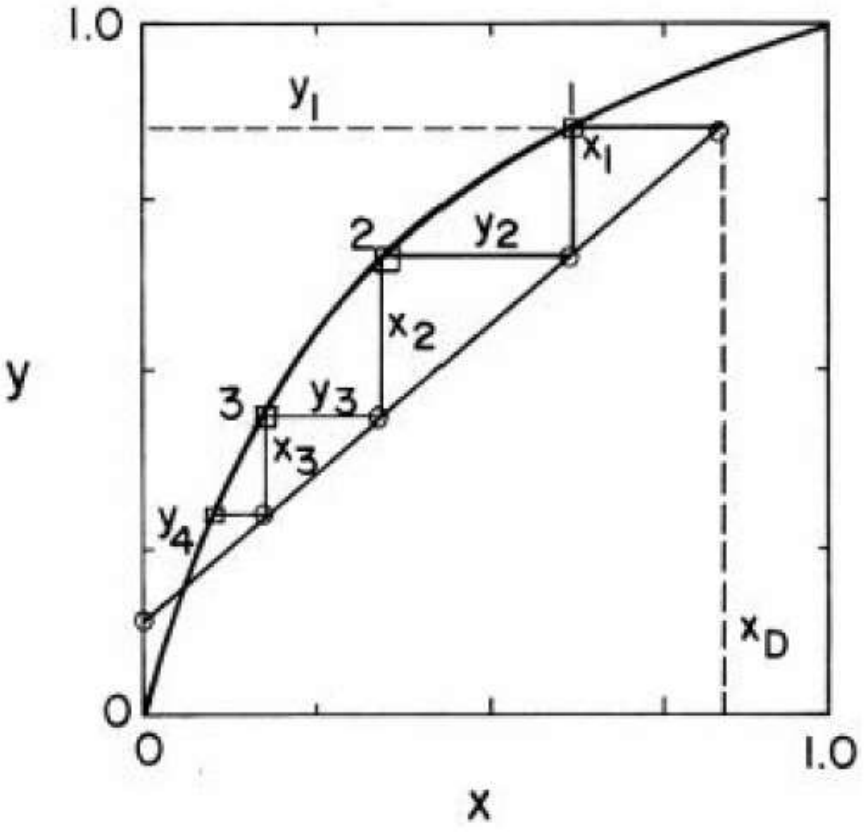
- The vapor leaving the first stage is in equilibrium with the liquid leaving the first stage.
- This liquid composition, x_1, can be determined from the equilibrium curve at $y = y_1$.
- Mass balance in the enriching section is represented by the OL
    - slope L/V
    - y intercept (x=0) $(1-L/V)x_D$
    - passing through the point (y_1, x_D).
- Once OL has been plotted, y_2 is easily found from the y value at $x = x_1$.





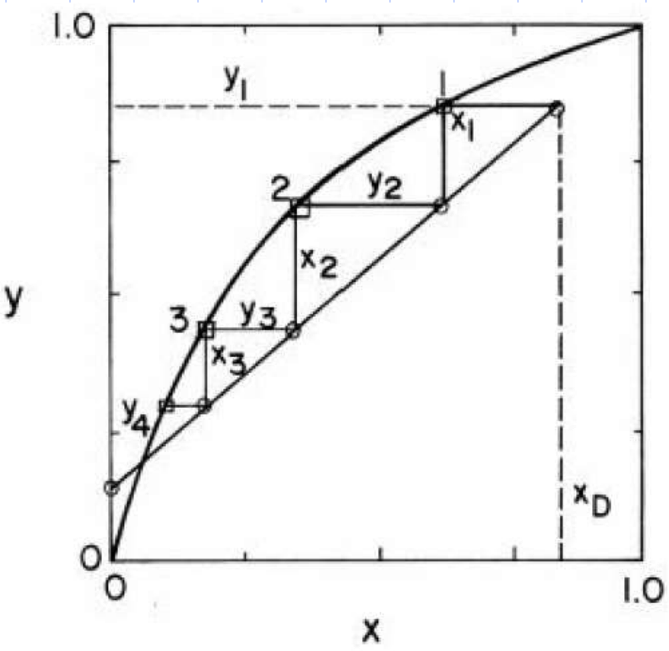
Introduction to McCabe Thiele method: enriching section

- With y_2 known we can proceed down the column.
  - Since x_2 and y_2 are in equilibrium, we easily obtain x_2 from the equilibrium curve.
  - Then we obtain y_3 from the operating line (mass balances), since x_2 and y_3 are the compositions of passing streams.
  - This procedure of *stepping off stages* is shown in Figure.
  - It can be continued as long as we are in the rectifying section.
  - Note that this produces a staircase on the y-x, or McCabe-Thiele, diagram.



Introduction to McCabe Thiele method: stripping section

- Note that the horizontal and vertical lines have no physical meaning.
  - The points on the equilibrium curve (squares) represent liquid and vapor streams leaving an equilibrium stage.
  - The points on the operating line (circles) represent the liquid and vapor streams passing each other in the column.
- In the stripping section the top operating line is no longer valid
  - since different mass balances and, hence, a different operating equation are required.

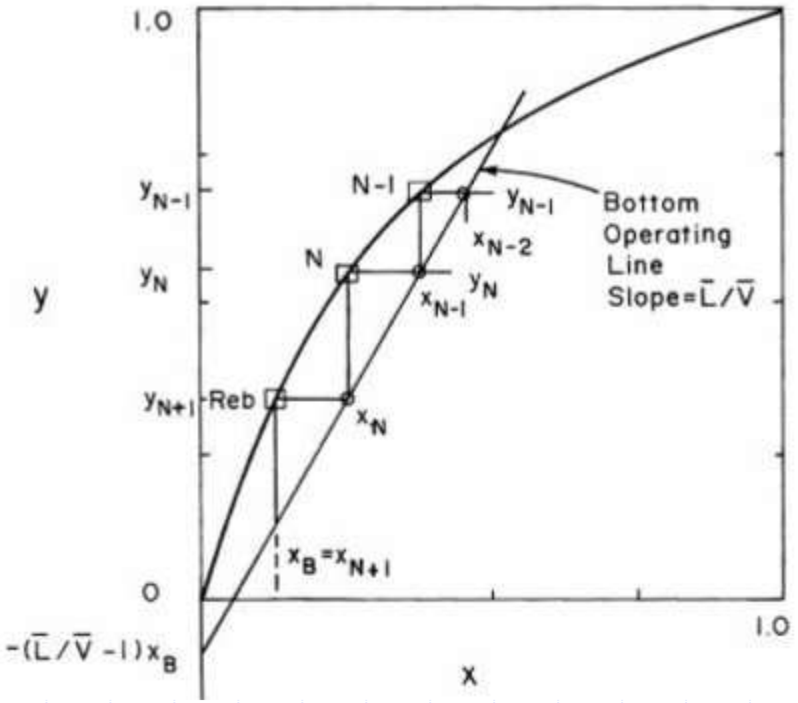


Introduction to McCabe Thiele method: stripping section

- Starting with the liquid leaving the partial reboiler, of mole fraction $x_B = x_{N+1}$,
  - we know that the vapor leaving the partial reboiler is in equilibrium with x_B.
  - Thus we can find y_{N+1} from the equilibrium curve.
  - x_N is easily found from the bottom operating line, since liquid of composition x_N is a passing stream to vapor of composition y_{N+1}.
  - We can continue alternating between the equilibrium curve and the bottom operating line as long as we are in the stripping section.

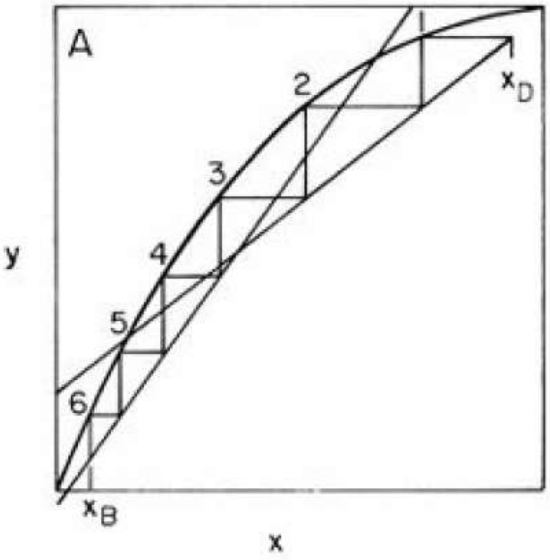
OL: slope $\underline{L}/\underline{V}$

y intercept (x=0) $-(\underline{L}/\underline{V}-1)X_B$



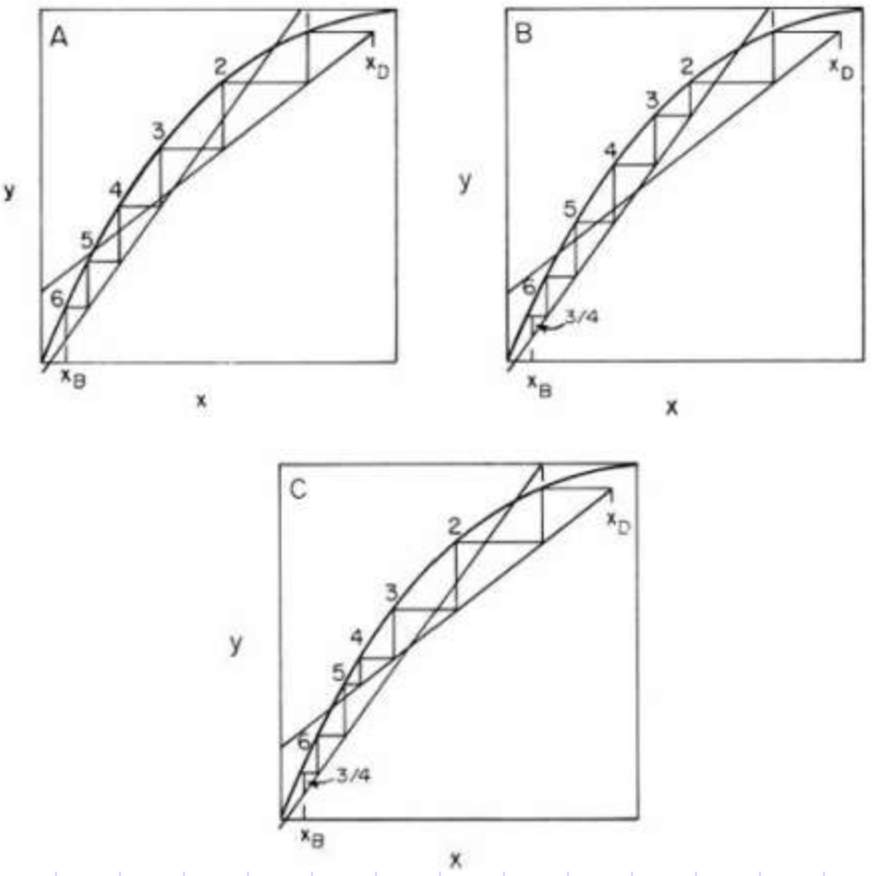
Introduction to McCabe Thiele method: feed section

- If we are stepping off stages down the column, **at the feed stage f**
  - we switch from the top operating line to the bottom operating line
  - above the feed stage, we calculate x_f-1 from equilibrium and y_f from the top operating line.
- Since liquid and vapor leaving the feed stage are assumed to be in equilibrium,
  - we can determine x_f from the equilibrium curve at $y = y_f$ and then find y_f+1 from the bottom operating line.
- In figure stage 3 is the feed stage.
  - The separation shown would require 5 equilibrium stages plus an equilibrium partial reboiler,
  - or 6 equilibrium contacts, when stage 3 is used as the feed stage.

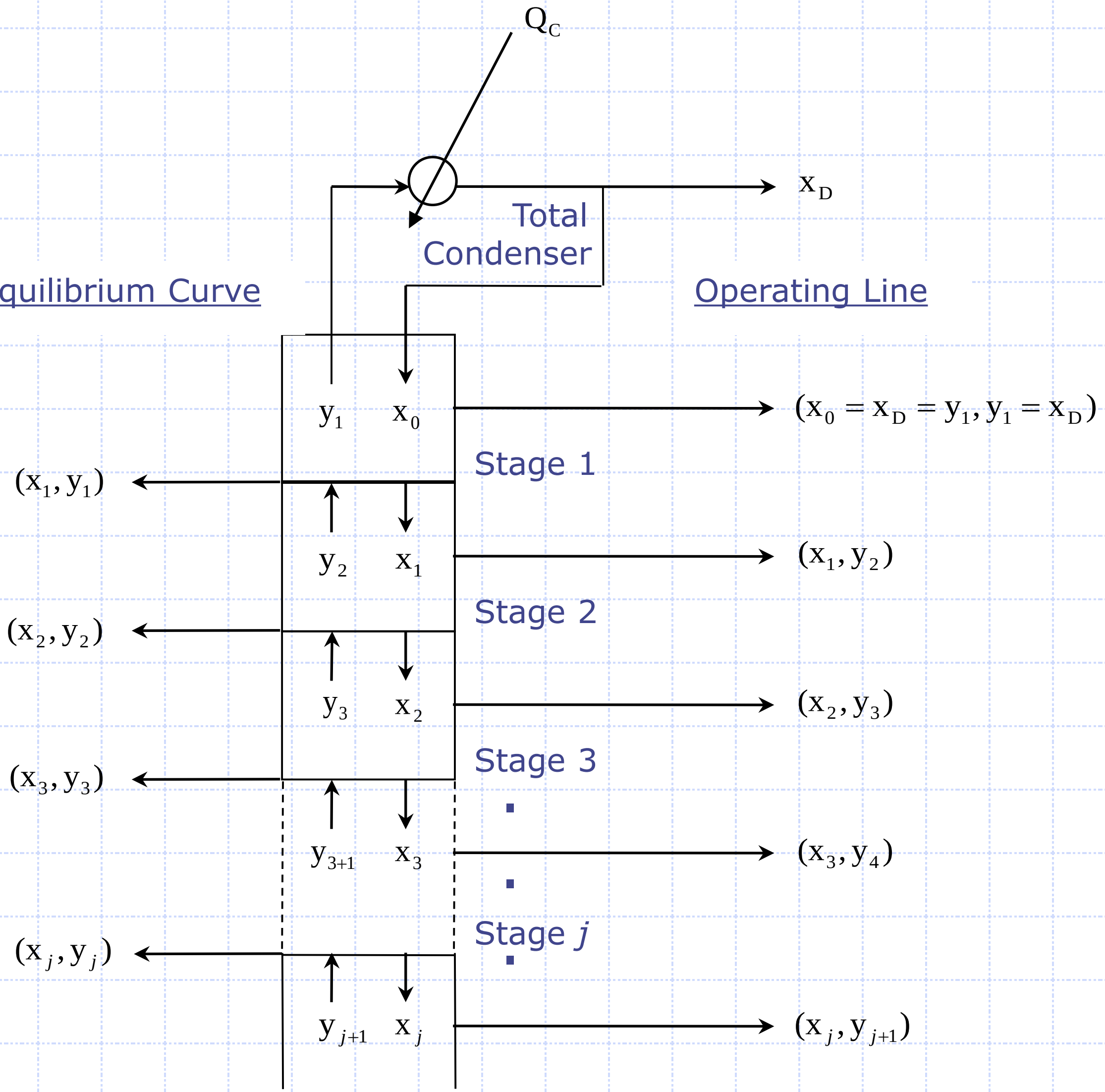


Introduction to McCabe Thiele method: feed section

- Stage 3 is the *optimum feed stage.*
  - That is, a separation will require the fewest total number of stages when feed stage 3 is used.
  - Note in B and C that if stage 2 or stage 5 is used, more total stages are required.
- For binary distillation the optimum feed plate is easy to determine;
  - it will always be the stage where the step in the staircase includes the point of intersection of the two operating lines
  - compare A to B and C



Stage Compositions – Total Condenser



Q_C

x_D

Total Condenser

Equilibrium Curve

Operating Line

y_1 x_0

$(x_0 = x_D = y_1, y_1 = x_D)$

Stage 1

(x_1, y_1)

y_2 x_1

(x_1, y_2)

Stage 2

(x_2, y_2)

y_3 x_2

(x_2, y_3)

Stage 3

(x_3, y_3)

y_{3+1} x_3

(x_3, y_4)

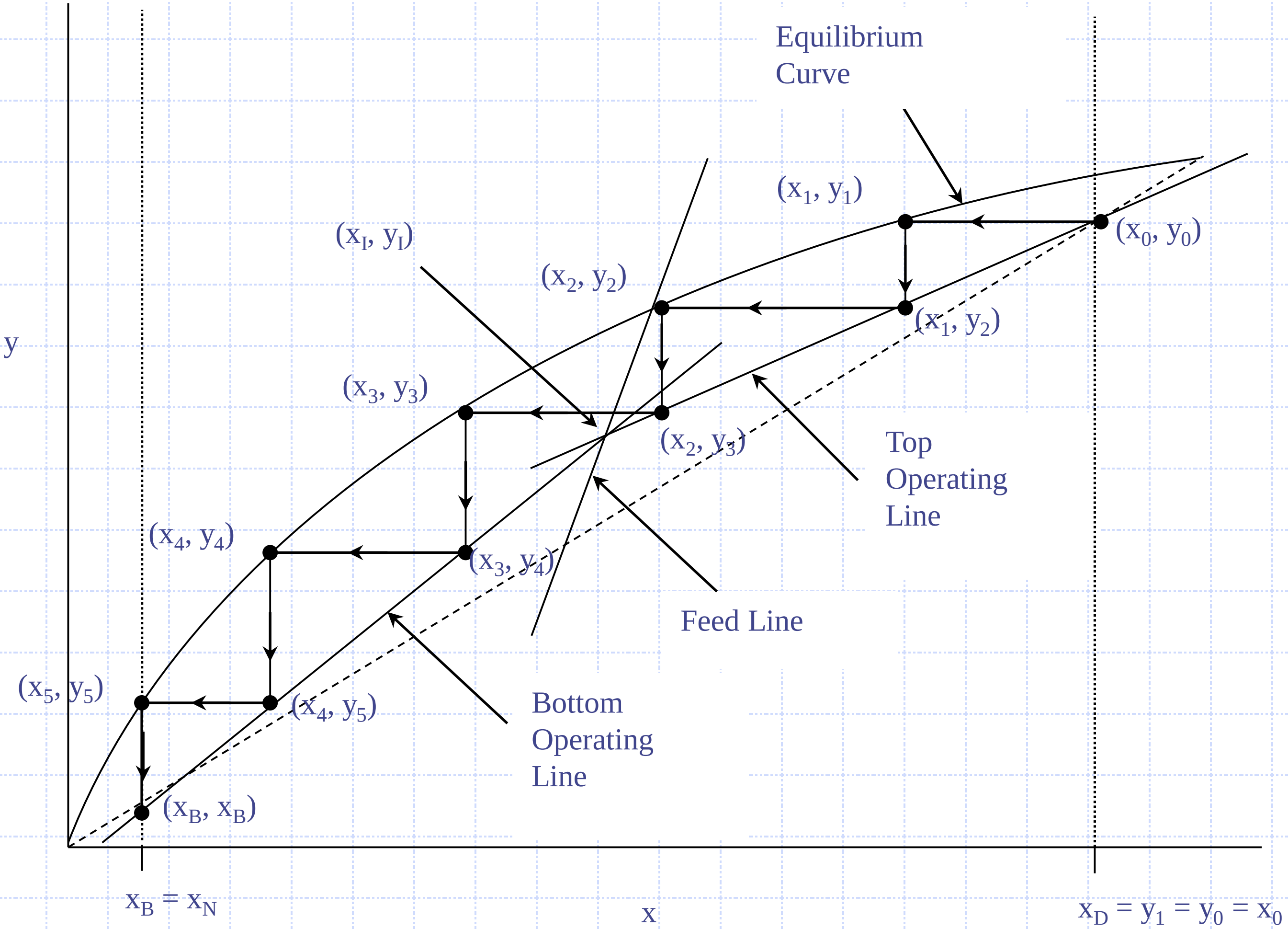
Stage *j*

(x_j, y_j)

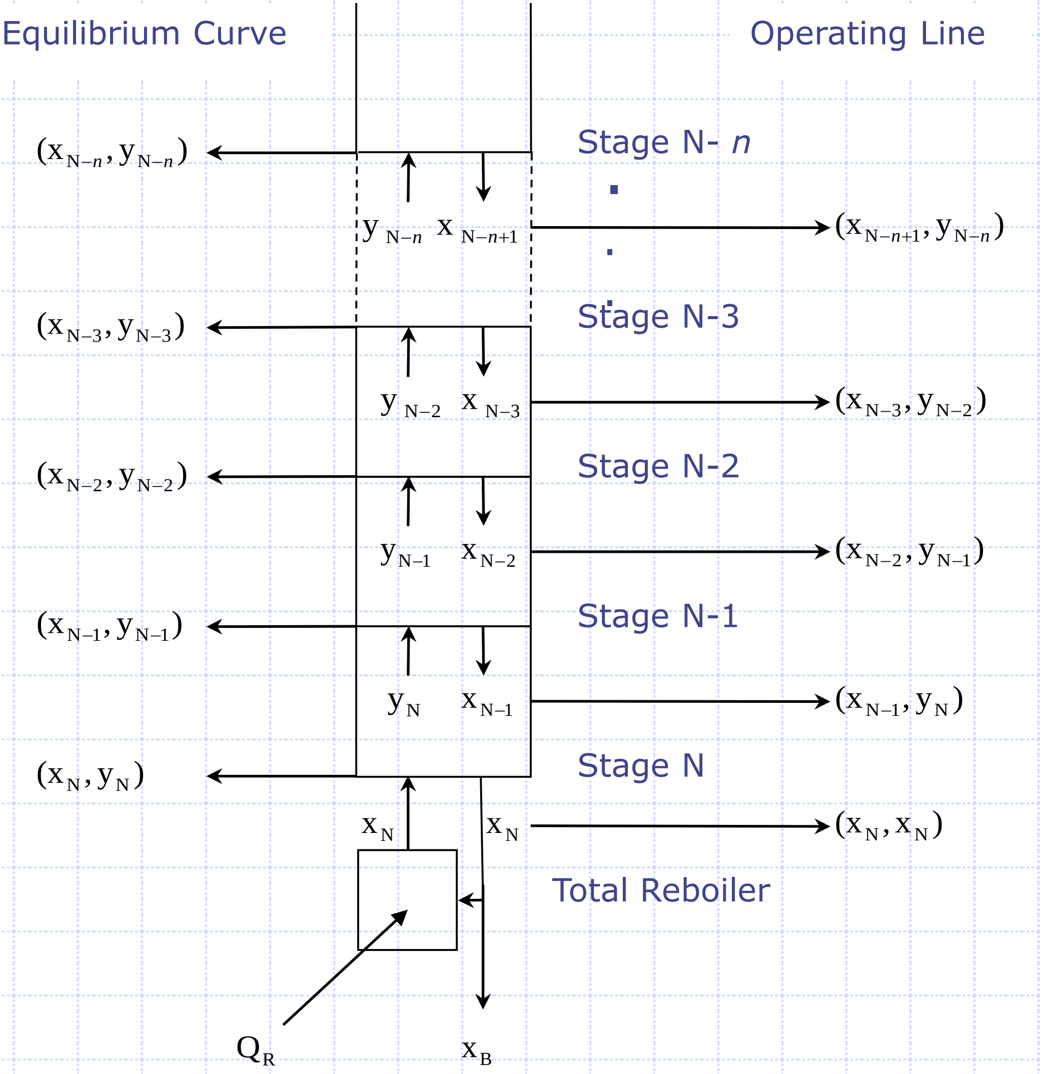
y_{j+1} x_j

(x_j, y_{j+1})

Complete McCabe-Thiele Solution Total Condenser



Stage Compositions – Total Reboiler



Equilibrium Curve

Operating Line

(x_{N-n}, y_{N-n})

Stage N- *n*

y_{N-n} x_{N-n+1}

(x_{N-n+1}, y_{N-n})

(x_{N-3}, y_{N-3})

Stage N-3

y_{N-2} x_{N-3}

(x_{N-3}, y_{N-2})

(x_{N-2}, y_{N-2})

Stage N-2

y_{N-1} x_{N-2}

(x_{N-2}, y_{N-1})

(x_{N-1}, y_{N-1})

Stage N-1

y_N x_{N-1}

(x_{N-1}, y_N)

(x_N, y_N)

Stage N

x_N x_N

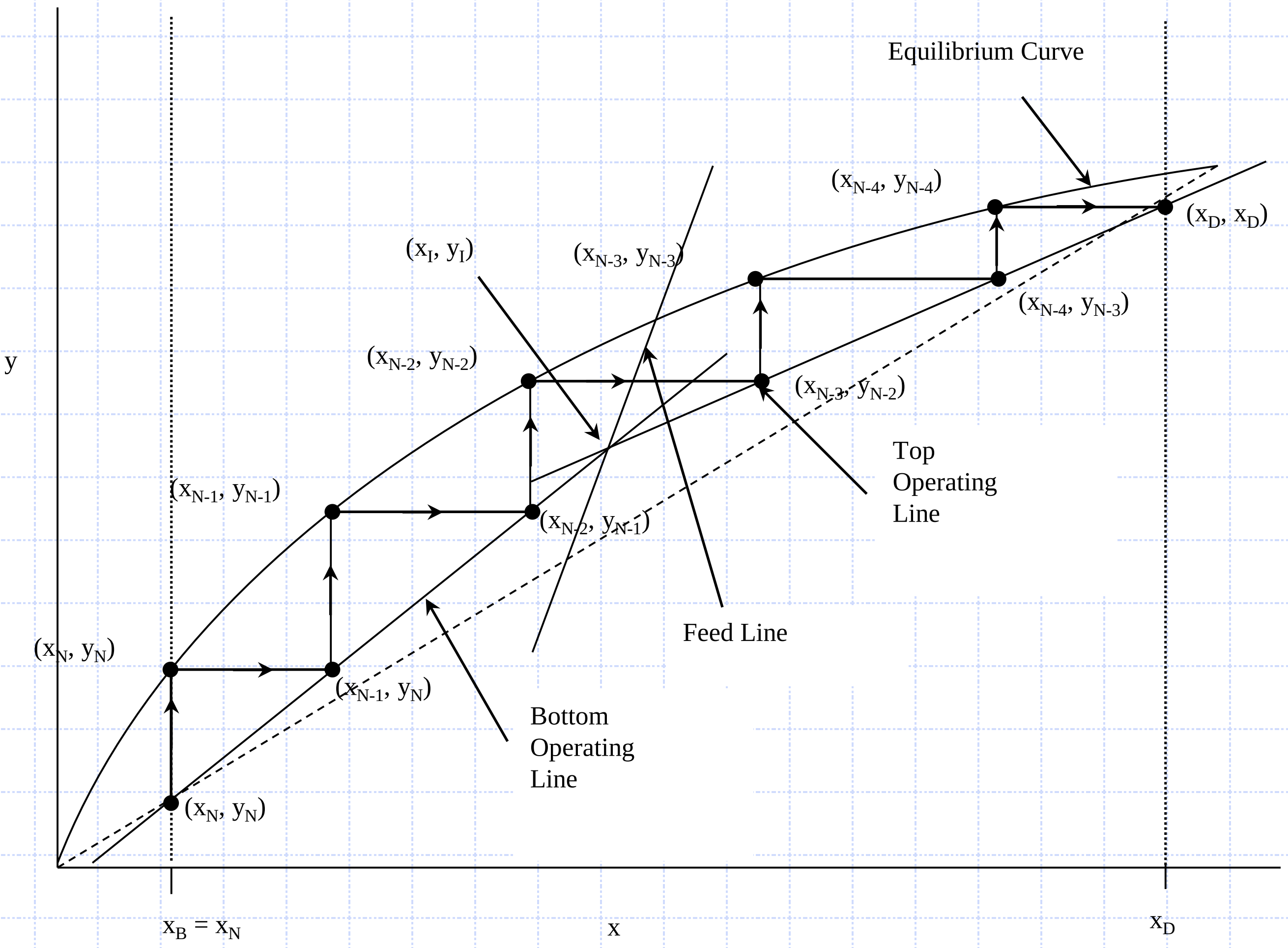
(x_N, x_N)

Total Reboiler

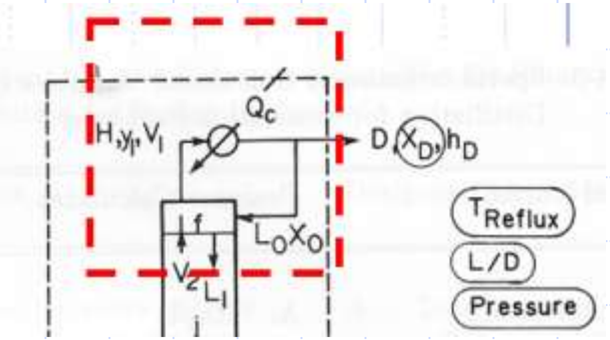
Q_R

x_B

Complete McCabe-Thiele Solution Total Reboiler



Introduction to McCabe Thiele method: design problem



- The **known** variables are
  - F, z, q, x_D, x_B, L_0/D, p, saturated liquid reflux, and the optimum feed location.
- The reflux is a saturated liquid
  - there will be no change in the liquid or vapor flow rates on stage 1 (CMO) and $L_0 = L_1$ and $V_1 = V_2$.
  - This allows us to calculate the internal reflux ratio, R=L/V, from the external reflux ratio, L_0/D, which is specified.

$$\frac{L}{V} = \frac{L}{L + D} = \frac{L/D}{L/D + 1}$$

- With L/V and x_D known, the top operating line is fully specified and can be plotted.
- The boilup ratio, $\underline{V}$/B, was not specified, → we cannot directly calculate $\underline{L}/\underline{V}$ (slope of the bottom OL)
  - The condition of the feed allows to determine flow rates in the stripping section.
  - The feed quality, q, is calculated from:

$$q \equiv \frac{\overline{L} - L}{F} \sim \frac{H - h_F}{H - h}$$

  - Then $\underline{L}$ is given by $\underline{L} = L + qF$, and $\underline{V} = \underline{L} - B$.
- With $\underline{L}/\underline{V}$ and x_B known, the bottom OL is fully specified → can be plotted.

General Feed line

At the feed stage, the enriching section OL and the stripping section OL must intersect. These OL's can be written as:

$Vy = Lx + Dx_D$ Enriching Section OL

$\underline{V}y = \underline{L}x - Bx_B$ Stripping Section OL

We can represent this point of intersection by subtracting the stripping section OL from the enriching section OL (essentially a simultaneous solution). Doing so and grouping terms yields:

$$y(V - \underline{V}) = (L - \underline{L})x + Dx_D + Bx_B$$

General Feed Line

The component mass balance around the column yields

$$Dx_D + Bx_B = Fz_F$$

Substituting this mass balance into the difference of the OL's yields, upon rearrangement,

$$y = \frac{(L - \underline{L})}{(V - \underline{V})} x + \frac{F}{(V - \underline{V})} z_F \qquad \text{Feed Line}$$

This equation is linear and in the form of an operating line.

It is one of the various forms, as we shall see, of the feed line and is the most general form.

General Feed Line

The total mass balance around the feed stage yields

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

Combining this mass balance with the previous feed line yields, upon rearrangement,

$$y = \frac{\dfrac{\underline{L} - L}{F}}{\left(\dfrac{\underline{L} - L}{F}\right) - 1} x + \frac{1}{1 - \left(\dfrac{\underline{L} - L}{F}\right)} z_F$$

or, from the definition of quality, q:

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

Feed Line

- The previous equation is the feed line for the column in terms of quality q.

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

- This should look familiar – it is the same as the operating line that we obtained from the mass balances for flash distillation!

$$q = \frac{\underline{L} - L}{F} = \frac{H_V - h_F}{H_V - h_L}$$

- We can use the conditions of the feed to determine q from its enthalpy relationship and then the slope of the feed line
  - E.g.: if the feed is saturated liquid → h_f=h and q =1 → slope is ∞ and the feed line is vertical

Feed Line Equations

- By inspection from the results of our flash distillation operating lines, the feed line can also be expressed in terms of fraction of feed vaporized, f = V/F.
  - This, as well as the other feed line equations, are summarized below:

$$y = \frac{(L - \underline{L})}{(V - \underline{V})} x + \frac{F}{(V - \underline{V})} z_F$$

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

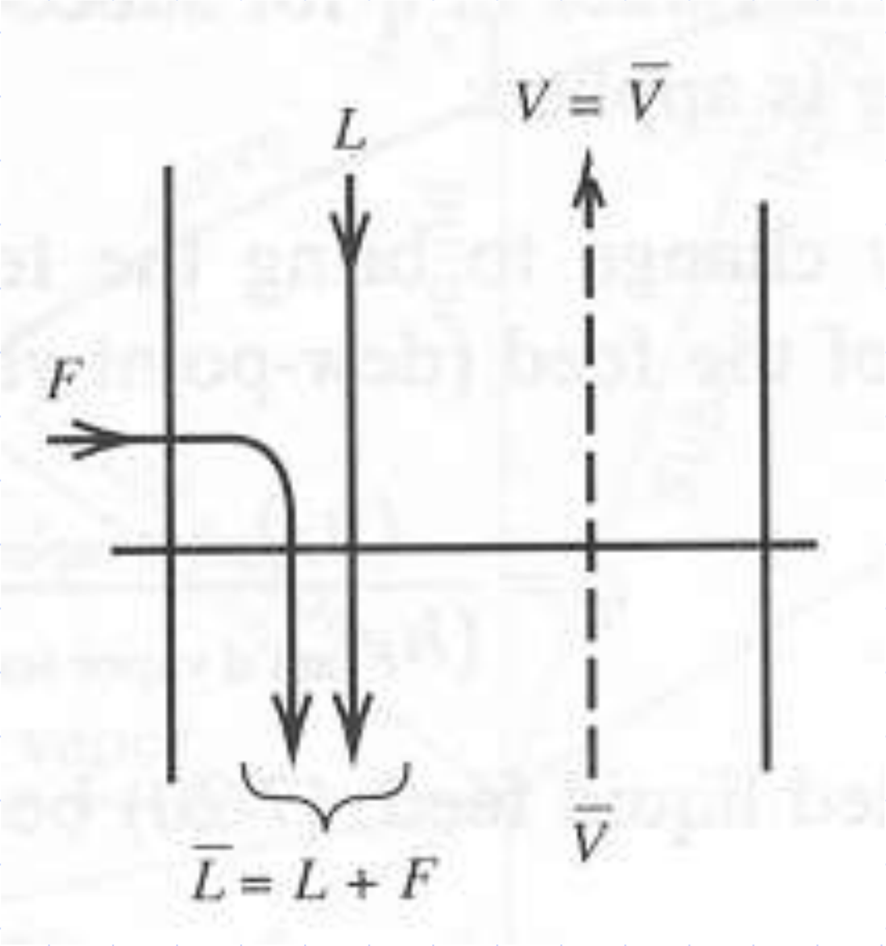
$$y = -\frac{1 - f}{f} x + \frac{1}{f} z_F$$

  - Remember that we derived these feed line equations from the intersection of the enriching section and stripping section OL’s.
  - It can be shown that the feed line also intersects the OL’s at their intersection – all three lines intersect at the same point.
  - We will need to use this intersection point in our solutions…

Possible Feed Stream Conditions

- We assume that the incoming feed is adiabatically flashed to the column pressure, P_{col}.
- We can have 5 possible feed stream conditions for a given feed composition z_F:
  - Subcooled liquid feed if $T_F < T_{bp}$
  - Saturated liquid feed if $T_F = T_{bp}$
  - Two-phase feed if $T_{bp} < T_F < T_{dp}$
  - Saturated Vapor if $T_F = T_{dp}$
  - Superheated Vapor if $T_F > T_{dp}$

Saturated Liquid Feed – Given $T_F = T_{bp}$



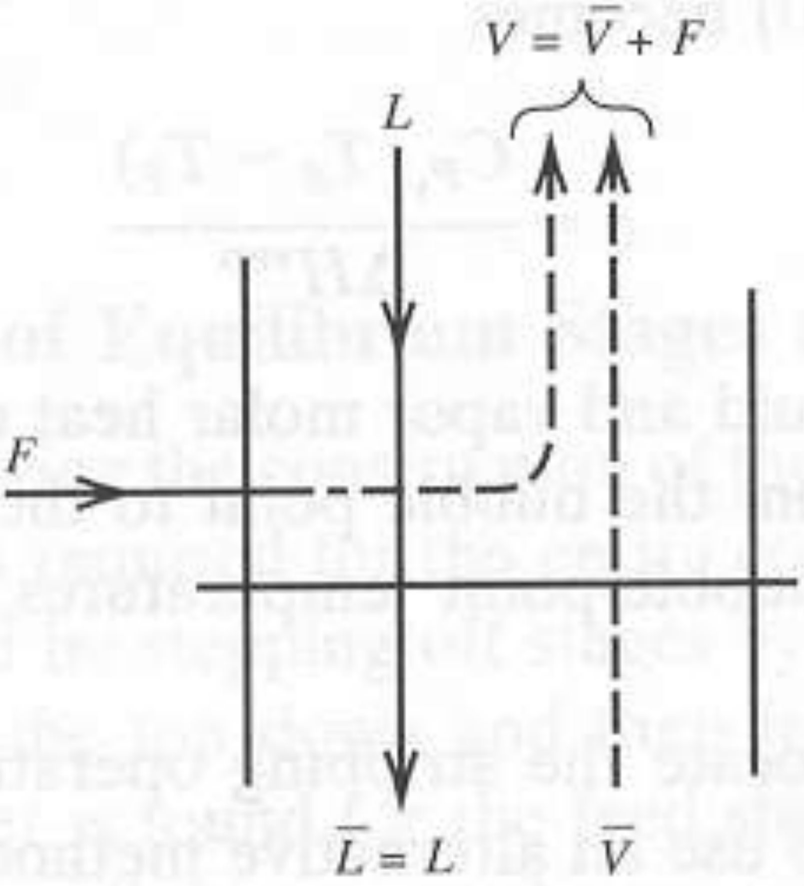
$$q = \frac{\underline{L} - L}{F} = \frac{(L + F) - L}{F} = 1$$

or since $h_F = h_L$

$$q = \frac{H_V - h_F}{H_V - h_L} = \frac{0 - h_F}{0 - h_L} = 1$$

Note that q = 1.

Saturated Vapor Feed – Given $T_F = T_{dp}$



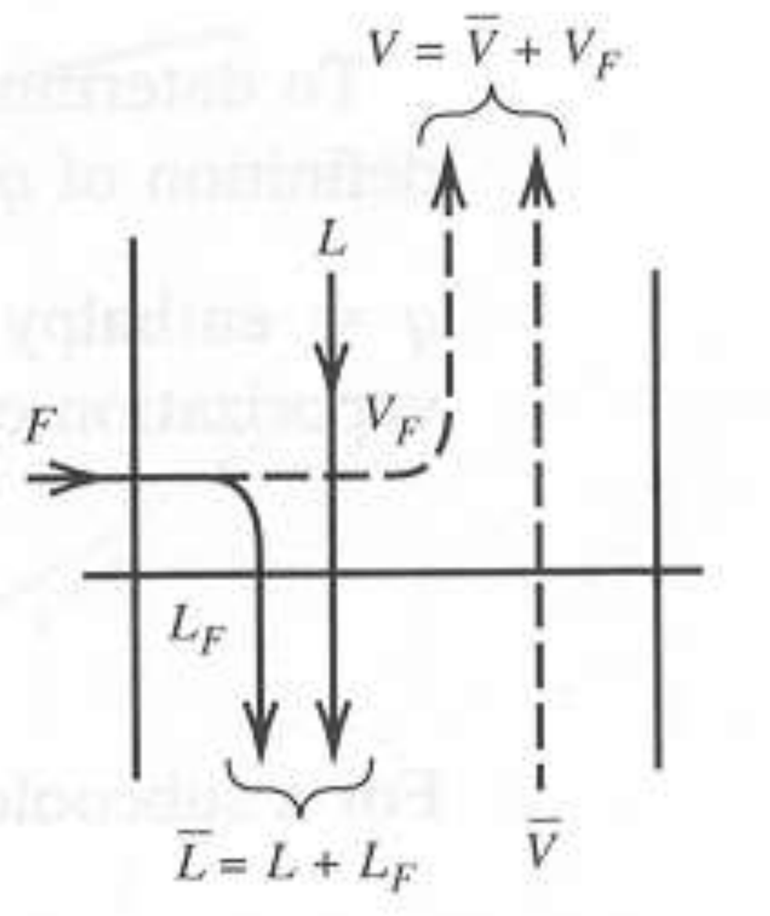
$$q = \frac{\underline{L} - L}{F} = \frac{\underline{L} - \underline{L}}{F} = 0$$

or since $H_V = h_F$,

$$q = \frac{H_V - h_F}{H_V - h_L} = \frac{H_V - H_V}{H_V - h_L} = 0$$

Note that q = 0.

Two-Phase Feed – Given f



f is the fraction of feed vaporized.

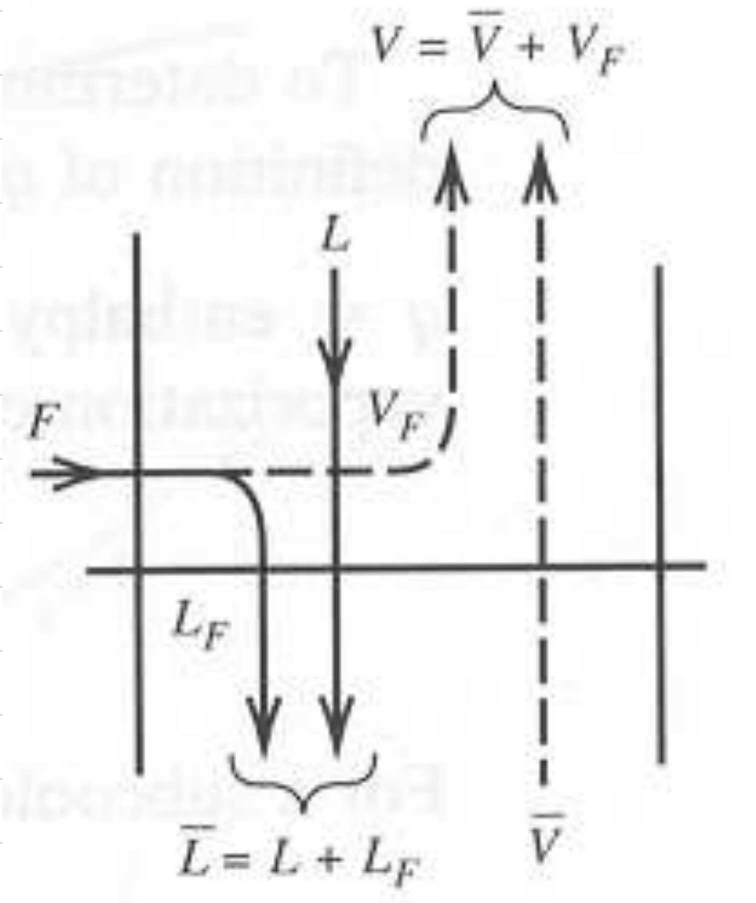
$$q = \frac{\underline{L} - L}{F} = \frac{(L + L_F) - L}{F} = \frac{L_F}{F}$$

$$q = 1 + \frac{\underline{V} - V}{F} = 1 + \frac{\underline{V} - (\underline{V} + V_F)}{F} = 1 - \frac{V_F}{F}$$

$$q = 1 - \frac{V_F}{F} = 1 - f$$

Note that $0 < q < 1$.

Two-Phase Feed – Given T_F



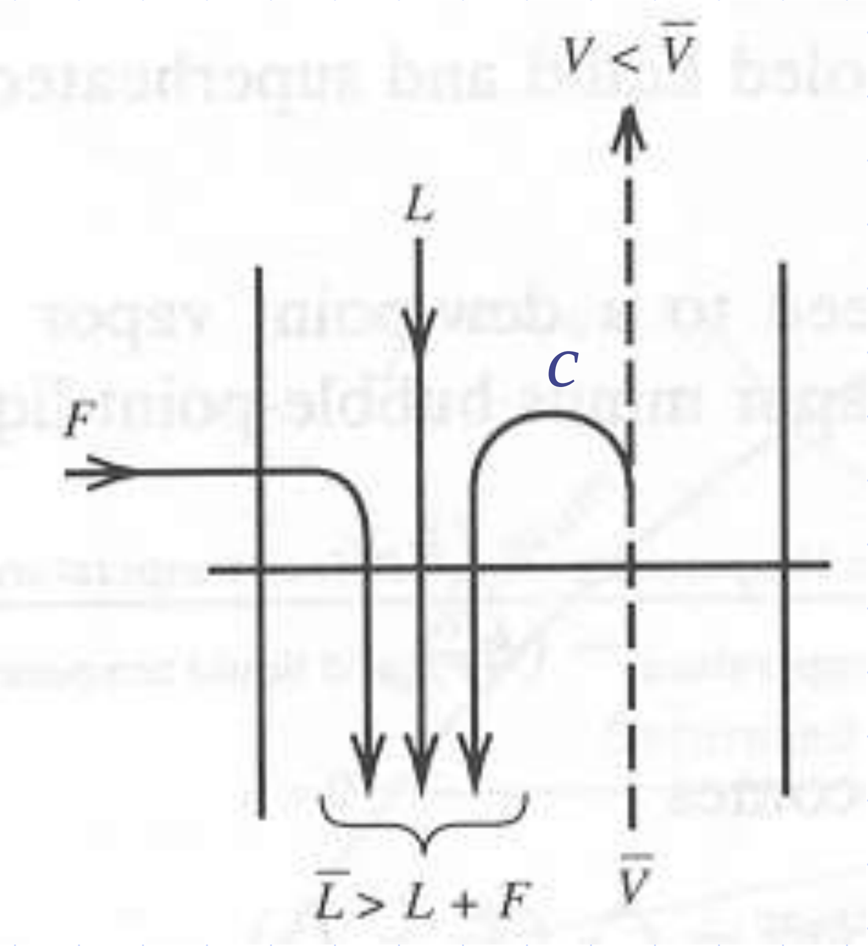
Since we assume CMO, all H_V's and h_L's are constant.

$$q = \frac{H_V - h_F}{H_V - h_L} = \frac{H_{V(\text{sat'd vapor})} - h_{F(\text{feed temp})}}{H_{V(\text{sat'd vapor})} - h_{L(\text{sat'd liquid})}}$$

all determined at z_F.

Note that $H_V > h_F > h_L$, $0 < q < 1$.

Subcooled Liquid Feed – Given *c*

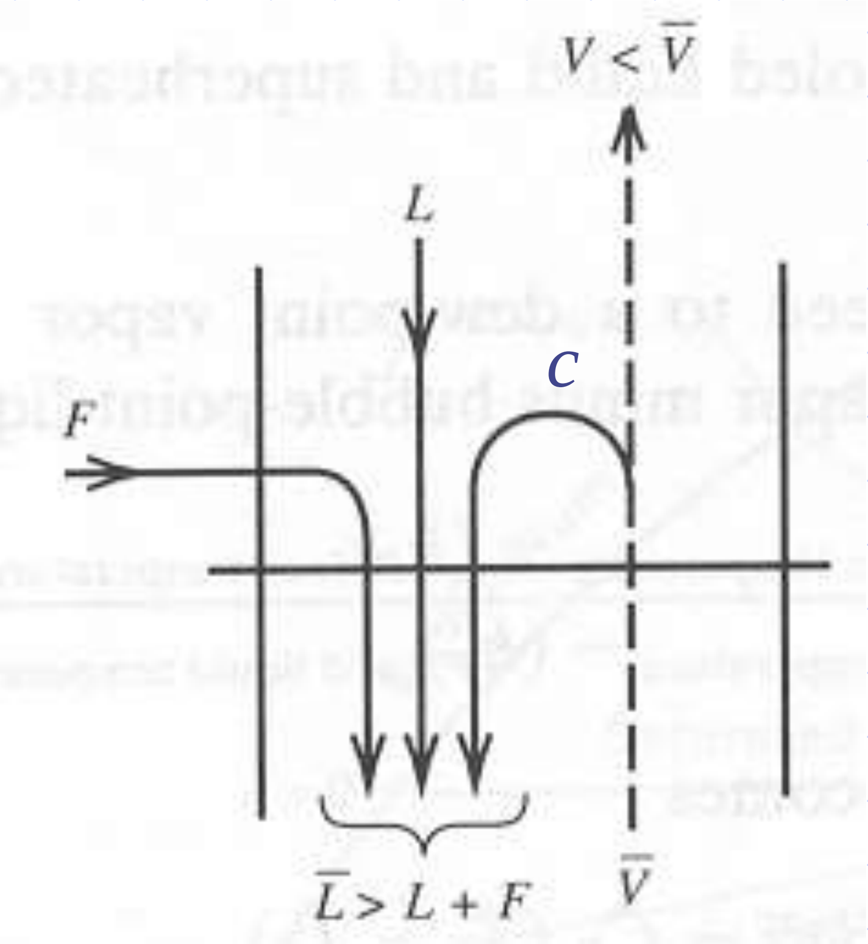


c is the amount of $\underline{V}$ condensed.

$$q = \frac{\underline{L} - L}{F} = \frac{(L + F + c) - L}{F} = 1 + \frac{c}{F}$$

Note that $q > 1$.

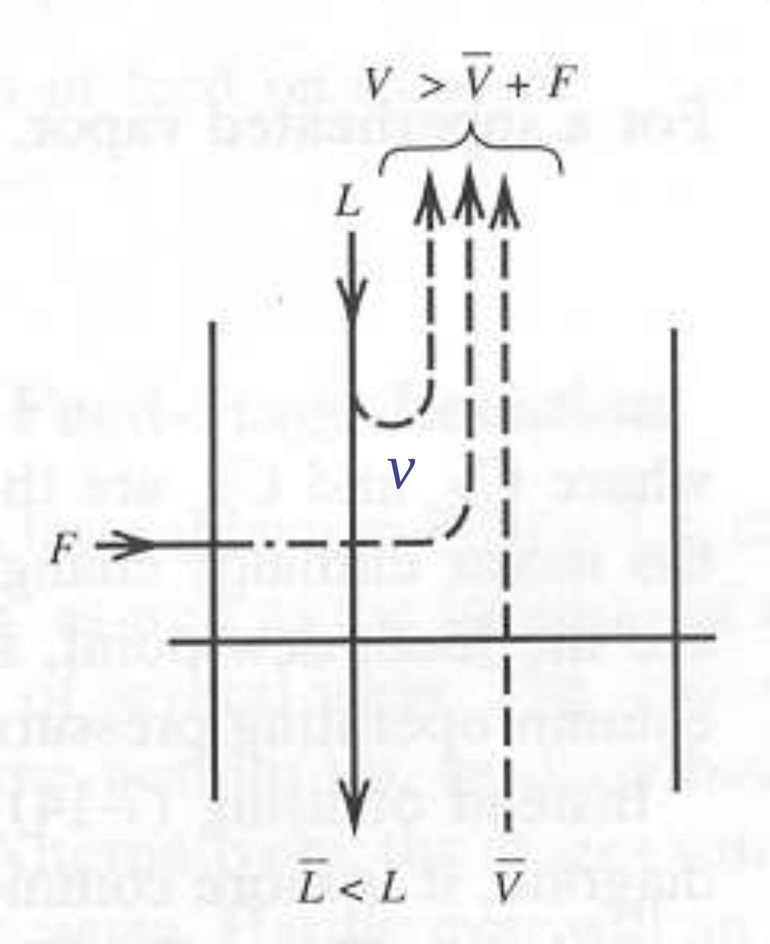
Subcooled Liquid Feed – Given $T_F < T_{bp}$



$$q = 1 + \frac{C_{PL}(T_{bp} - T_F)}{\lambda}$$

Note that $T_F < T_{bp}$, $q > 1$.

Superheated Vapor Feed – Given *v*

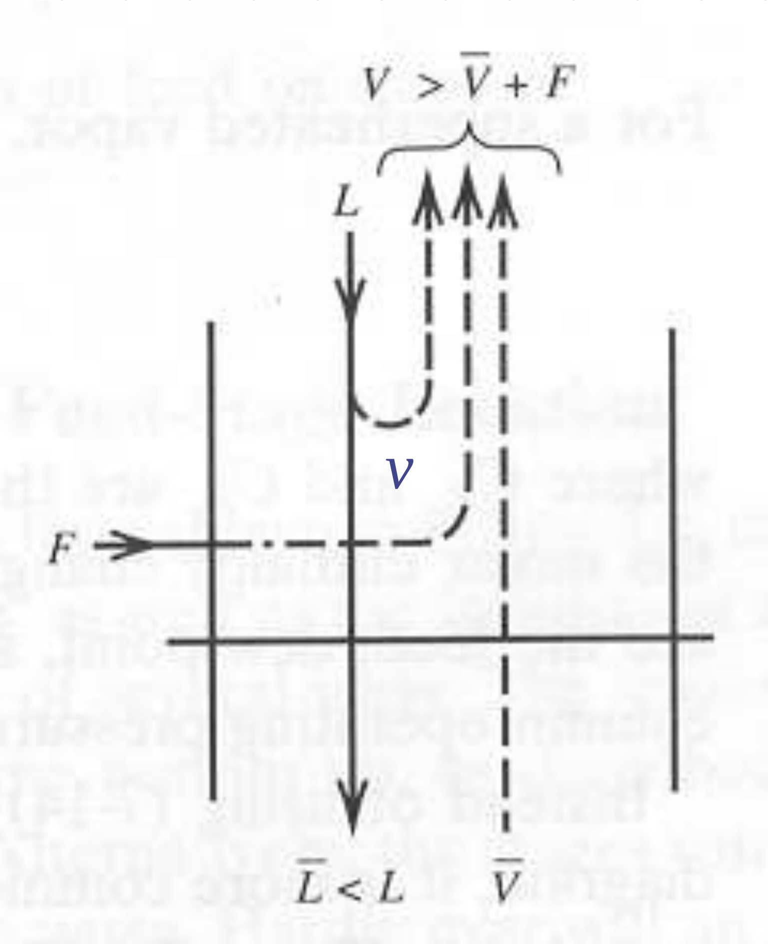


v is the amount of L vaporized.

$$q = \frac{\underline{L} - L}{F} = \frac{(L - v) - L}{F} = -\frac{v}{F}$$

Note that q < 0.

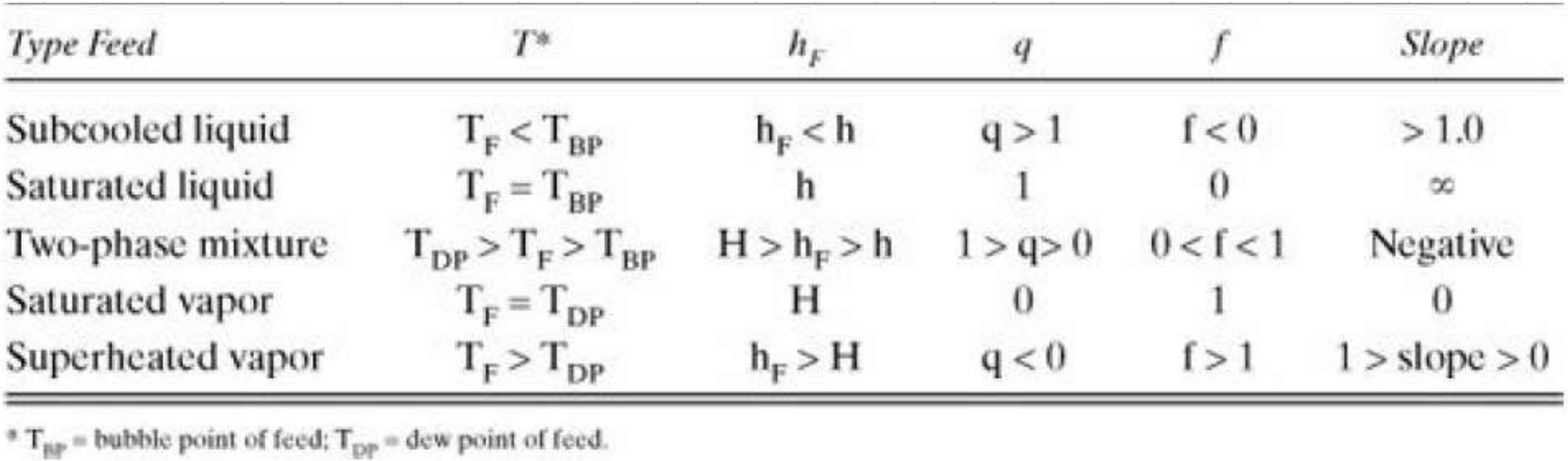
Superheated Vapor Feed – Given $T_F > T_{dp}$



$$q = \frac{C_{PV}(T_{dp} - T_F)}{\lambda}$$

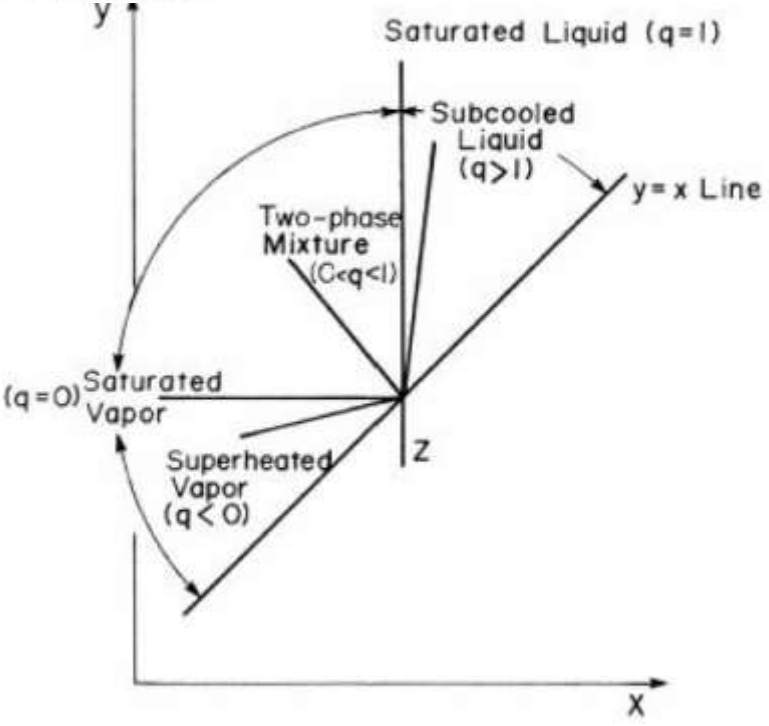
Note that $T_F > T_{dp}$, $q < 0$.

Possible Feed Lines: summary



Type Feed	*T**	h_F	*q*	*f*	*Slope*
Subcooled liquid	$T_F < T_{BP}$	$h_F < h$	$q > 1$	$f < 0$	> 1.0
Saturated liquid	$T_F = T_{BP}$	h	1	0	∞
Two-phase mixture	$T_{DP} > T_F > T_{BP}$	$H > h_F > h$	$1 > q > 0$	$0 < f < 1$	Negative
Saturated vapor	$T_F = T_{DP}$	H	0	1	0
Superheated vapor	$T_F > T_{DP}$	$h_F > H$	$q < 0$	$f > 1$	$1 > \text{slope} > 0$

* T_{BP} = bubble point of feed; T_{DP} = dew point of feed.



MC Cabe Thiele method: assumptions

- *Main assumptions:*
  - *Total condenser*
  - *Pressure is constant in the column*
  - *VLE data for the binary system are available (y-x diagram)*
  - *CMO OL stripping and enriching*
  - Optimum feed location: intersection point of the two OL
- Principle of operation:
  - Internal reflux ratio R is calculated from external L/D
  - Stair procedure starting from x_d y_1
  - Switch off to the stripping section when feed is encountered
- Some definitions:
  - R_{min} is the L/V which is obtained when the OL goes though the intersection of the feed line with the equilibrium curve.
  - R cannot be lower than this value.
  - Optimum value of R must be higher than R_{min}: slope must be higher.

McCabe Thiele: Determine all of the information stated in the problem

- Configuration of the column
  - Operating Pressure
  - Total, partial or no condenser
  - Total, partial or no reboiler
  - Location of feed stream(s)
  - Location of side stream(s)
  - Location of product stream(s)
- Condition of streams (saturated, superheated or subcooled)
  - Distillate
  - Bottoms
  - Feed
  - Reflux
  - Boilup
- Flow rates and composition of streams
  - Distillate, x_D and D
  - Bottoms, x_B and B
  - Feed, z_F and F
  - Reflux, L/V or L/D
  - Boilup, $\underline{L}/\underline{V}$ or $\underline{V}/B$

Methodology for Complete McCabe-Thiele Solution

- Determine equilibrium relationship
  - Use convenient equilibrium equation – e.g., given relative volatility, α
  - Curve fit equilibrium data at P_{col} – y vs x and/or x vs y
- Setup operating line equations and equilibrium curves in proper format for stepping down or stepping up the column…
- Assume CMO when applicable

Methodology for Complete McCabe-Thiele Solution

- Determine Top Operating Line
  - Choose convenient TOL equation or derive
  - Utilize total and/or component mass balances to determine required variables (e.g., L, V, L/V, L/D) in TOL if not given
- Determine Bottom Operating Line
  - Choose convenient BOL equation or derive
  - Utilize total and/or component mass balances to determine required variables (e.g., L, V, L/V, V/B) in BOL if not given
- Determine Feed Line
  - Choose convenient feed line equation or derive
  - Utilize total and/or component mass balances to determine required variables (e.g., F or z_F,) for feed if not given
  - Utilize total and/or component mass balances to determine required variables (e.g., L, V, $\underline{L}$, $\underline{V}$, L_F, V_F,) for feed if not given
  - Use feed-stage relationships to determine q or f at feed conditions

Methodology for Complete McCabe-Thiele Solution

- Stepping Up the Column from the Reboiler
  - Equilibrium Curve

    $y_{Eq} = y_{Eq}(x_{Eq})$ – as normally expressed
  - Operating Line

    $x_{OL} = x_{OL}(y_{OL})$ – solve operating line for x
- Stepping Down the Column from the Condenser
  - Equilibrium Curve

    $x_{Eq} = x_{Eq}(y_{Eq})$ – solve equilibrium relationship for x
  - Operating Line

    $y_{OL} = y_{OL}(x_{OL})$ – as normally expressed
- Determine intersection of operating lines and/or feed line to determine when to switch from the TOL to the BOL by:
  - Solving TOL, BOL, and/or feed line equations algebraically

Intersection of OL's and Feed Line

Simultaneous solution of the enriching section and stripping section OL's and feed line yields their intersections, x_I and y_I:

$$x_I = \frac{\left(1-\frac{L}{V}\right)x_D + \left(\frac{\underline{L}}{\underline{V}}-1\right)x_B}{\frac{\underline{L}}{\underline{V}}-\frac{L}{V}}$$

Intersection of TOL with BOL

$$y_I = \frac{L}{V}x_I + \left(1-\frac{L}{V}\right)x_D$$

$$x_I = \frac{-(q-1)\left(1-\frac{L}{V}\right)x_D - z_F}{(q-1)\left(\frac{L}{V}\right)-q}$$

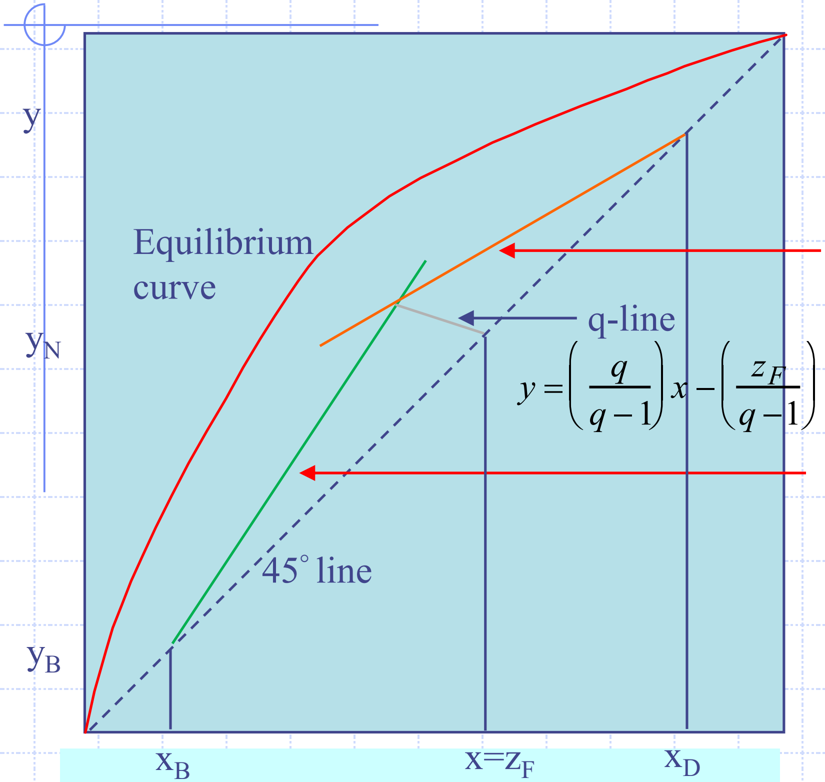
Intersection of TOL and FL

$$y_I = \frac{z_F + \frac{x_D q}{L_0/D}}{1+\frac{q}{L_0/D}}$$

Methodology for Complete McCabe-Thiele Solution

- Plot the equilibrium curve, TOL, BOL, and feed line
- Check the equations and plot by verifying that the:
  - TOL intersects $y = x$ at x_D
  - BOL intersects $y = x$ at x_B
  - Feed line intersects $y = x$ at z_F
  - OL's and feed line all intersect at x_I and y_I
- Implement McCabe-Thiele algorithm and plot stages
- Determine
  - total number of equilibrium stages
  - optimum feed stage
  - any fractional stages
- Answer specific questions,
  - e.g., liquid and/or vapor compositions for a given stage, number of stages above reboiler, condenser, etc.
- Keep in mind that a partial condenser and/or partial reboiler are each counted as an equilibrium stage outside the column!

Construction Lines for McCabe-Thiele Method



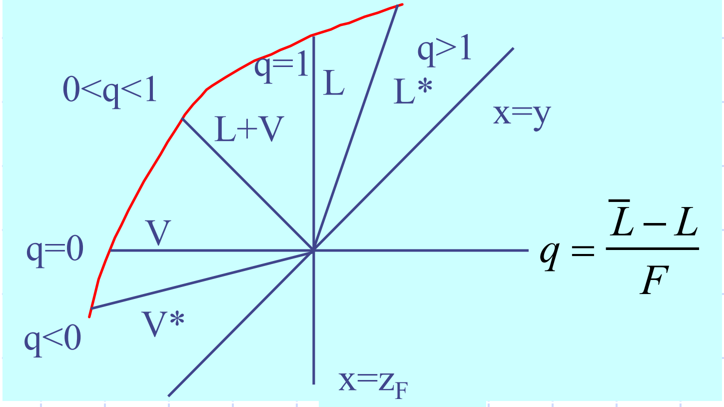
$$y=\left(\frac{q}{q-1}\right)x-\left(\frac{z_F}{q-1}\right)$$

Rectifying Section:
Operating line
Slope=L/V=R/(R+1)<1
With R= L/D

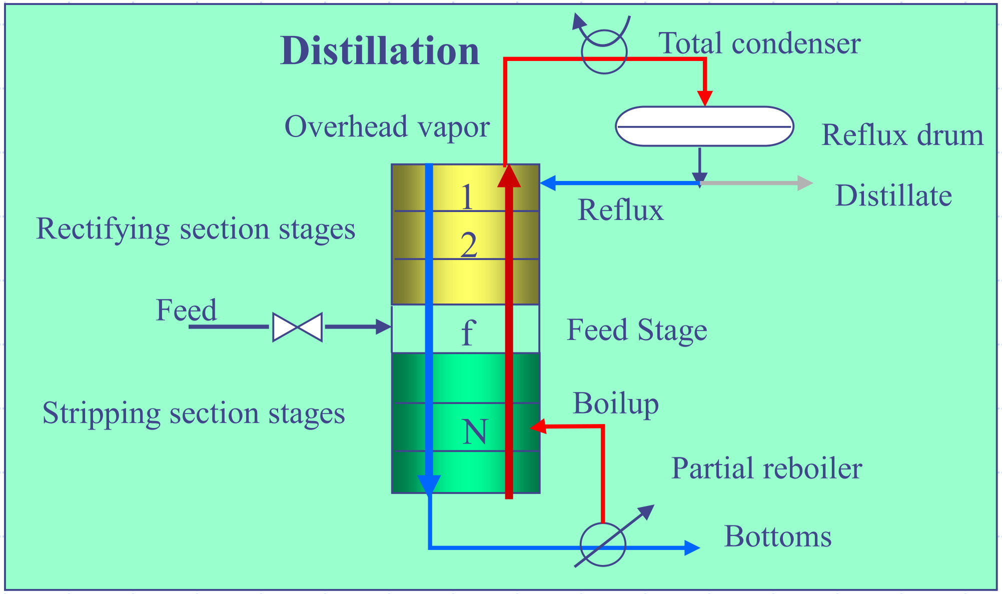
$$y=\frac{L}{V}x+\frac{D}{V}x_D$$

Stripping Section:
Operating line
Slope=$\underline{L}/\underline{V}=(V_B+1)/V_B$

$$y=\frac{\bar{L}}{\bar{V}}x-\frac{B}{\bar{V}}x_B$$

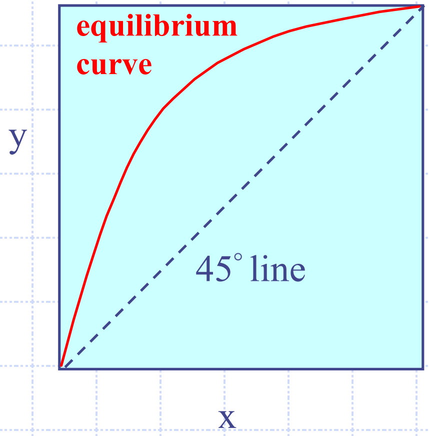


$$q=\frac{\bar{L}-L}{F}$$



Construction for the McCabe-Thiele Method

1.



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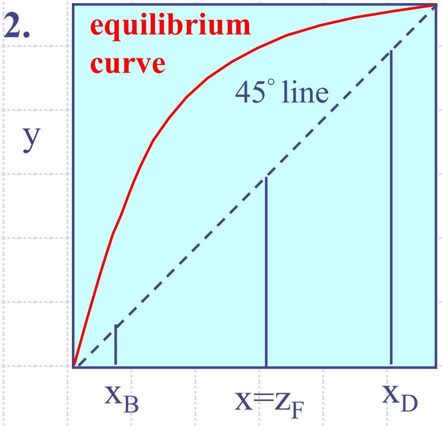
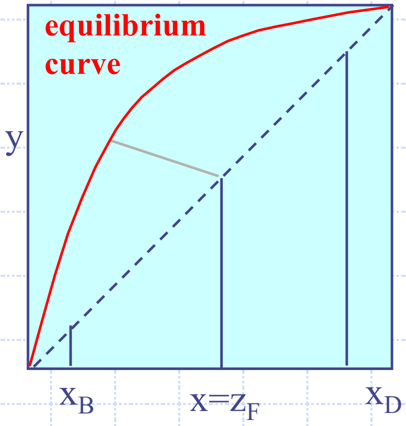
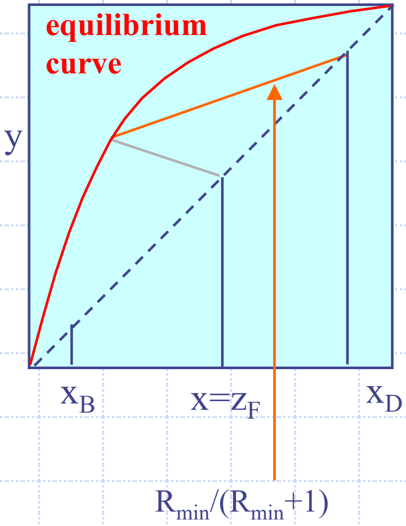


Step 1: Plot **equilibrium curve** and 45 degree line.
Step 2: Plot given compositions (F, B, and D)
Step 3: Draw **q-line** from L_F and V_F
Step 4: Determine R_{min} from intersection of the rectifying section OL and the equilibrium curve.
Step 5: Determine R from R/R_{min}
Step 6: Draw OL for **Rectifying section**
Step 7: Draw OL for **Stripping section**

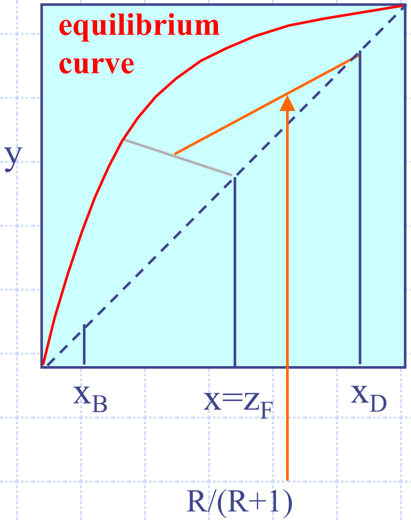
3.



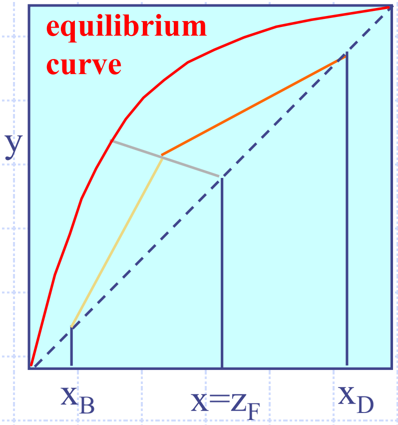
4.



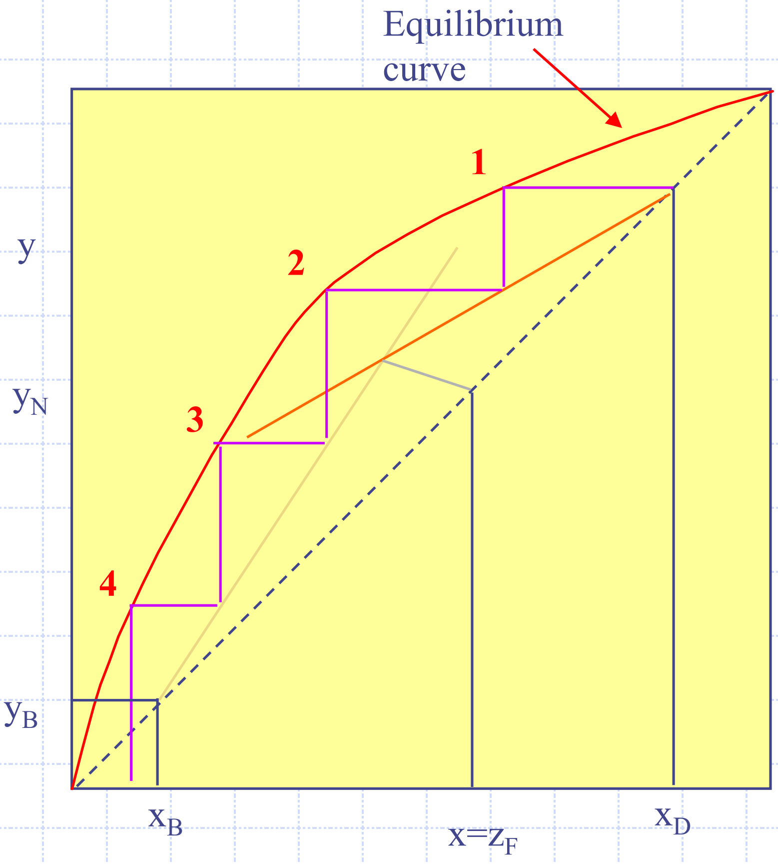
5. and 6.



7.



Determination of N and x_B for McCabe-Thiele



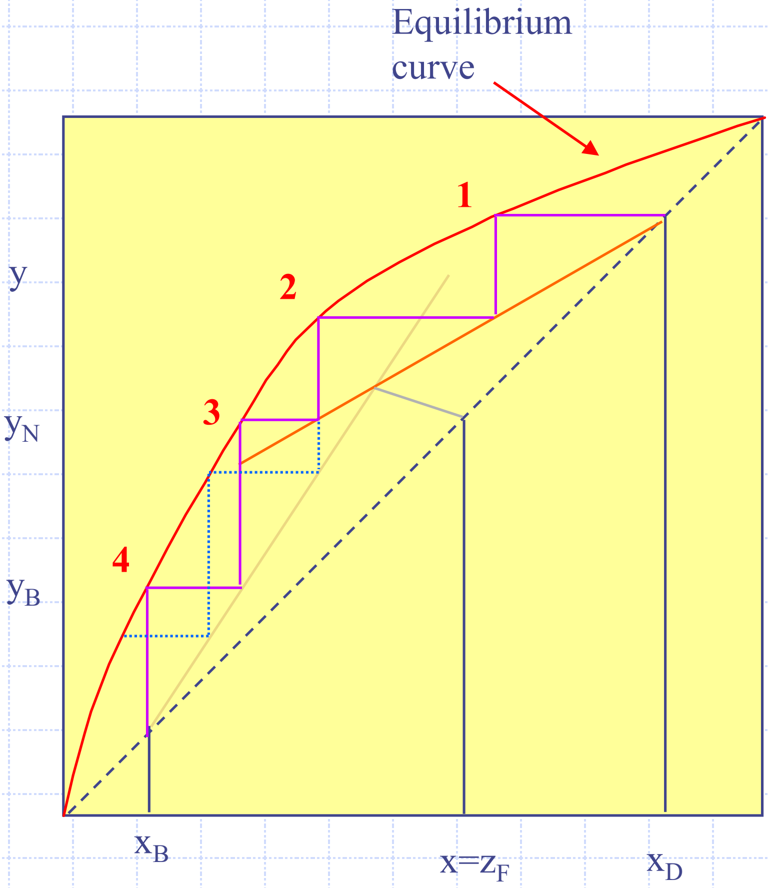
Construction:

Step 1: Plot **equilibrium curve** and 45 degree line.
Step 2: Plot given compositions (F, B, and D)
Step 3: Draw **q-line** from L_F and V_F
Step 4: Determine R_{min} from intersection of the Rectifying section OL and the equilibrium curve.
Step 5: Determine R from R/R_{min}
Step 6: Draw OL for **Rectifying section**
Step 7: Draw OL for **Stripping section**

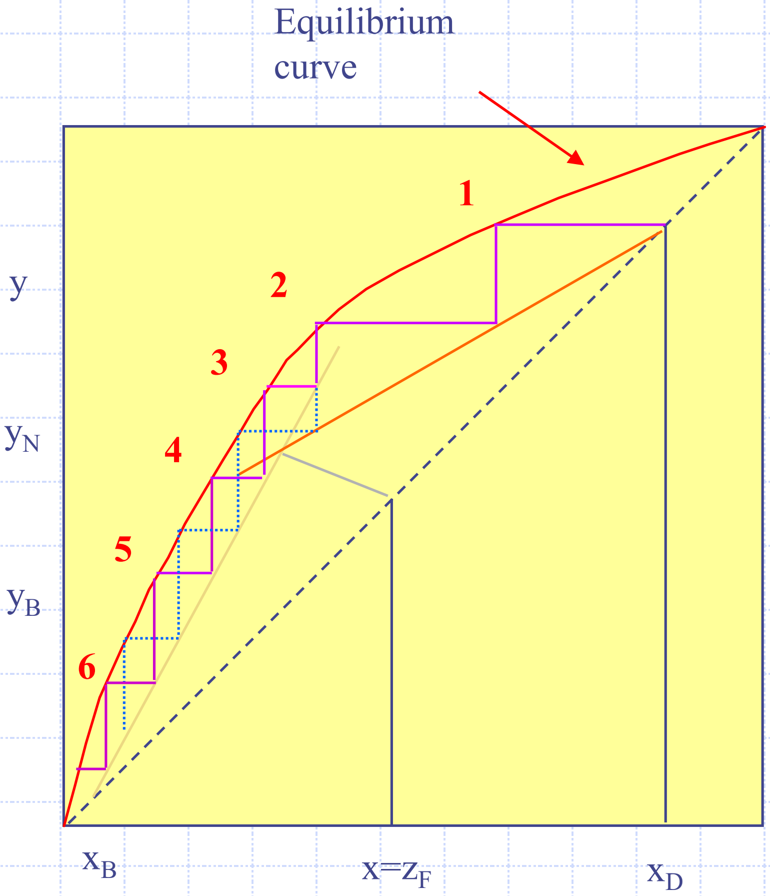
Solution:

Step 1: From x_D locate x_1 and y_1 drawing a horizontal line to the equilibrium condition for stage 1.
Step 2: Find y_2 drawing a vertical line to the rectifying OL locate the mass balance condition between x_1 and y_2.
Step 3: From y_2 draw a horizontal line to the equilibrium condition for stage 2 to locate x_2.
Step 4: Return to step 2 and cycle through steps 2 and 3 until $x_i < z_F$. Draw subsequent vertical lines to the **stripping section OL.**
Step 5: End after predetermined number of stages, or when x_i is less than x_B.

Feed Location for the McCabe-Thiele Method

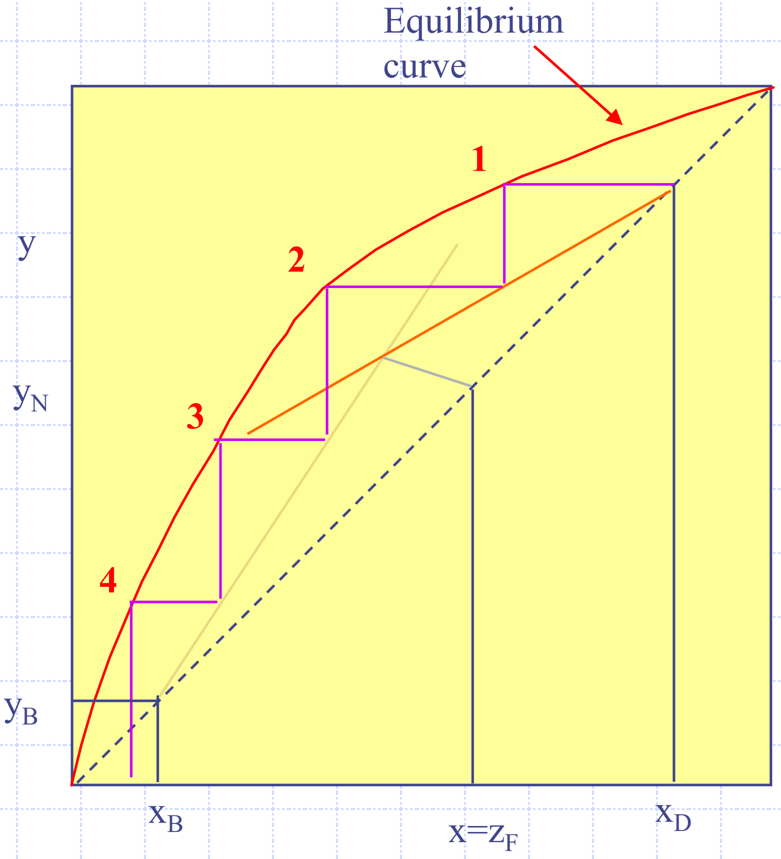


Feed stage located one tray too low.



Feed stage located one tray too high.

Optimum Feed Location for McCabe-Thiele



Optimum feed stage location.

Total Reflux: design case

- At total reflux:

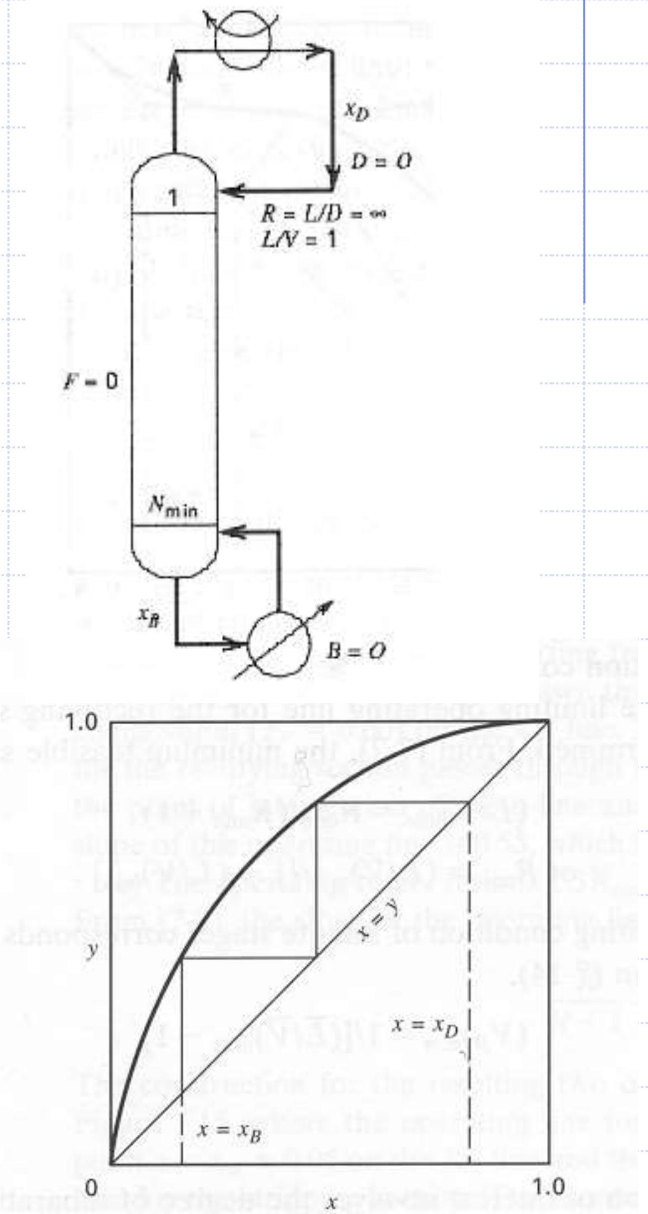
$$R = L/D = \infty$$

$$L/V = 1.0$$

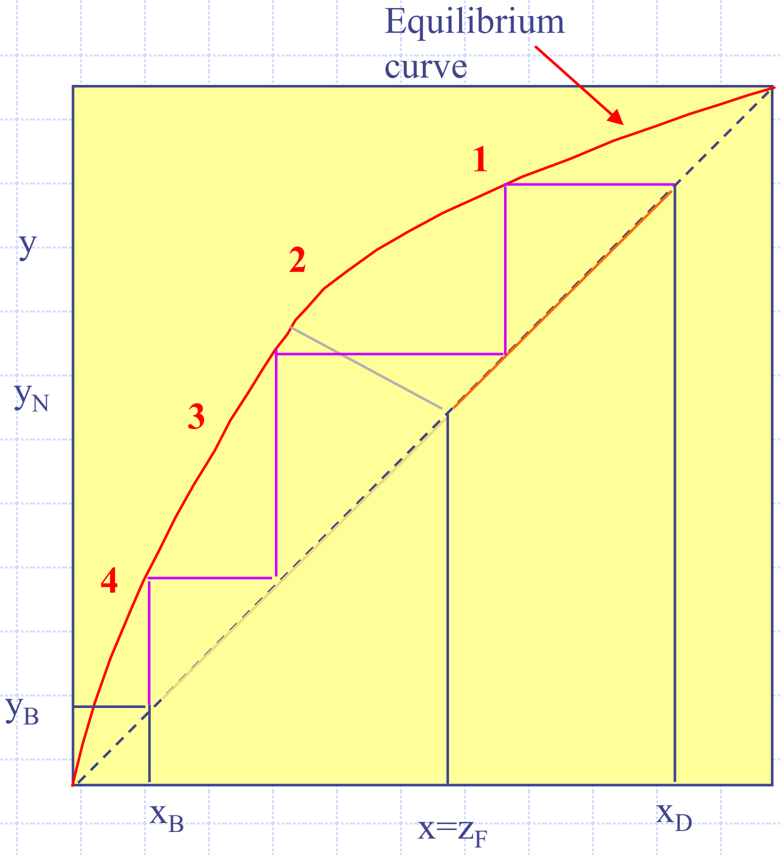
$$\bar{L} = \bar{V}$$

$$\bar{L}/\bar{V} = 1.0$$

- Both operating lines, TOL and BOL, become the y=x auxiliary line.
- Operating a column under total reflux yields the minimum number of equilibrium stages for a particular column.



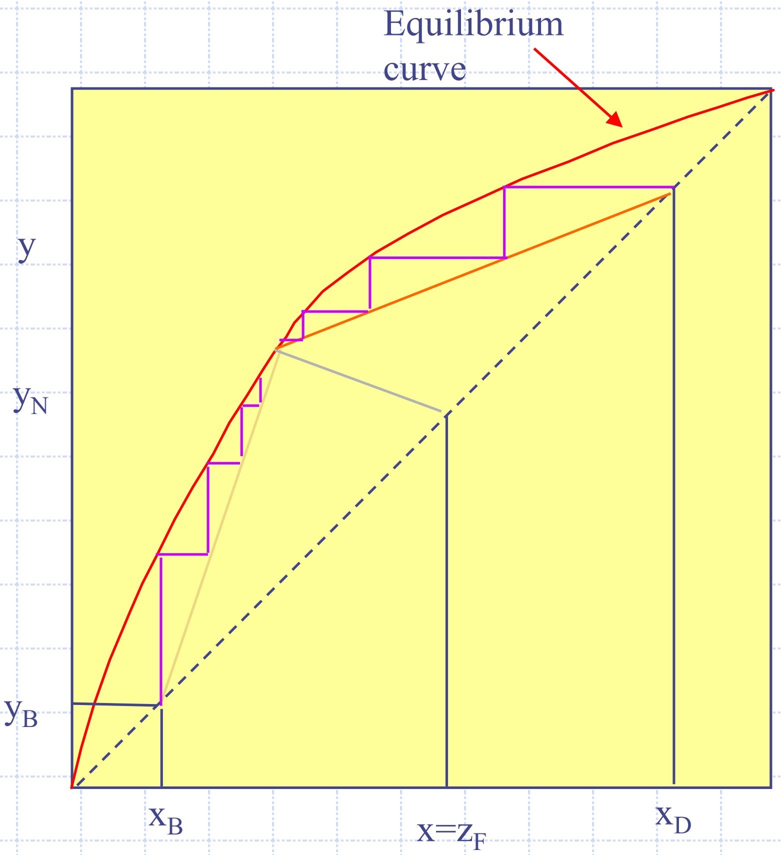
Minimum Number of Stages for McCabe-Thiele



By returning all the exiting vapor as reflux and all the exiting liquid as boilup the operating lines have slope of one.

Although this is the minimum number of stages, no product is produced (note the feed must then go to zero).

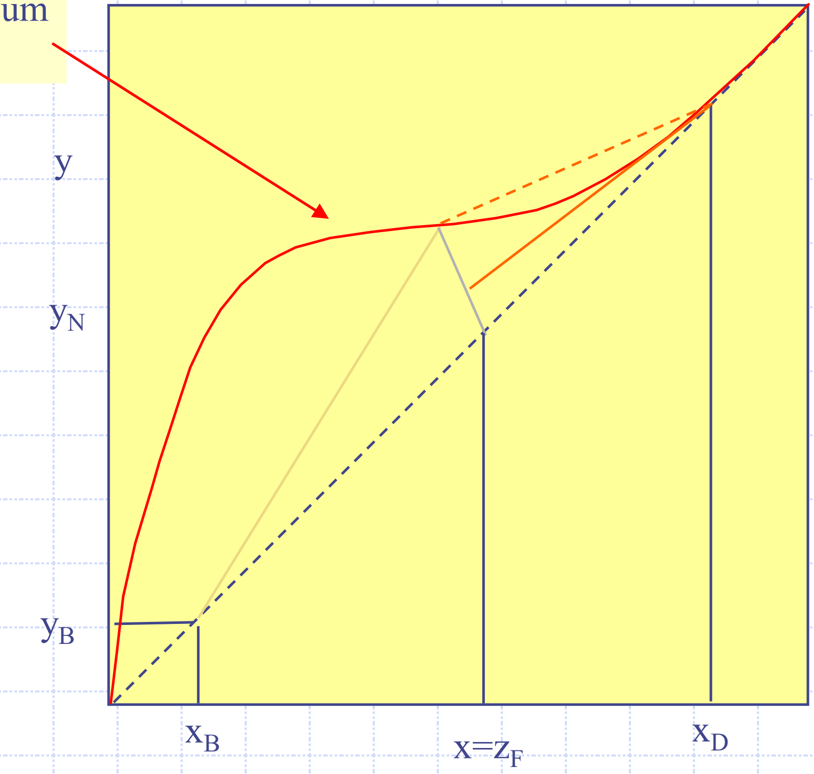
Minimum Reflux for McCabe-Thiele



By returning no exiting vapor as reflux and no exiting liquid as boilup the operating line intersection is as far to the left as equilibrium allows.

Although this is the minimum amount of reflux, it takes infinite stages (note the pinch point between the operating lines and equilibrium).

Minimum Reflux for Non-ideal McCabe-Thiele



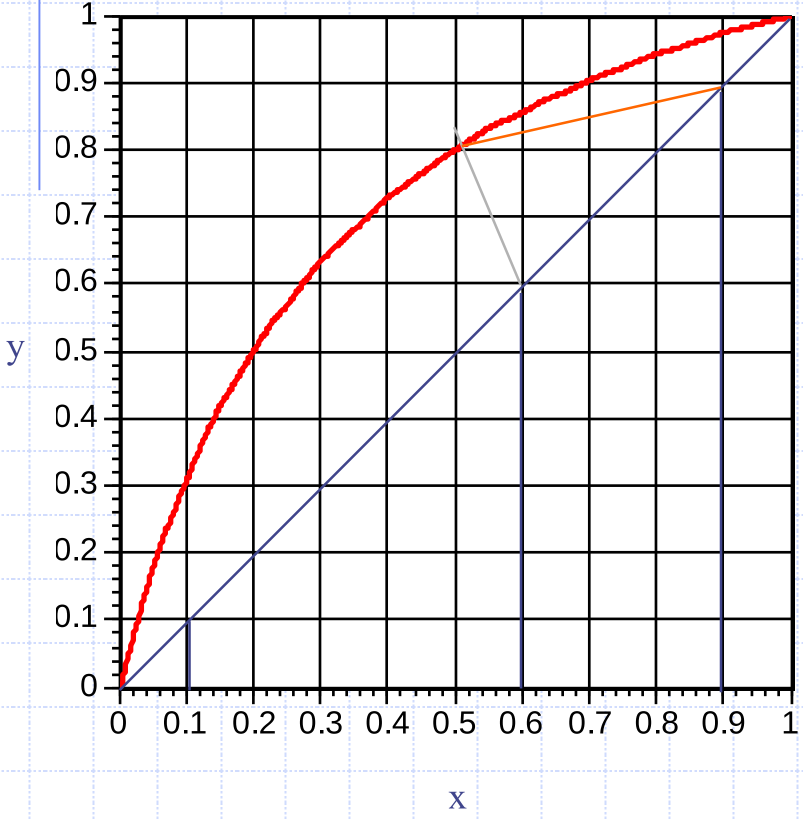
Equilibrium curve

Although this is the minimum amount of reflux, it takes infinite stages (note the pinch point between the operating lines and equilibrium).

Example: Determination of N and x_B for McCabe-Thiele

Given:

100 Kmol/hr of a feed of 60% benzene and 40% heptane is to be separated by distillation. The distillate is to be 90% benzene and The bottoms 10% benzene. The feed enters the column as 30mol% vapor. Use R 1.5 times the minimum. Assume a constant relative Volatility of $\propto$ of 4 and that the pressure is constant throughout the column at 1atm.



Construction:

Step 1: Plot **equilibrium curve** and 45 degree line.

The equilibrium curve is found using:

$$y = \frac{\alpha x}{1 + x(\alpha - 1)}$$

Step 2: Plot given compositions (F, B, and D)

Step 3: Draw **q-line** from L_F and V_F. Use

$$q = \frac{\bar{L} - L}{F} = \frac{L + L_F - L}{F} = \frac{L_F}{F} = 0.7$$

to find q. Then plot the q-line using:

$$y = \left(\frac{q}{q-1}\right)x - \left(\frac{z_F}{q-1}\right) = -2.333x + 2$$

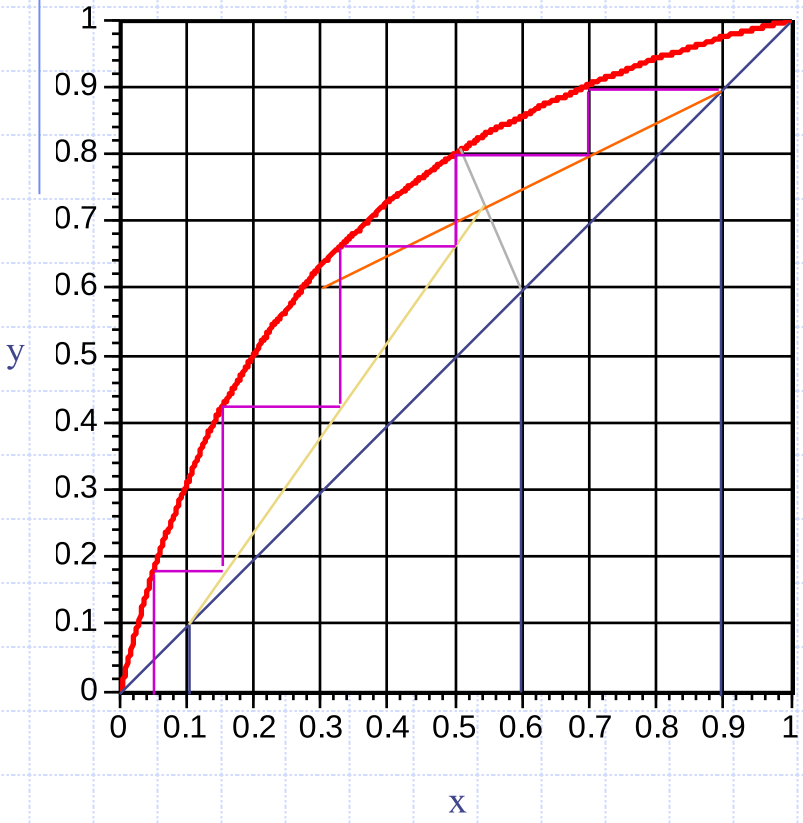
Step 4: Determine R_{min} from intersection of the rectifying section OL and the equilibrium curve. This happens at a slope of about .25

$$0.25 = \frac{R_{\min}}{R_{\min} + 1} \Rightarrow R_{\min} = 0.333$$

Example: Determination of N and x_B for McCabe-Thiele

Given:

100 Kmol/hr of a feed of 60% benzene and 40% heptane is to be separated by distillation. The distillate is to be 90% benzene and The bottoms 10% benzene. The feed enters the column as 30mol% vapor. Use R 3 times the minimum. Assume a constant relative Volatility of $\propto$ of 4 and that the pressure is constant throughout the column at 1atm.



Construction:

Step 5: From R_{min}=0.333 and $R=3R_{min}$ we have R=1 And the slope of rectifying section OL is 0.5

Step 6: Draw the line with slope 0.5 which is the rectifying section OL.

Step 7. Draw the stripping section operating line from the Bottoms composition to the intersection of the rectifying section OL and the q-line.

Solution:

Step 1: From x_D locate x_1 and y_1 drawing a horizontal line to the equilibrium condition for stage 1.

Step 2: Find y_2 drawing a vertical line to the rectifying OL locate the mass balance condition between x_1 and y_2.

Step 3: From y_2 draw a horizontal line to the equilibrium condition for stage 2 to locate x_2.

Step 4: Return to step 2 and cycle through steps 2 and 3 until $x_i < z_F$.

Results:

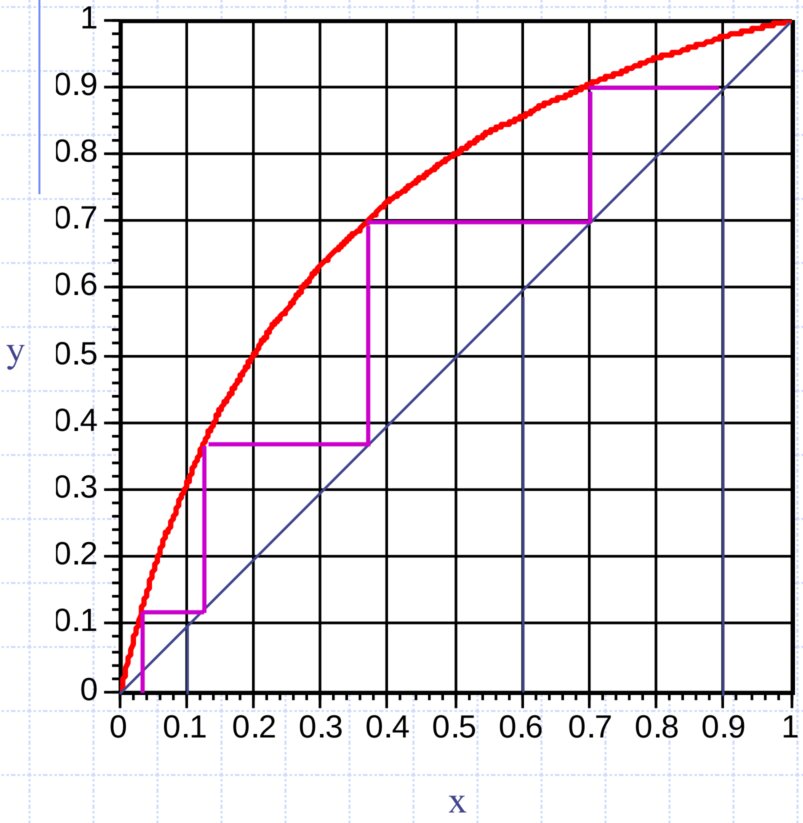
Feed at stage between 2 and 3. 5 stages (minimum stages = 3.2)

x_B=0.05% benzene

Example: Determination of N and x_B for McCabe-Thiele

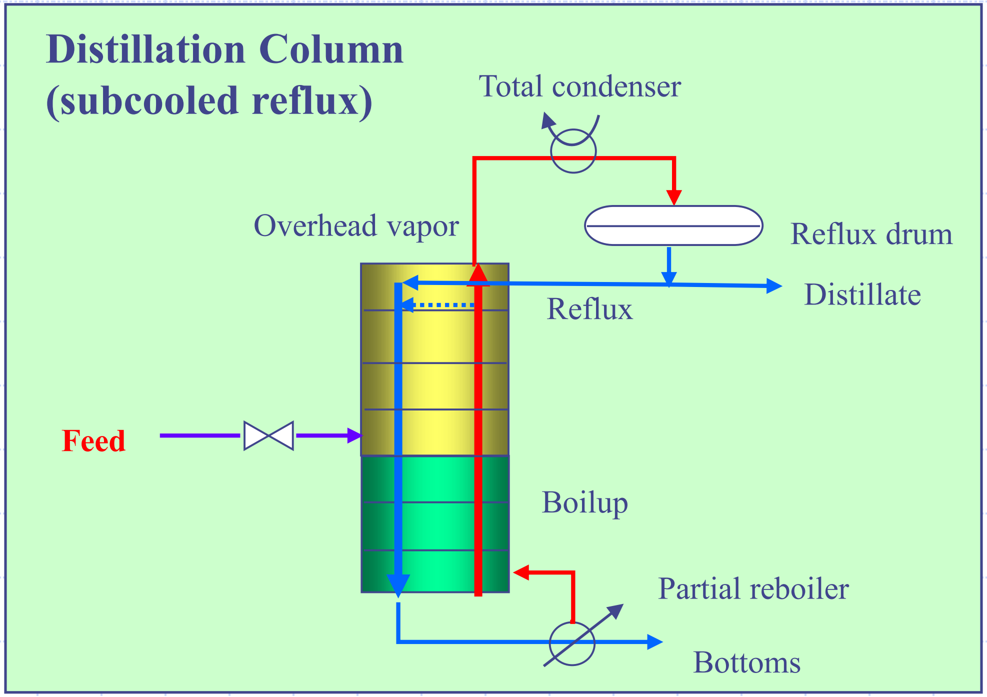
Given:

100 Kmol/hr of a feed of 60% benzene and 40% heptane is to be separated by distillation. The distillate is to be 90% benzene and The bottoms 10% benzene. The feed enters the column as 30mol% vapor. Use R 3 times the minimum. Assume a constant relative Volatility of ∝ of 4 and that the pressure is constant throughout the column at 1atm.



Minimum number of stages is determined by stepping off between the equilibrium curve and the 45 degree line.The result is 3.2 stages.

McCabe-Thiele Method: Subcooled Reflux



If the liquid reflux is colder than the bubble-point temperature, then it will condense some vapor in the top stage. This changes the reflux ratio to the internal reflux ratio.

McCabe-Thiele Method: Subcooled Reflux

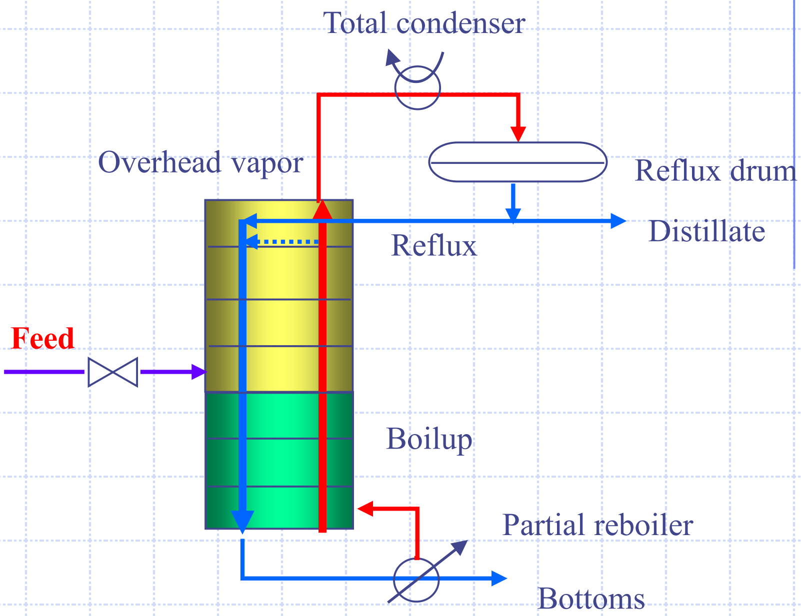
The amount of extra reflux that is produced depends on the heat capacity of the liquid, and the heat of vaporization of the vapor.

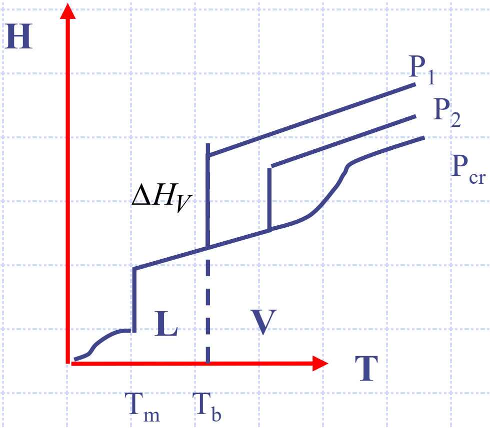
$$R' \Delta H^{vap} = R C_P^L \Delta T_{sub}$$

The total amount of reflux, called the internal reflux is the sum of the reflux ratio and the vapor condensed by the subcooled reflux:

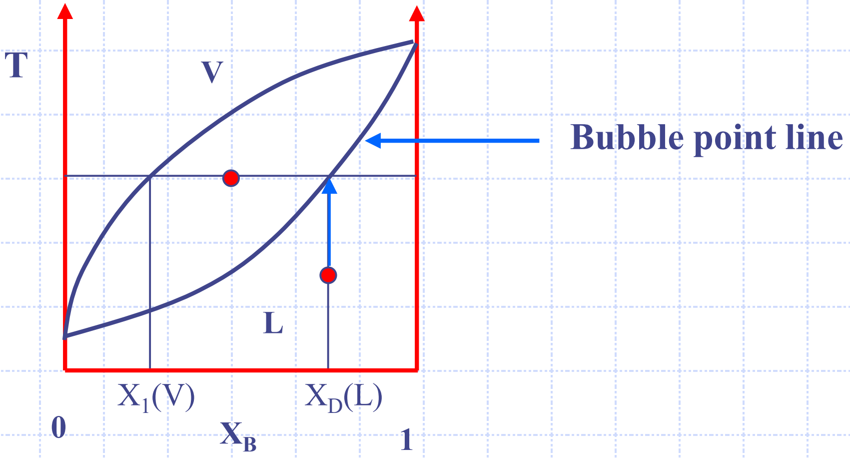
$$R_{\text{int}} = R + R'$$

$$R_{\text{int}} = R\left(1 + \frac{C_P^L \Delta T_{sub}}{\Delta H^{vap}}\right)$$

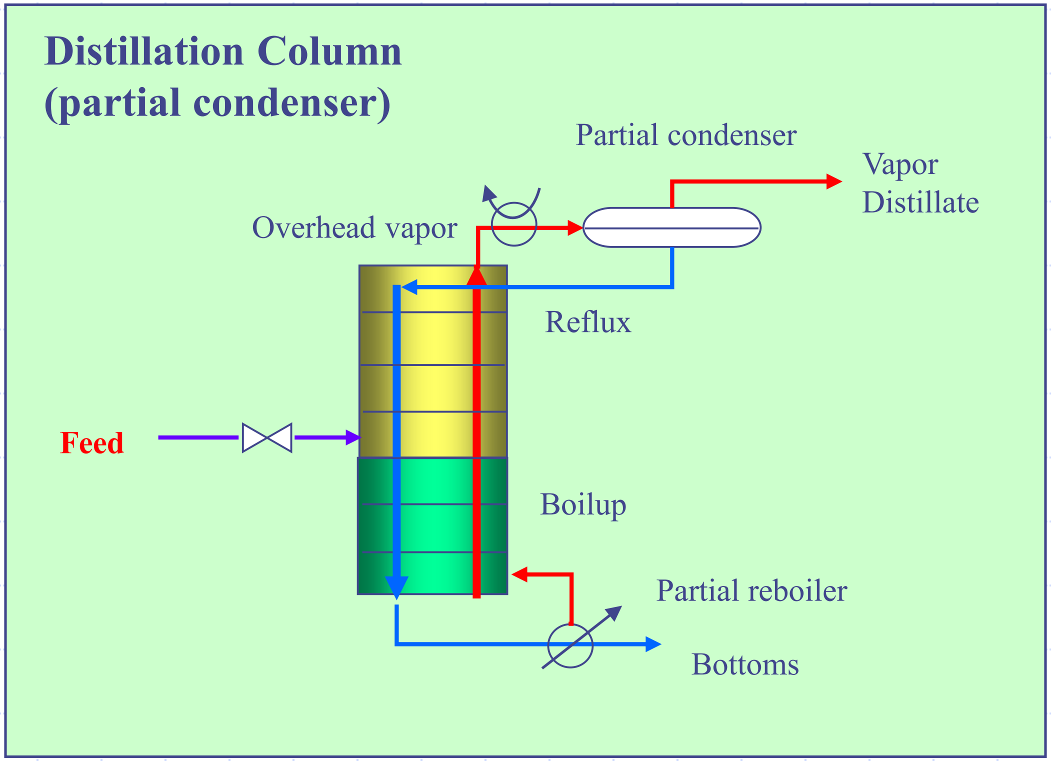




$$dH = C_P dT + V(1 - T\alpha)dP$$



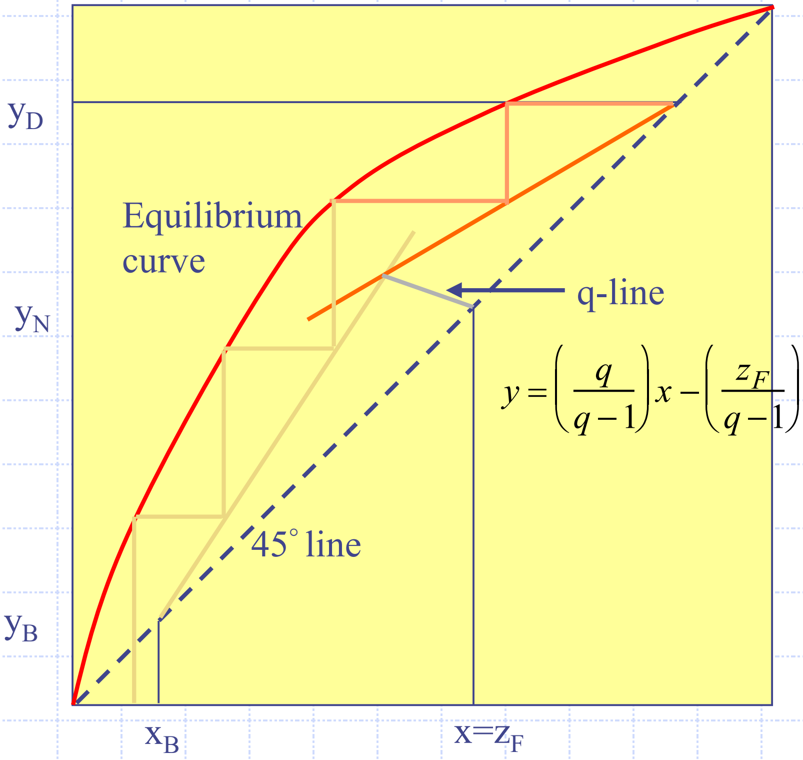
McCabe-Thiele Method: Partial Condenser



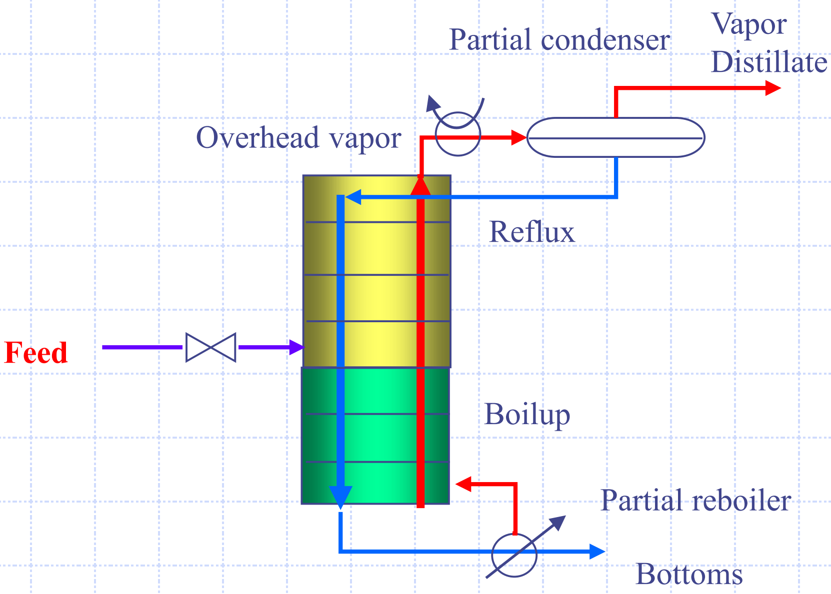
If the liquid reflux is obtained from a partial condenser, then the reflux is produced as the liquid in equilibrium with the vapor distillate in the condenser.

McCabe-Thiele Method: Partial Condenser

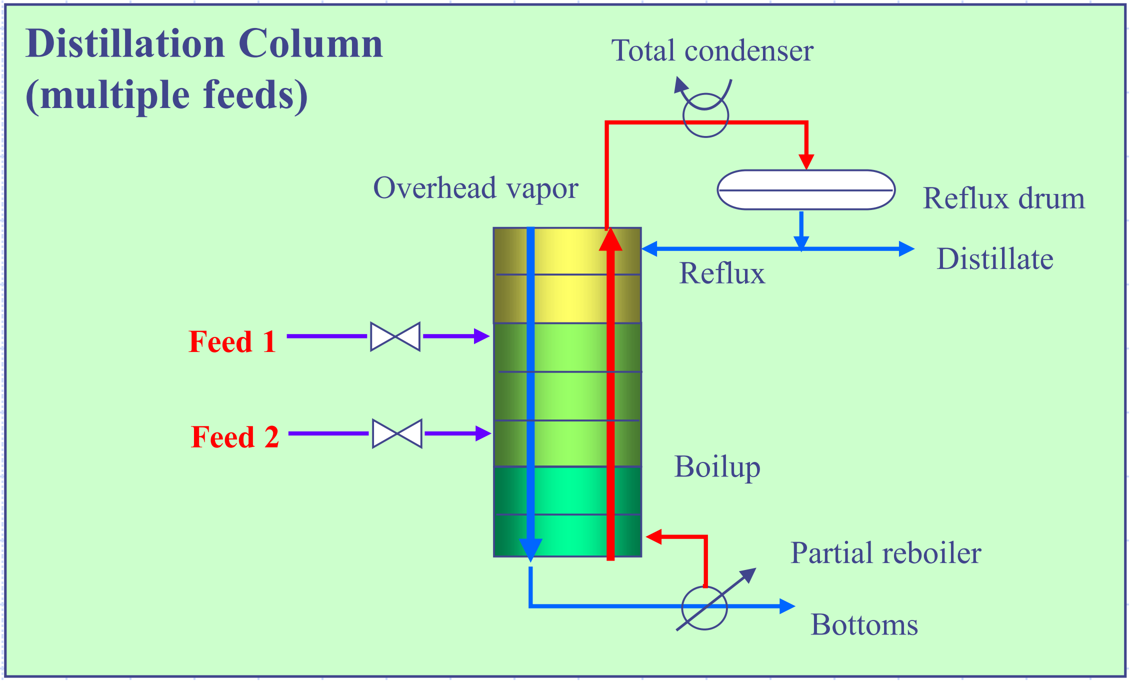
The vapor distillate composition then determines the y_D and stages are stepped off from the intersection of y_D and the equilibrium curve.



$$y=\left(\frac{q}{q-1}\right)x-\left(\frac{z_F}{q-1}\right)$$



McCabe-Thiele Method: Multiple Feeds



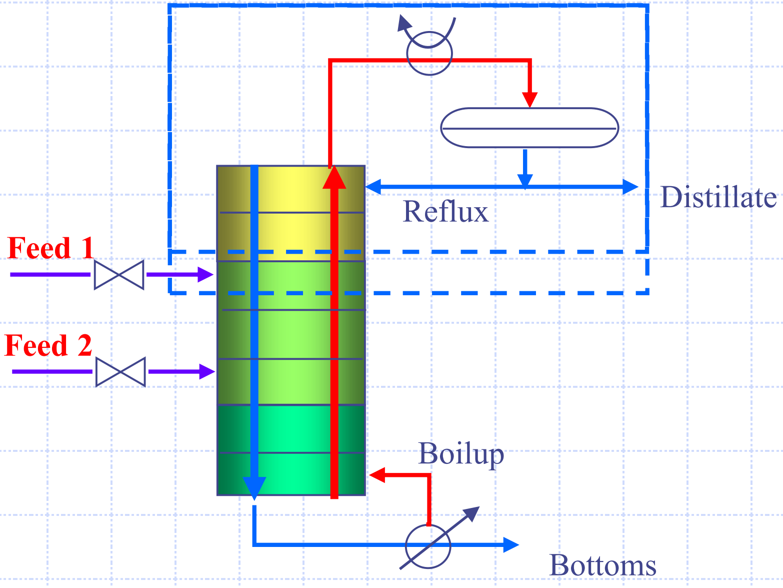
The McCabe-Thiele method for cascades can be applied to systems with more than two sections. Here, we show a cascade with 2 feeds: A 3 section cascade.

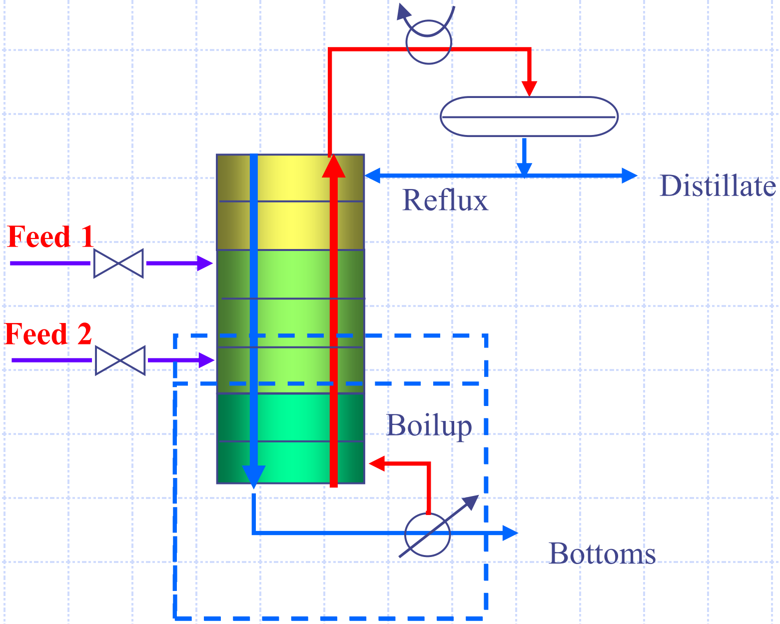
How do you make the McCabe-Thiele graphical construction for such a cascade?

McCabe-Thiele Method: Multiple Feeds

First, note that each feed stream changes the slope of the operating line from section to section.

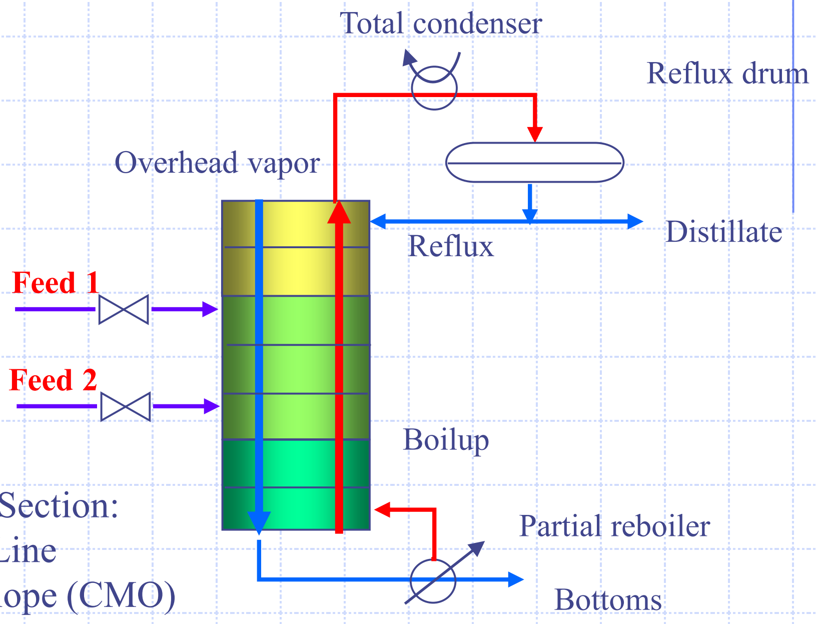
The feed stream changes the flow rates in the stages above and below it. Consequently, it changes the mass balances and the slopes of the operating lines.

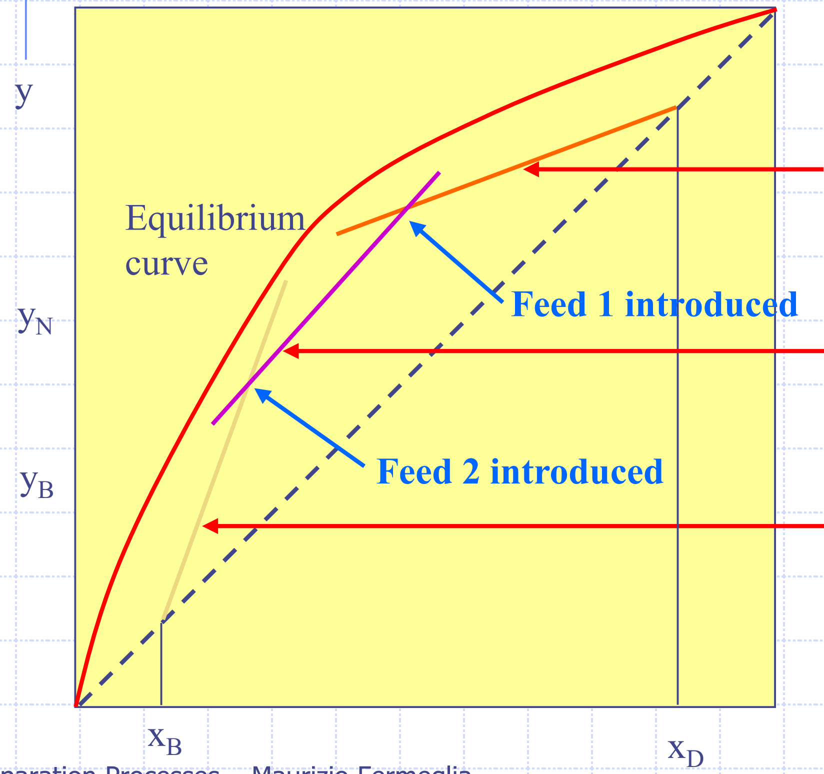




McCabe-Thiele Method: Multiple Feeds

The flow rates above Feed 1 are constant due to constant molar overflow (CMO). The feed changes the slope depending on the feed condition. Flow rates in the intermediate section are constant, but change when Feed 2 is introduced.





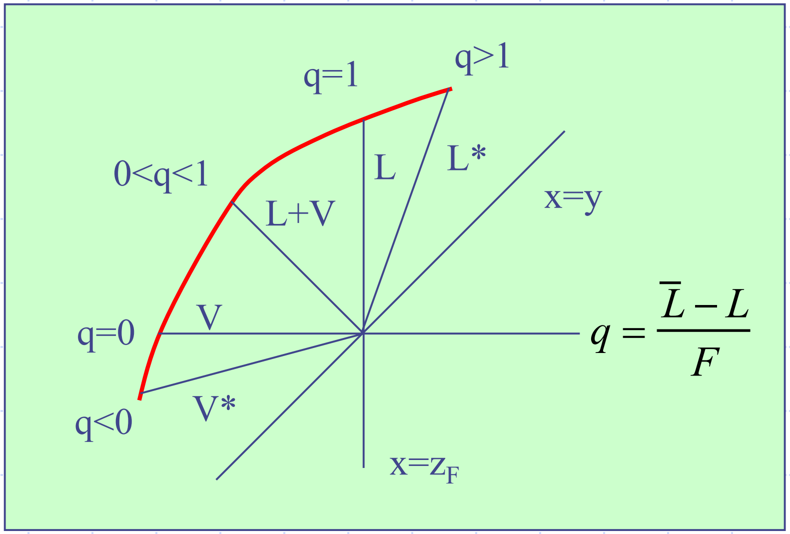
Rectifying Section:
Operating Line
Constant Slope (CMO)

Intermediate section:
Operating Line
Constant Slope (CMO)

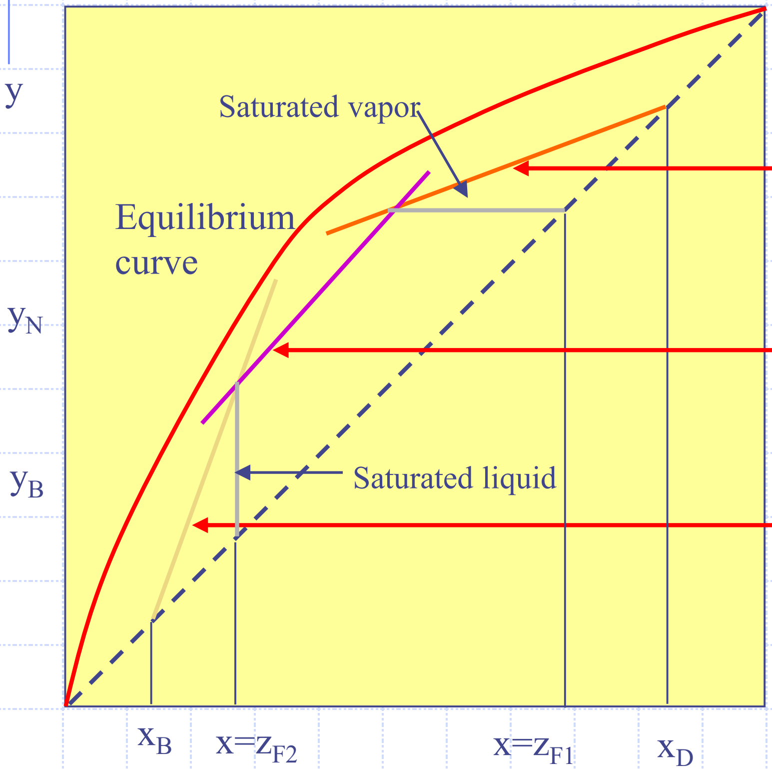
Stripping Section:
Operating Line
Constant Slope (CMO)

McCabe-Thiele Method: Multiple Feeds

Example: Feed 1 a saturated vapor of composition z_{F1}, and Feed 2 a saturated liquid of composition z_{F2}



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



Rectifying Section:
Operating line
Slope=L/V=R/(R+1)<1

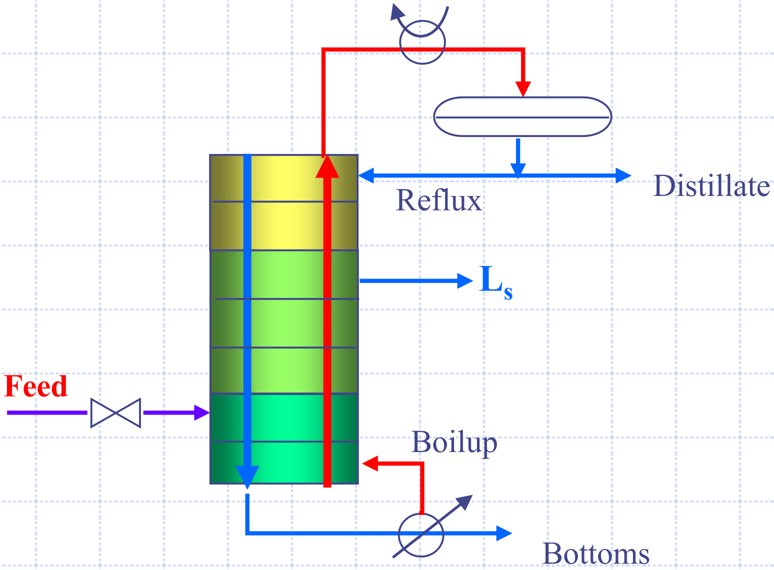
Intermediate section:
Operating line
Slope=L'/V'

Stripping Section:
Operating line
Slope=$\underline{L}/\underline{V}=(V_B+1)/V_B$

McCabe-Thiele Method: Side Stream

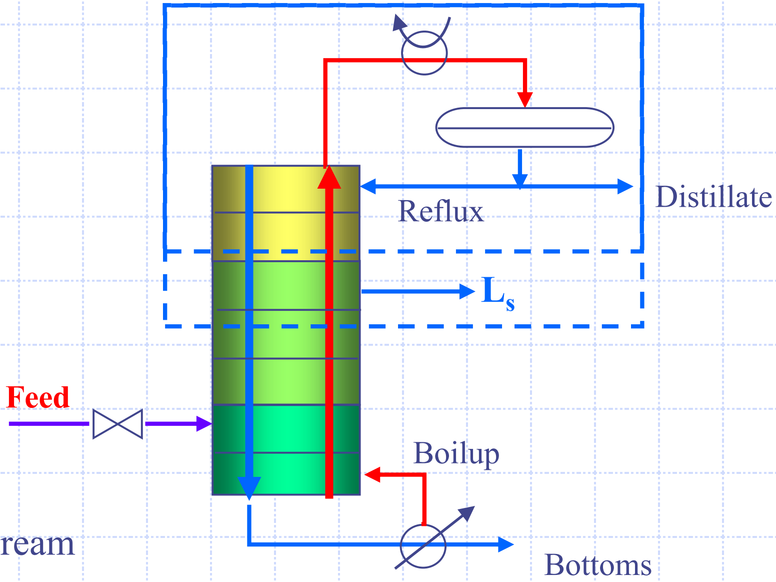
Occasionally a cascade is configured such that an intermediate side stream of intermediate composition is removed from the column.

How do we analyze this configuration?



Use the multiple mass balance envelopes and assume a constant molar overflow condition.

If we perform a **material balance** in the light key around the stages above the side stream including the condenser:



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

Which we can rearrange to find:

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

For L and V constant from stage to stage, then:

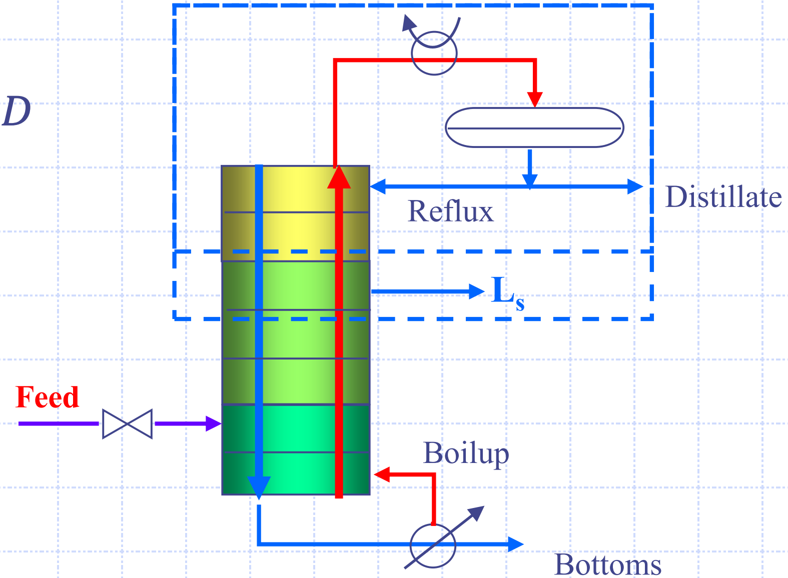
$$y = \frac{L}{V} x + \frac{D}{V} x_D$$

Operating line above side stream

McCabe-Thiele Method: Side Stream

If we perform a **material balance** in the light key around the stages above the side stream including the side stream and condenser:

$$V_{n+1}y_{n+1} = L_n x_n + L_s x_s + D x_D$$



Which we can rearrange to find:

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

For L and V constant from stage to stage, then:

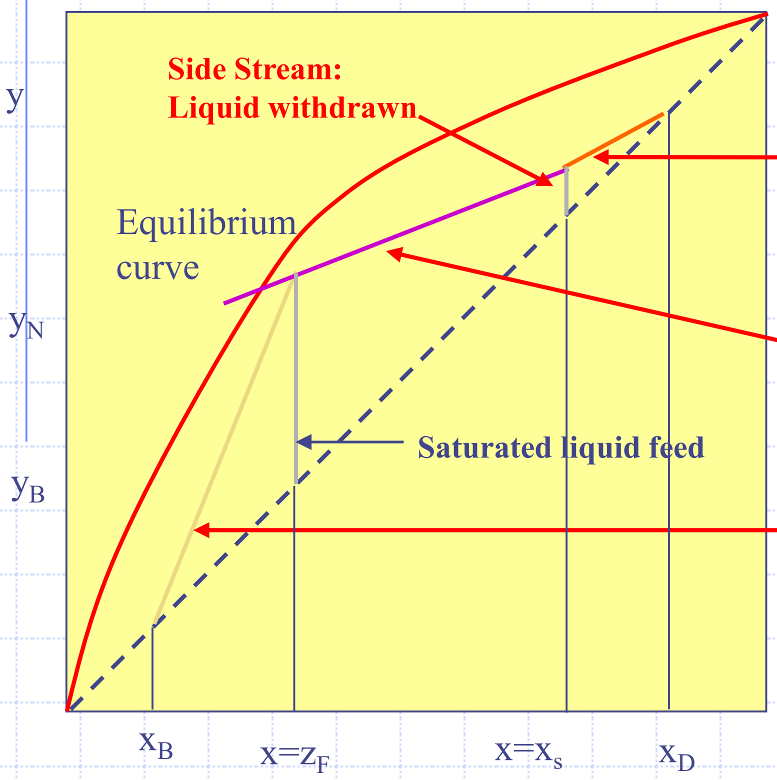
$$y = \frac{L'}{V} x + \frac{L_s x + D x}{V}$$

Operating line below side stream

The two operating lines intersect at :

$$x = x_s$$

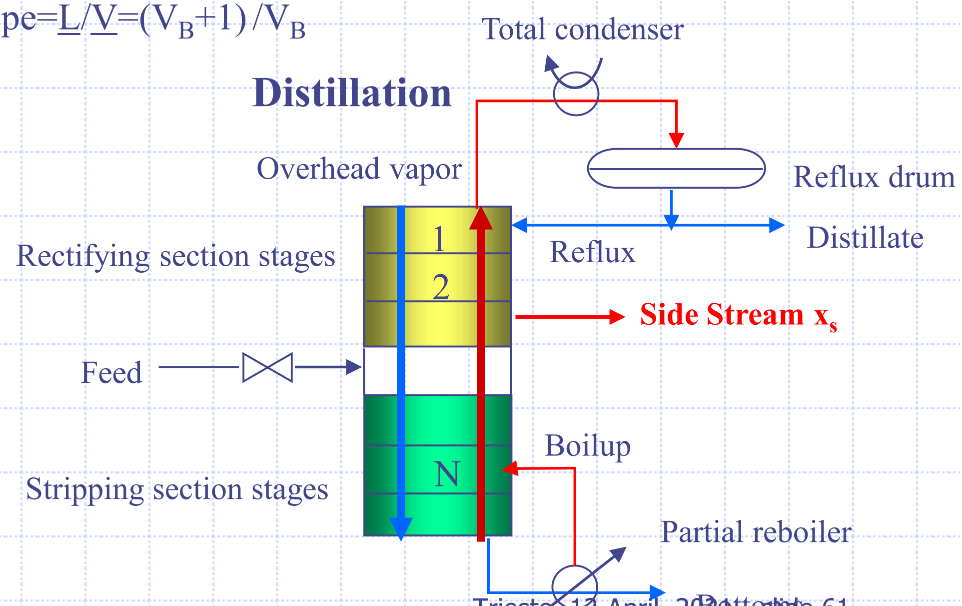
McCabe-Thiele Method: Side Stream



Rectifying Section:
Operating line
Slope=L/V=R/(R+1)<1

Intermediate section:
Operating line
Slope=L'/V

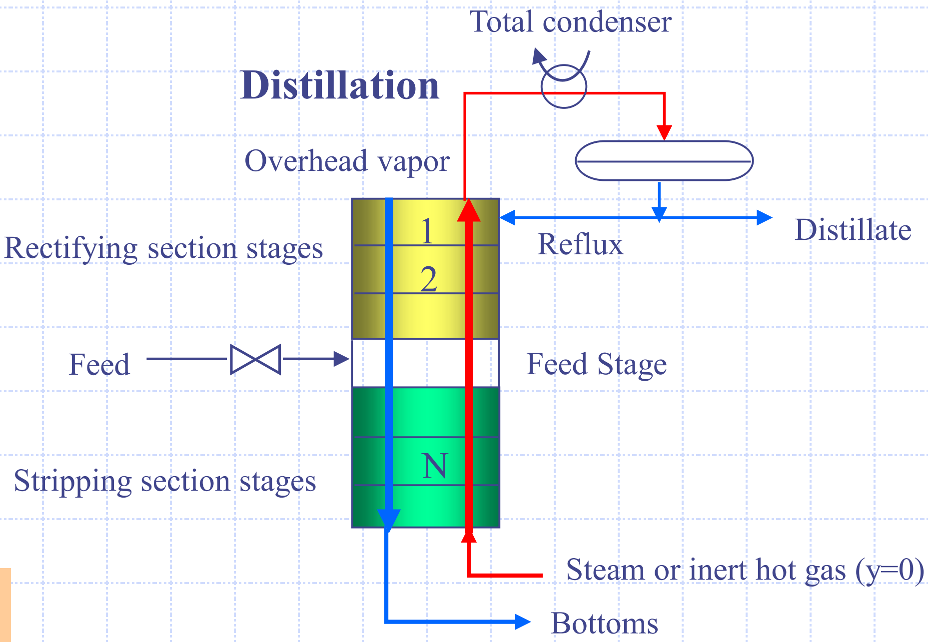
Stripping Section:
Operating line
$\text{Slope}=\underline{L}/\underline{V}=(V_B+1)/V_B$



McCabe-Thiele Method: Open Steam

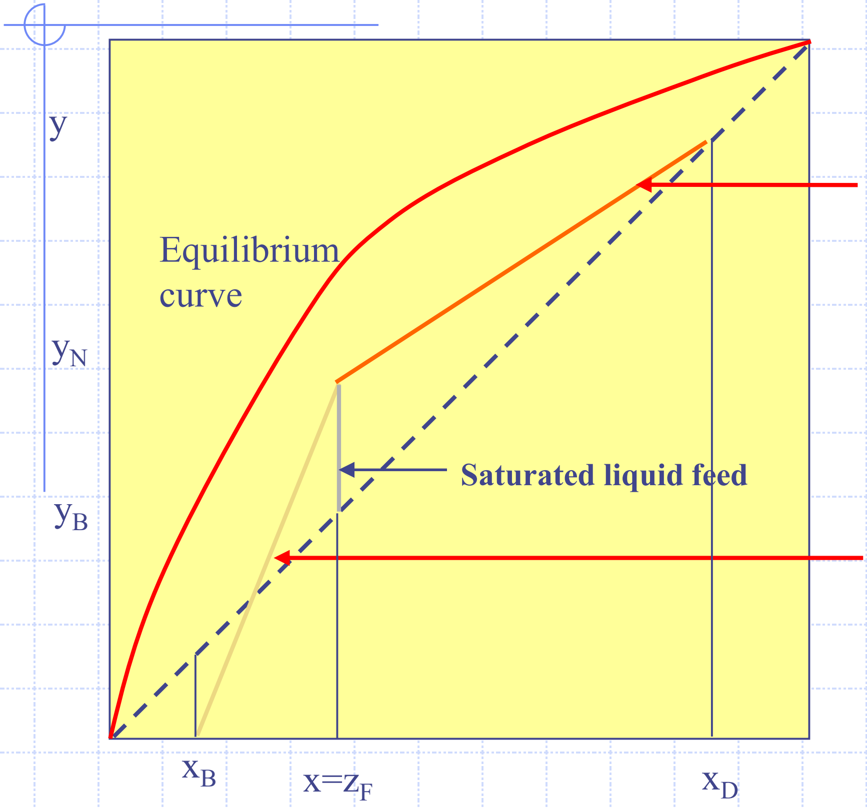
Consider the cascade shown on the left:

In this example, the reboiler is replaced by a source of hot steam or an inert gas. In this case, the vapor entering the bottom stage of the column has no light key and so y_B is zero, although x_B is non-zero.



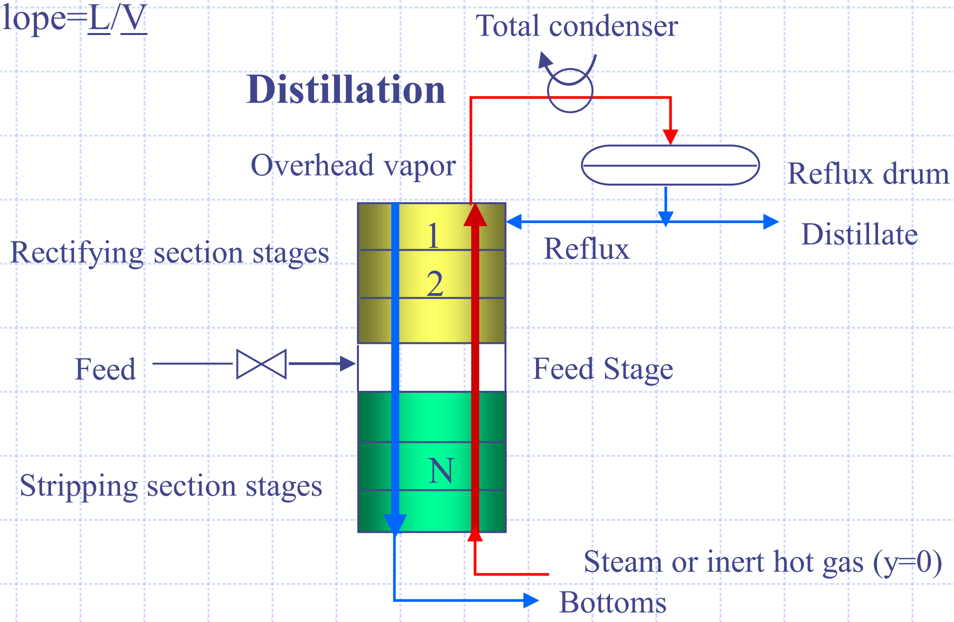
Does the slope of the rectifying section operating line increase or decrease?

McCabe-Thiele Method: Open Steam

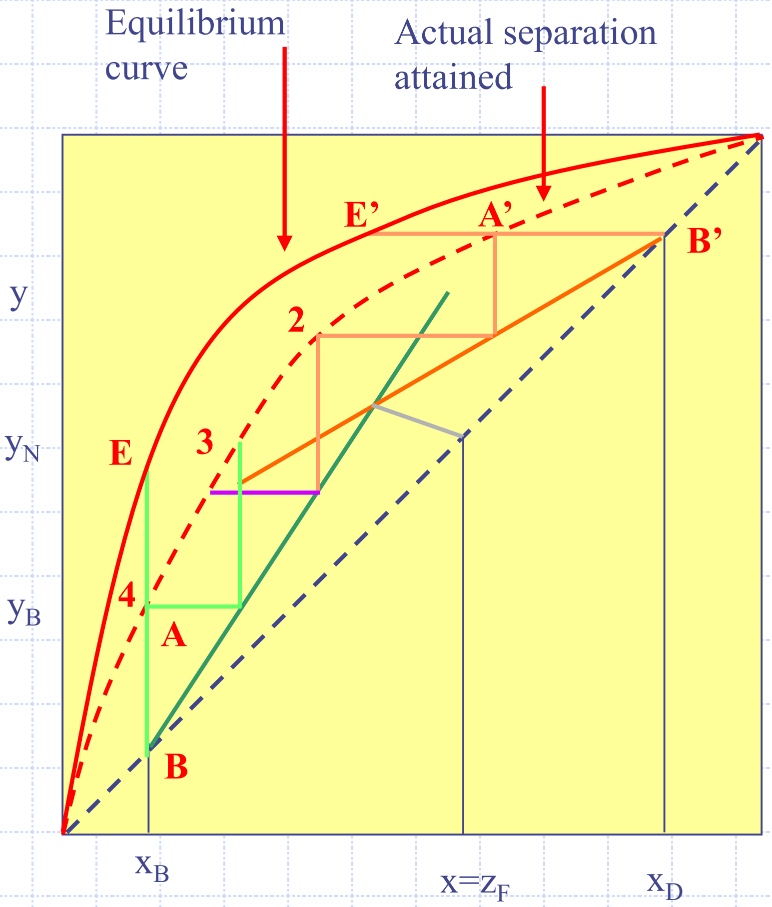


Rectifying Section:
Operating line
Slope=L/V=R/(R+1)<1

Stripping Section:
Operating line
Slope=$\underline{L}/\underline{V}$



Non-equilibrium McCabe-Thiele: Murphree Efficiency



Component distribution obtained less than theoretical limit described by equilibrium

The Murphree Plate Efficiency gives the ratio of the actual composition difference between two sequential plates, and that predicted by equilibrium.

For the vapor efficiency:

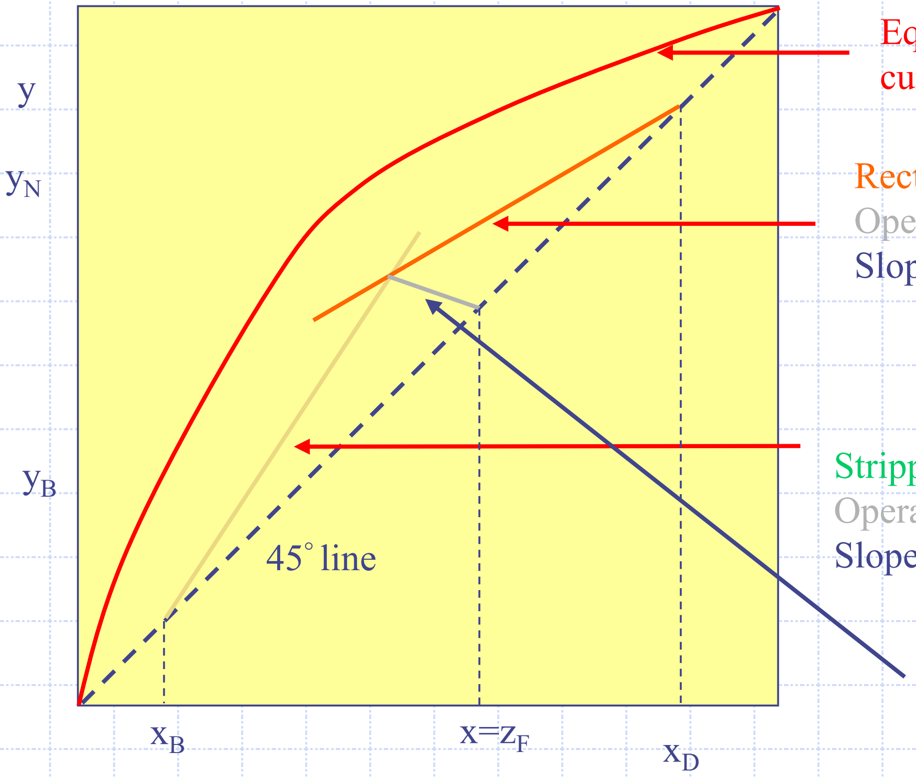
$$E_{MV} = \frac{y_n - y_{n+1}}{y_n - y_{n+1}} = \frac{\overline{AB}}{\overline{EB}}$$

For the liquid efficiency:

$$E_{ML} = \frac{x_n - x_{n+1}}{x_n - x_{n+1}} = \frac{\overline{A'B'}}{\overline{E'B'}}$$

McCabe-Thiele Algebraic Method

We have already developed the McCabe-Thiele **Graphical Method** for cascades. The same equations we used for the operating lines, q-line, and equilibrium curve can be used to solve for the compositions in each stage **algebraically**.



Equilibrium curve

$$y = \frac{\alpha x}{1 + x(\alpha - 1)}$$

Rectifying Section:
Operating line
Slope=L/V=R/(R+1)<1

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

Stripping Section:
Operating line
Slope=$\bar{L}/\bar{V}=(V_B+1)/V_B$

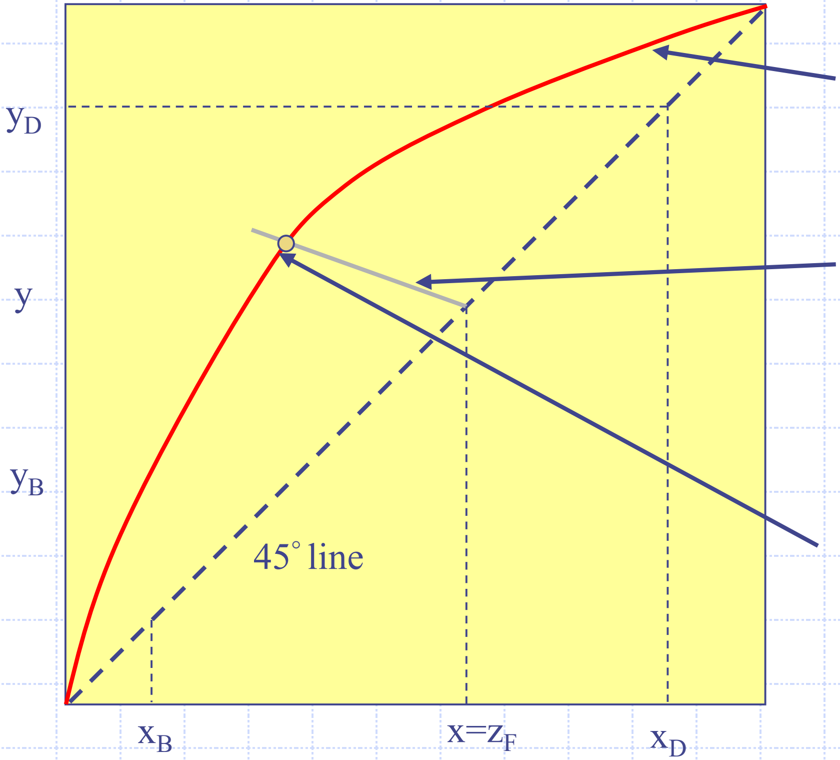
$$y = \frac{\bar{L}}{\bar{V}}x - \frac{B}{\bar{V}}x_B$$

$$y = \left(\frac{q}{q-1}\right)x - \left(\frac{z_F}{q-1}\right)$$

McCabe-Thiele: Minimum Reflux

To carry out the algebraic method we need to determine the slopes of the operating lines algebraically. This can be done finding the intersections between the q-line and equilibrium curve, and the q-line and the rectifying section operating line.

$$y=\left(\frac{q}{q-1}\right)x-\left(\frac{z_F}{q-1}\right)=\frac{\alpha x}{1+x(\alpha-1)}$$



$$y=\frac{\alpha x}{1+x(\alpha-1)}$$

$$y=\left(\frac{q}{q-1}\right)x-\left(\frac{z_F}{q-1}\right)$$

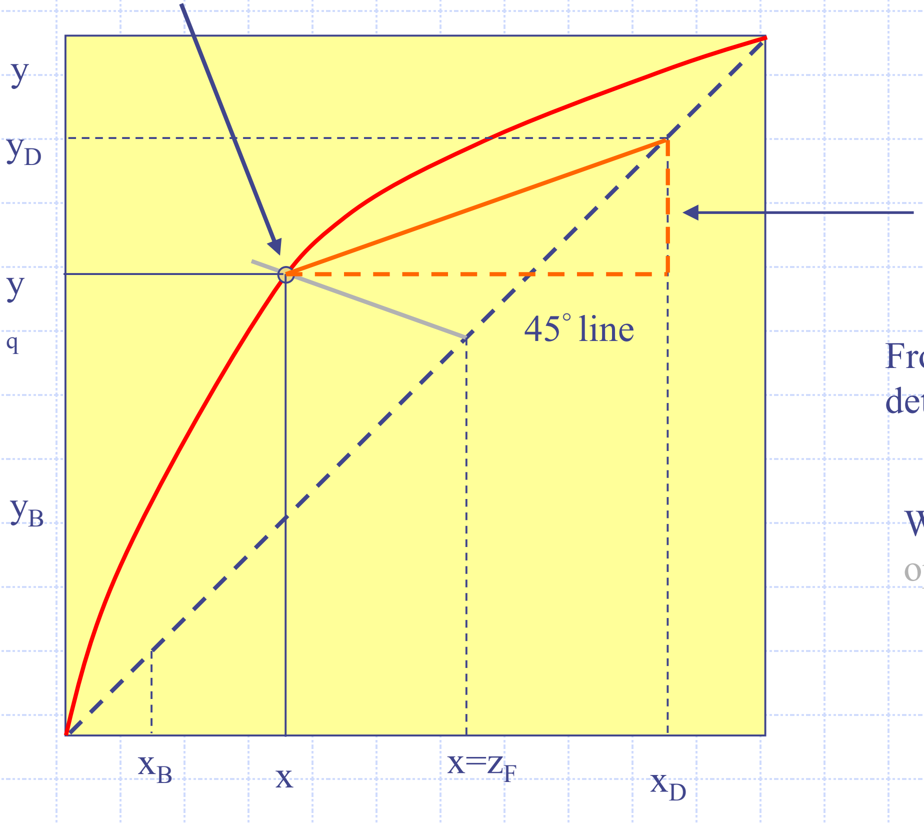
$$y=\left(\frac{q}{q-1}\right)x-\left(\frac{z_F}{q-1}\right)=$$

$$=\frac{\alpha x}{1+x(\alpha-1)}$$

McCabe-Thiele: Rectifying Section Operating Line

The slope of the operating line for the rectifying section with minimum reflux can be determined from the rise over run. We can then also find the minimum reflux from this slope.

$$y = \left(\frac{q}{q-1}\right)x - \left(\frac{z_F}{q-1}\right) = \frac{\alpha x}{1 + x(\alpha - 1)}$$



$$\frac{y_D - y_q}{x_D - x_q} = \frac{R_{\min}}{R_{\min} + 1}$$

From the minimum reflux, and R/R_{min} we can determine the reflux R.

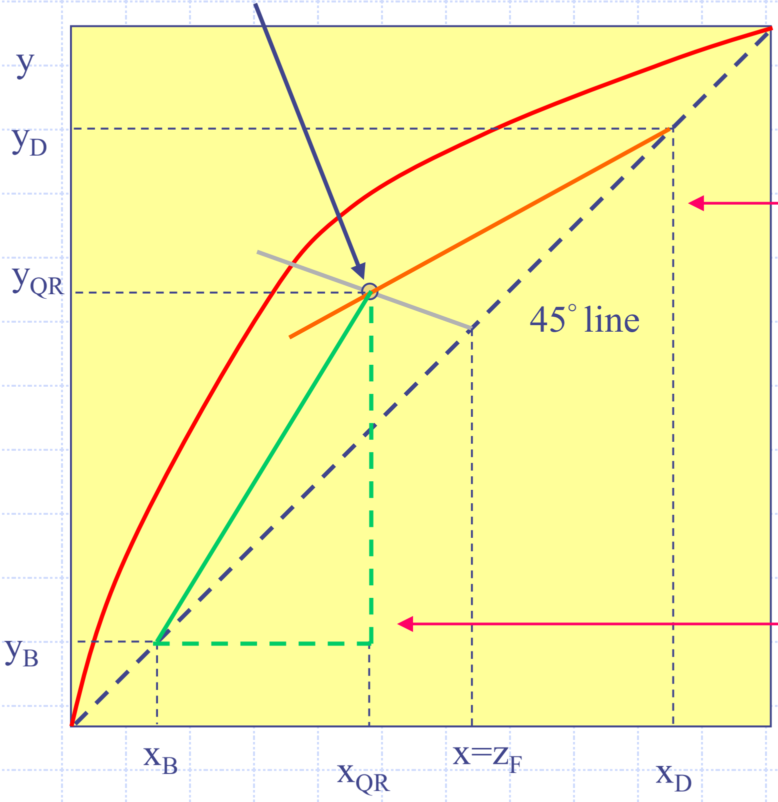
We determine the slope of the rectifying section operating line from:

$$slope = \frac{R}{R+1}$$

McCabe-Thiele: Rectifying Section Operating Line

We can find the intersection of the operating line and the q-line to determine the stripping section operating line:

$$y = \left(\frac{q}{q-1}\right)x - \left(\frac{z_F}{q-1}\right) = \frac{R}{R+1}x + \frac{1}{R+1}x_D$$



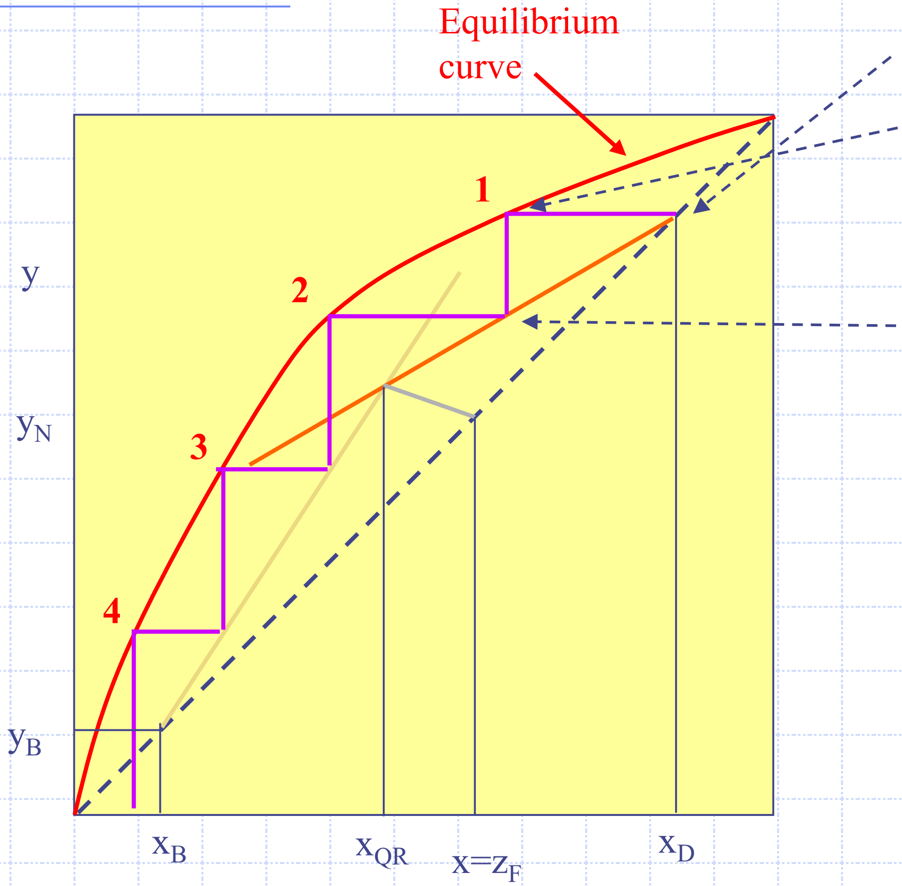
$$slope = \frac{R}{R+1}$$

From the minimum reflux, and R/R_{min} we can determine the reflux R.

We determine the slope of the stripping section operating line from:

$$\frac{y_{QR} - y_B}{x_{QR} - x_B} = slope$$

McCabe-Thiele: Algebraic Method



1. In total condenser $y_1=x_0$

2. x_1 is determined from the equilibrium curve:

$$y_1 = \frac{\alpha x_1}{1 + x_1(\alpha - 1)}$$

3. y_2 is determined from operating line for the rectifying section:

$$y_2 = \frac{R}{R+1} x_1 + \frac{1}{R+1} x_D$$

4. Repeat steps 2 and 3 until x_n is less than x_{QR} (you are on a point of the equilibrium curve to the left of the intersection of the OL and the q-line).

5. y_3 is determined from operating line for the stripping section:

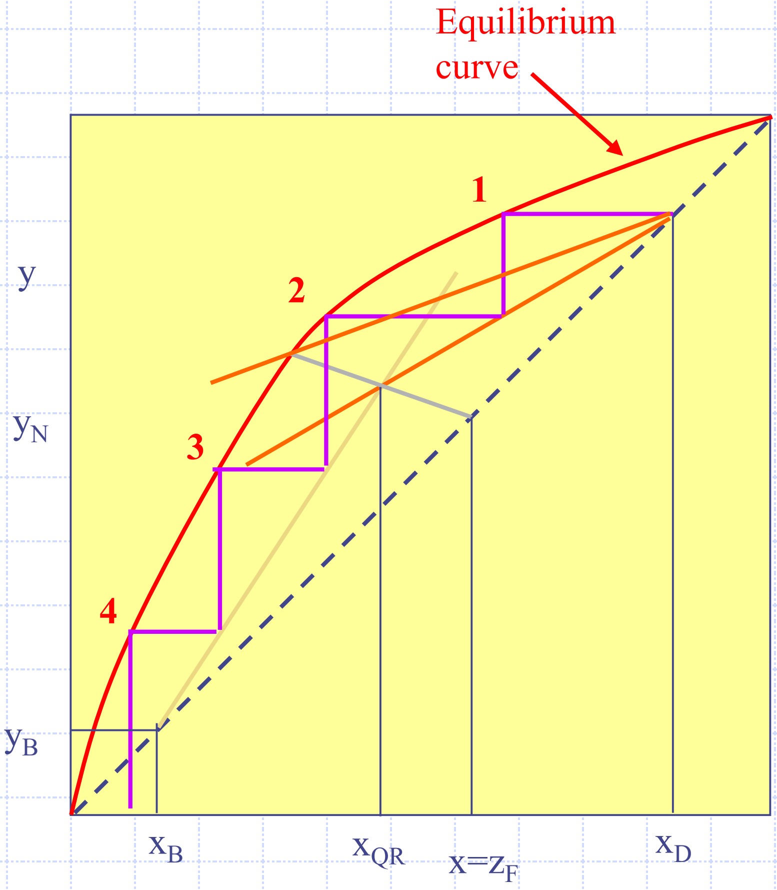
$$y_3 = \frac{\bar{L}}{\bar{V}} x_2 - \frac{B}{\bar{V}} x_B$$

6. x_3 is determined from the equilibrium curve:

$$y_3 = \frac{\alpha x_3}{1 + x_3(\alpha - 1)}$$

7. Repeat steps 5 and 6 until x_n is less than x_B

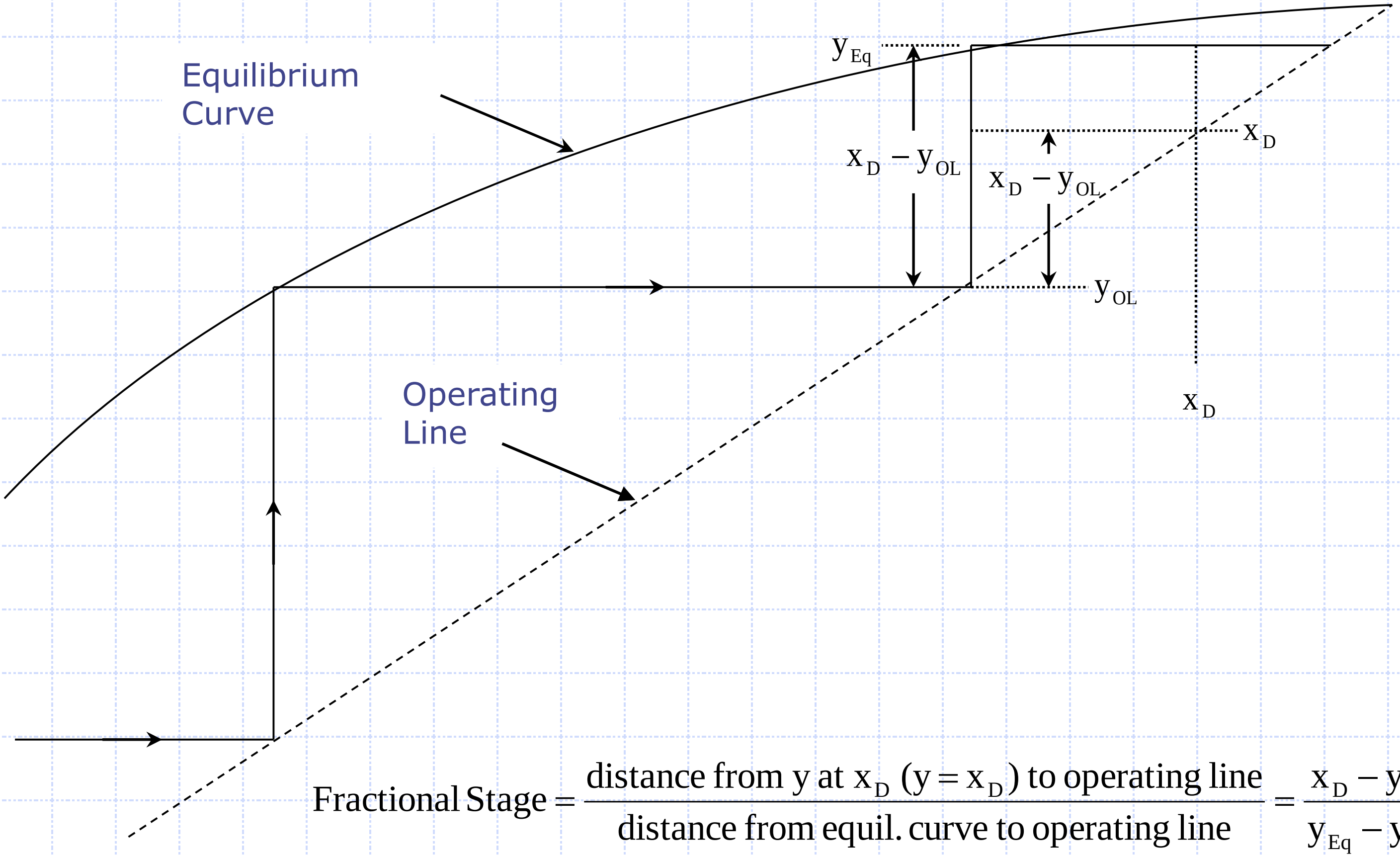
McCabe-Thiele Algebraic Method: Examples



x_D=0.9, x_B=0.1, z_F=0.5, q=0.8

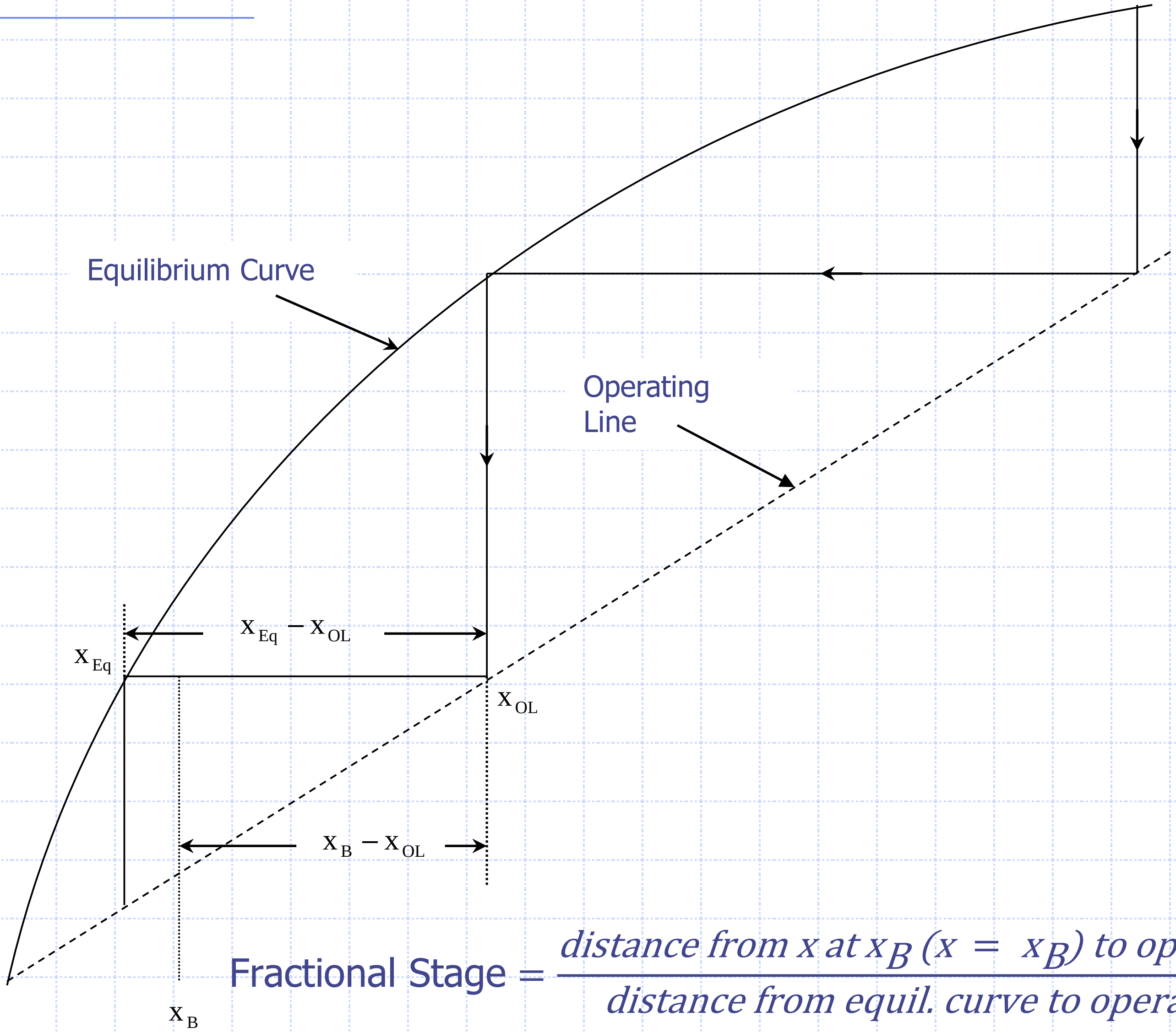
1. Alpha = 4, R = R_{min}
2. Alpha = 4, R = 2 R_{min}
3. Alpha = 4, R = 4 R_{min}
4. Alpha = 4, R = 20 R_{min}
5. Alpha = 1.1,R = 3 R_{min}

Fractional Stage at Top of Column



$$\text{Fractional Stage} = \frac{\text{distance from y at } x_D\ (y = x_D) \text{ to operating line}}{\text{distance from equil. curve to operating line}} = \frac{x_D - y_{OL}}{y_{Eq} - y_{OL}}$$

Fractional Stage at Bottom of Column



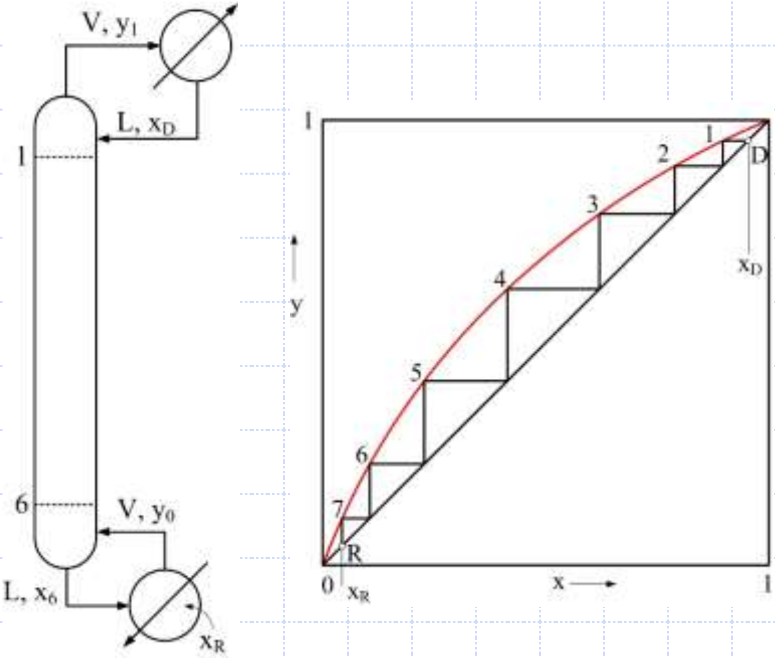
$$\text{Fractional Stage} = \frac{\textit{distance from x at } x_B\ (x = x_B) \textit{ to operating line}}{\textit{distance from equil. curve to operating line}} = \frac{x_B - x_{OL}}{x_{Eq} - x_{OL}}$$

Limiting Conditions – Reflux Ratios

- The external **reflux ratio**, L/D, is often a parameter that **is specified** for column operation since it is perhaps the **easiest to change** under column operation and changing L/D often has a **substantial effect** on the overall column behavior and separation.
- There are **two limiting conditions** with respect to the reflux ratio, L/D, that one obtains:
  - Total reflux ratio, D = 0, L/V = 1, and L/D → ∞
  - Minimum reflux ratio, $(L/D)_{min}$.
- One will often see an external reflux specification as a **multiple of the minimum reflux ratio**,
  - for example, $L/D = 2(L/D)_{min}$, etc.

Total Reflux and Boilup – Limiting Condition

- A column which has total reflux and boilup has no feed
  - the distillate, bottoms, and feed flow rates are zero.
- This is a **limiting condition** which provides one with the minimum number of equilibrium stages that can be obtained for a given column.
- While one would **not typically operate** under such conditions, total reflux and boilup are used for **starting up** a column, for operating the **column off-line** when other unit operations are off-line, and for **testing** column efficiency.



Total Reflux: design case

- At total reflux:
  - If α=constant, the minimum number of stages are calculated analytically

$$\frac{y_1}{1-y_1} = \alpha \frac{x_1}{1-x_1} \xrightarrow{y_1 = x_D \quad x_1 = y_2} \frac{x_D}{1-x_D} = \alpha \frac{y_2}{1-y_2}$$

$$\frac{y_2}{1-y_2} = \alpha \frac{x_2}{1-x_2} \xrightarrow{\qquad} \frac{x_D}{1-x_D} = \alpha^2 \frac{x_2}{1-x_2}$$

……

$$\frac{x_D}{1-x_D} = \alpha^N \frac{x_N}{1-x_N} = \alpha^N \frac{x_R}{1-x_R} \Rightarrow N = \frac{1}{\ln\alpha} \ln \frac{x_D(1-x_R)}{x_R(1-x_D)}$$

Fenske equation

Limiting Conditions – Minimum Reflux

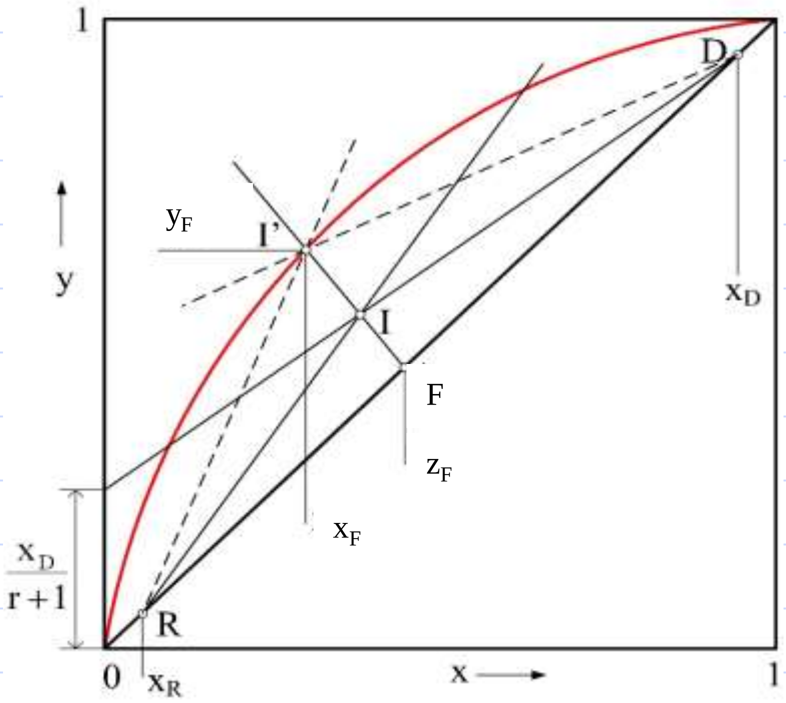
- Minimum reflux, R_{min} or $(L/D)_{min}$, is defined as the external reflux ratio at which the specified separation could just be obtained with an infinite number of stages.

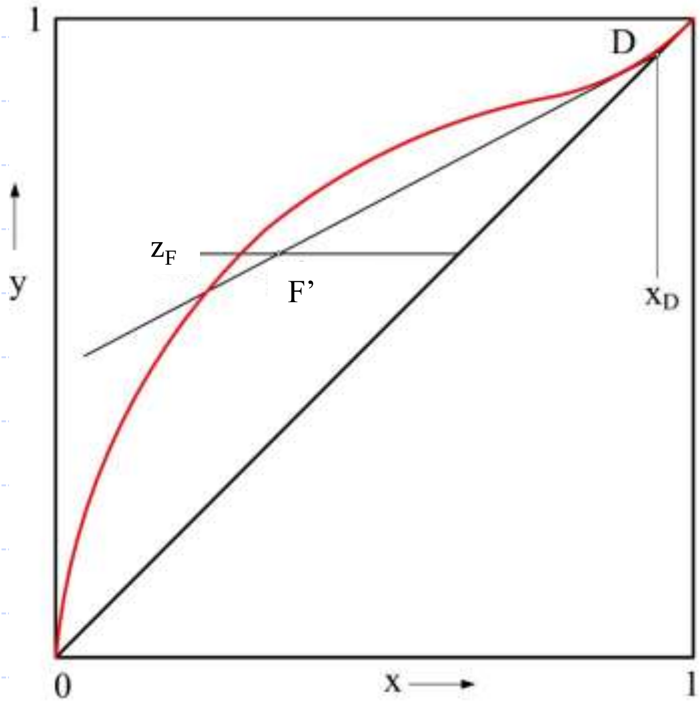
$$R_{min} = (L/D)_{min} = \frac{(L/V)_{min}}{1-(L/V)_{min}}$$

  - We obtain an infinite number of stages if our operating lines touch the equilibrium curve.
- The point on the equilibrium curve that this occurs is called a “pinch” point.

Minimum Reflux: design case

- At minimum reflux:





Pinch point

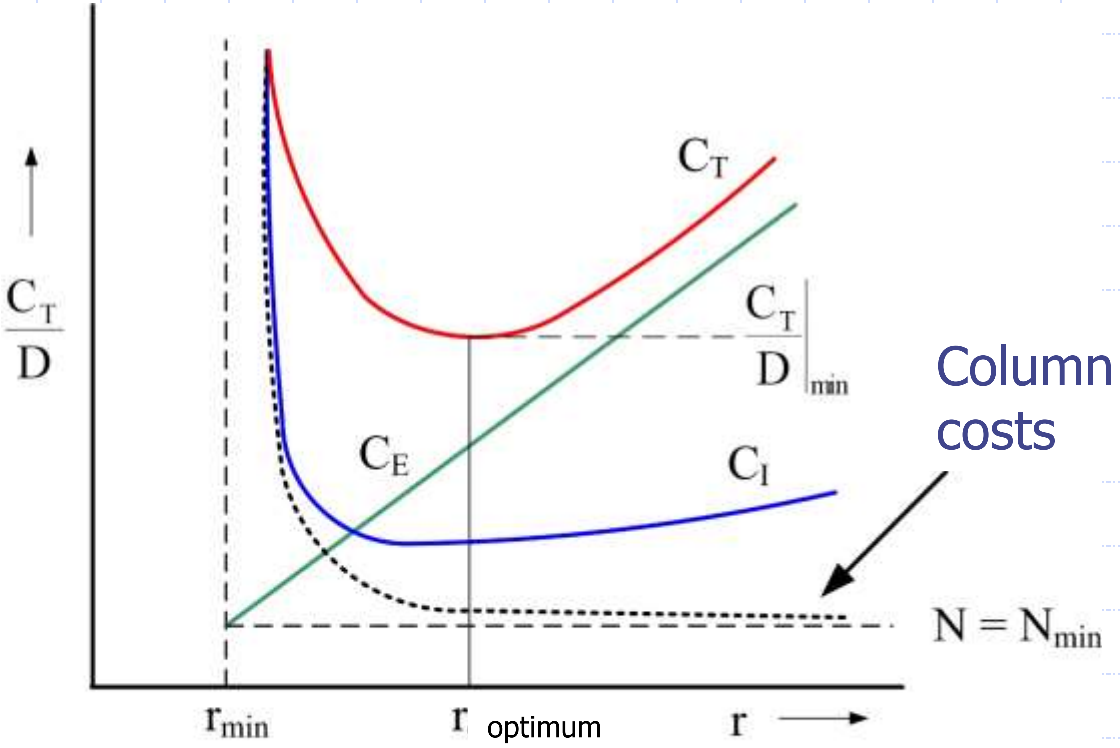
$$\left(\frac{r}{r+1}\right)_{min}=\frac{x_D-y_F}{x_D-x_F} \longrightarrow \boxed{r_{min}=\frac{x_D-y_F}{y_F-x_F}}$$

Optimum Reflux ratio: design case

- Calculation is based on total production costs minimization.
  - Defined as the sum of capital costs CI and operating costs CE per unit of distillate product.
  - The key variable is the reflux ratio, as it influences N, L and V.
- For a given production rate (F, D, R, flow rates and compositions), higher values of r implies:
  - Decrease of number of stages and therefore column height
  - Increase flow rates V, V ', L, L' and therefore:
    - Larger column diameter (proportional to $V^{0.5}$)
    - Higher thermal consumption at the condenser, with larger heat exchanger area and cooling water use
    - Higher thermal consumption at the reboiler with larger heat exchanger area and steam use
    - Increase of reflux flow rate with larger capital costs (for pumps, piping and valves) and operating costs.

Optimum Reflux ratio: design case

- Calculation is based on total production costs minimization.
  - C_I and C_E (r), is plotted to find the value of r that minimizes the total costs.



Column costs

$$C_T = C_I + C_E$$

$$r_{opt} = Kr_{min}$$

$$K = 1.2 \div 1.3$$

Rule of Thumb

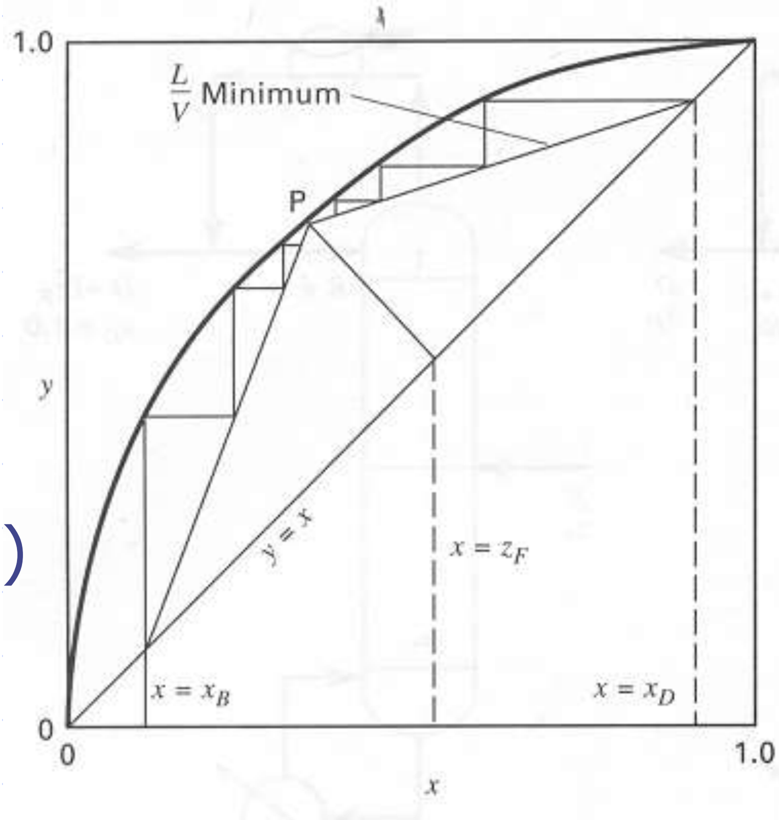
- The best operating condition lies between minimum and total reflux.
- As a rule of thumb, the optimum reflux ratio lies between 1.05 and 1.25 (L/D)min.
- Too low of an L/D results in a large number of equilibrium stages, while too high of an L/D increases the reboiler duty as well as the required diameter of the column.

Two Types of Pinch Points

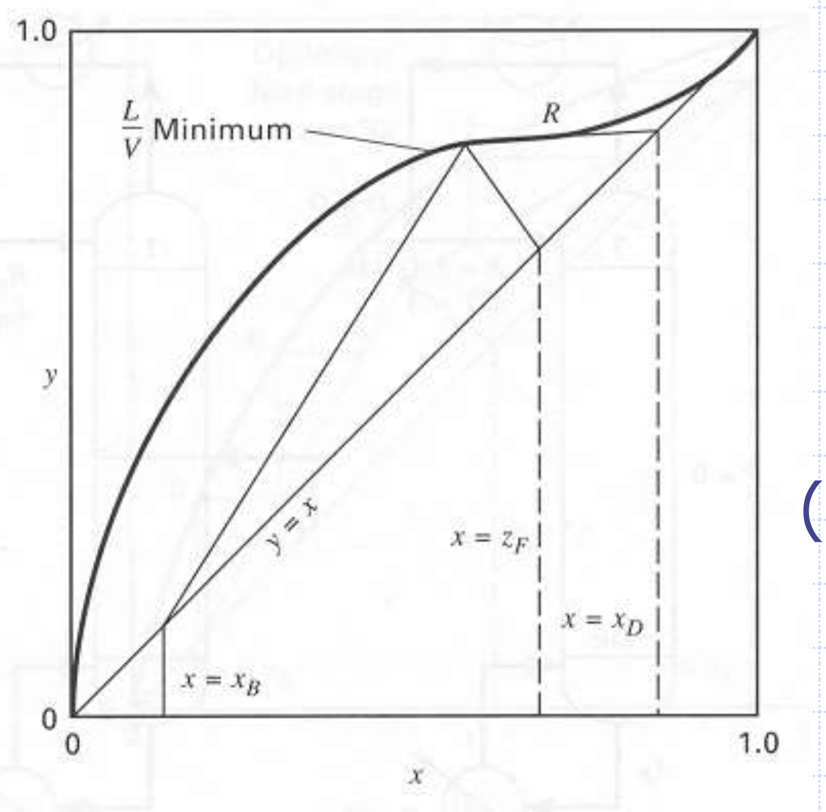
- For many systems, the pinch point will occur where the feed line crosses the equilibrium curve.
- A second type of pinch point can occur in “non-ideal” system where the operating line touches the equilibrium curve before the intersection of the feed line and the equilibrium curve.
- One should always look at a system to determine if a non-ideal pinch point occurs…
- Just don’t blindly assume it will be at the intersection of the feed line and equilibrium curve.

Minimum Reflux: Infinite Number of Equilibrium Stages

- (a) Typical ideal or near ideal pinch point at the feed stage
- (b) Typical non ideal system, pinch point above the feed stage



(a)



(b)

Limiting Conditions: Minimum Boilup

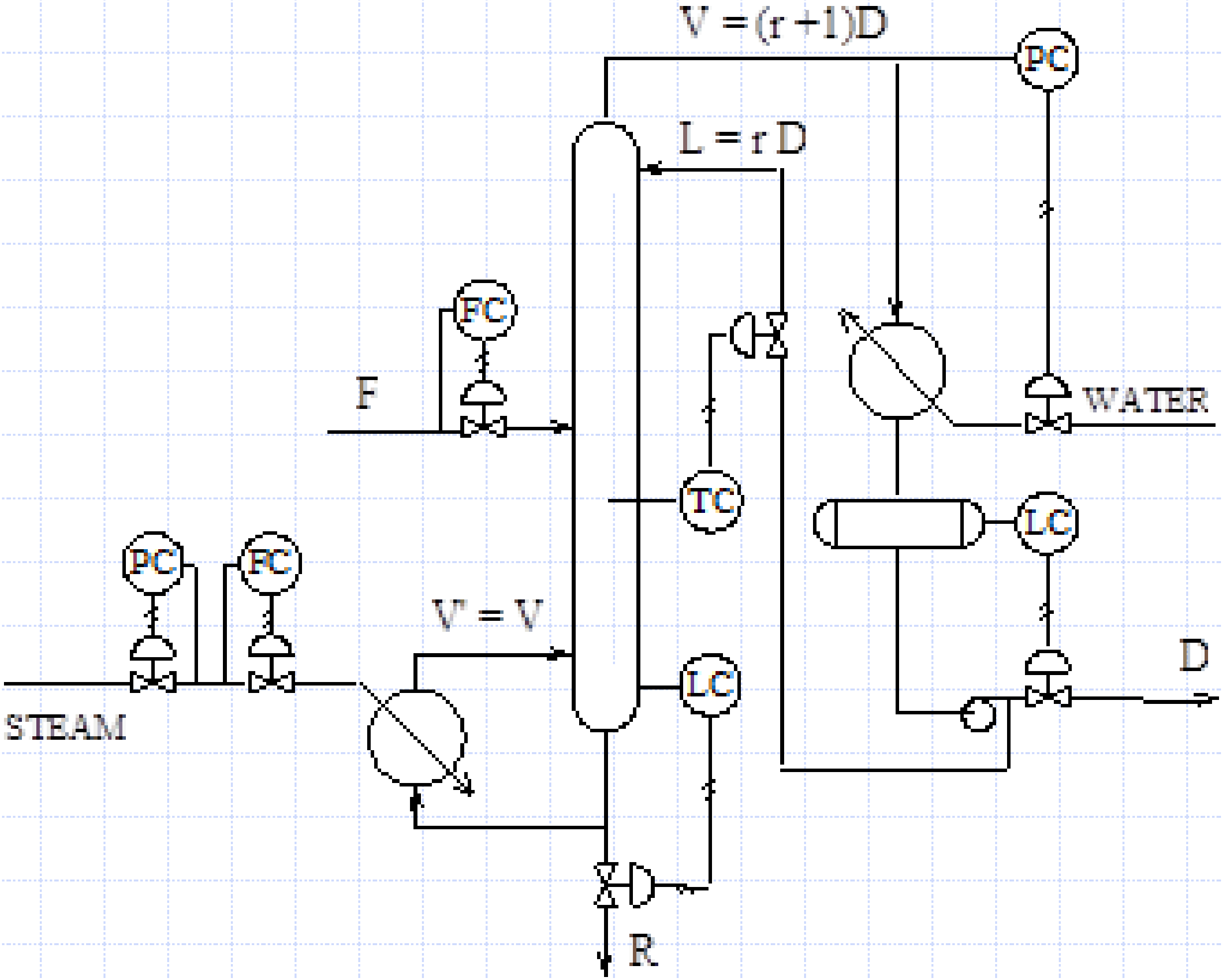
- A **minimum boilup ratio**, $(V/B)_{min}$, can be similarly defined as the boilup ratio at which the specified separation could just be obtained with an infinite number of stages.

$$(\underline{V}/B)_{min} = \frac{1}{(\underline{L}/\underline{V})_{max} - 1}$$

  - Because of this relationship of the BOL's slope, L/V, to the boilup ratio, V/B, we have a maximum L/V at minimum boilup, V/B.

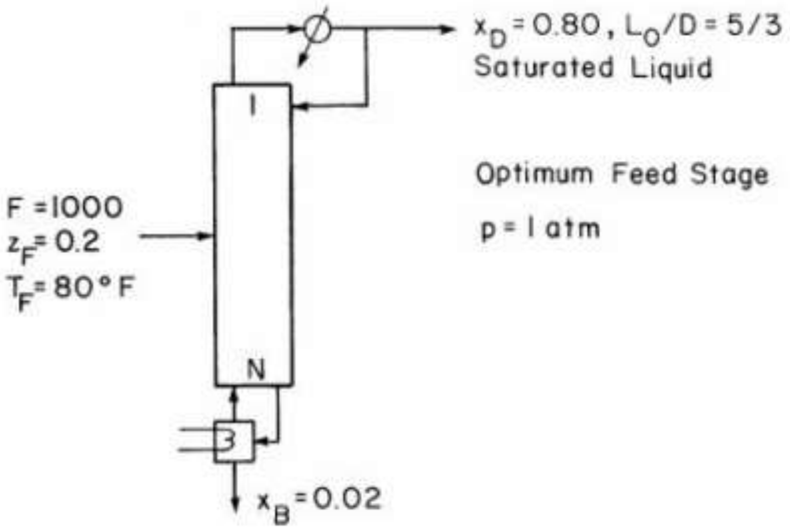
Distillation column control schema

- Schema of automatic control of a continuum distillation column.



Example: McCabe Thiele

- A distillation column with a total condenser and a partial reboiler is separating an ethanol-water mixture.
  - The feed is 20 mol% ethanol, feed rate is 1000 kmol/h, and feed temperature is 80°F (26.7 °C).
  - A distillate composition of 80 mol% ethanol and a bottoms composition of 2 mol% ethanol are desired.
  - The external reflux ratio is 5/3. The reflux is returned as a saturated liquid and CMO can be assumed.
  - Pressure is 1 atm.
  - The column is well isolated.
- Find the optimum feed plate location and the total number of equilibrium stages required.

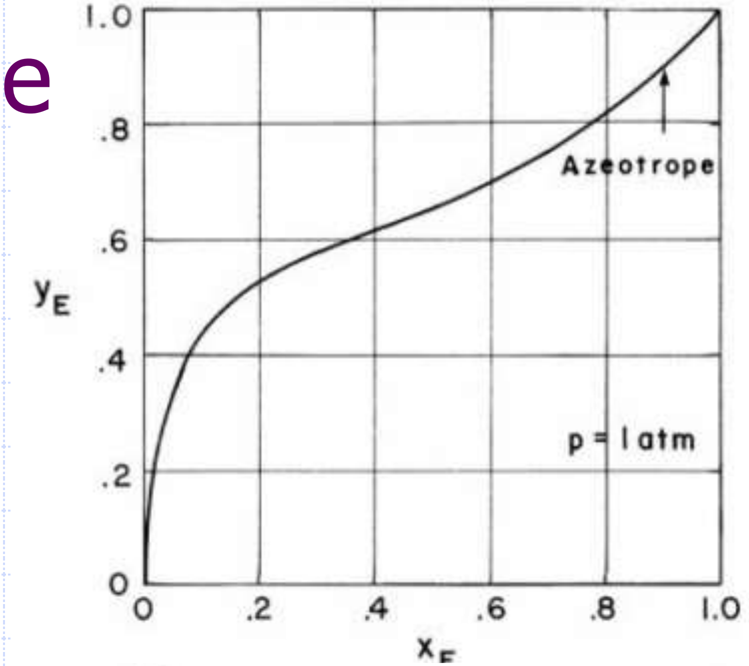


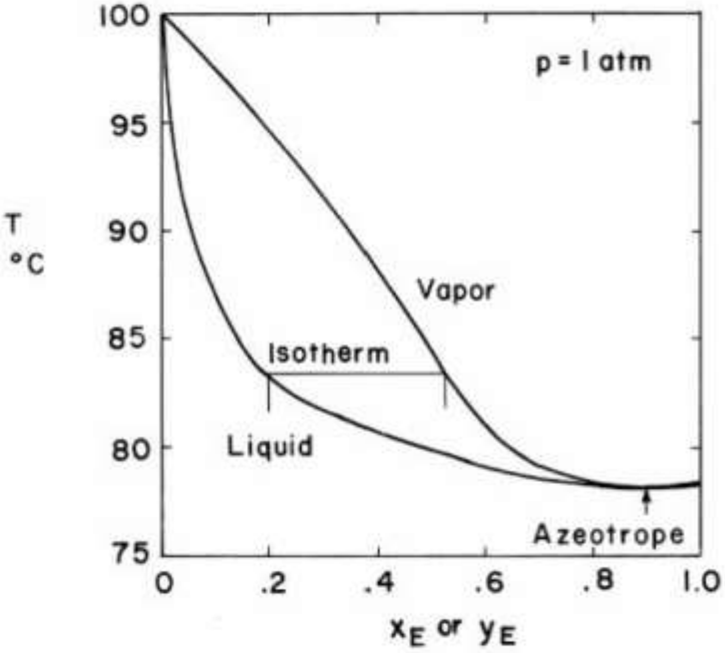
Example: McCabe Thiele

- Equilibrium data

x_{Etoh}	x_w	y_{Etoh}	y_w	$T, °C$
0	1.0	0	1.0	100
0.019	0.981	0.170	0.830	95.5
0.0721	0.9279	0.3891	0.6109	89.0
0.0966	0.9034	0.4375	0.5625	86.7
0.1238	0.8762	0.4704	0.5296	85.3
0.1661	0.8339	0.5089	0.4911	84.1
0.2337	0.7663	0.5445	0.4555	82.7
0.2608	0.7392	0.5580	0.4420	82.3
0.3273	0.6727	0.5826	0.4174	81.5
0.3965	0.6035	0.6122	0.3878	80.7
0.5198	0.4802	0.6599	0.3401	79.7
0.5732	0.4268	0.6841	0.3159	79.3
0.6763	0.3237	0.7385	0.2615	78.74
0.7472	0.2528	0.7815	0.2185	78.41
0.8943	0.1057	0.8943	0.1057	78.15
1.00	0	1.00	0	78.30

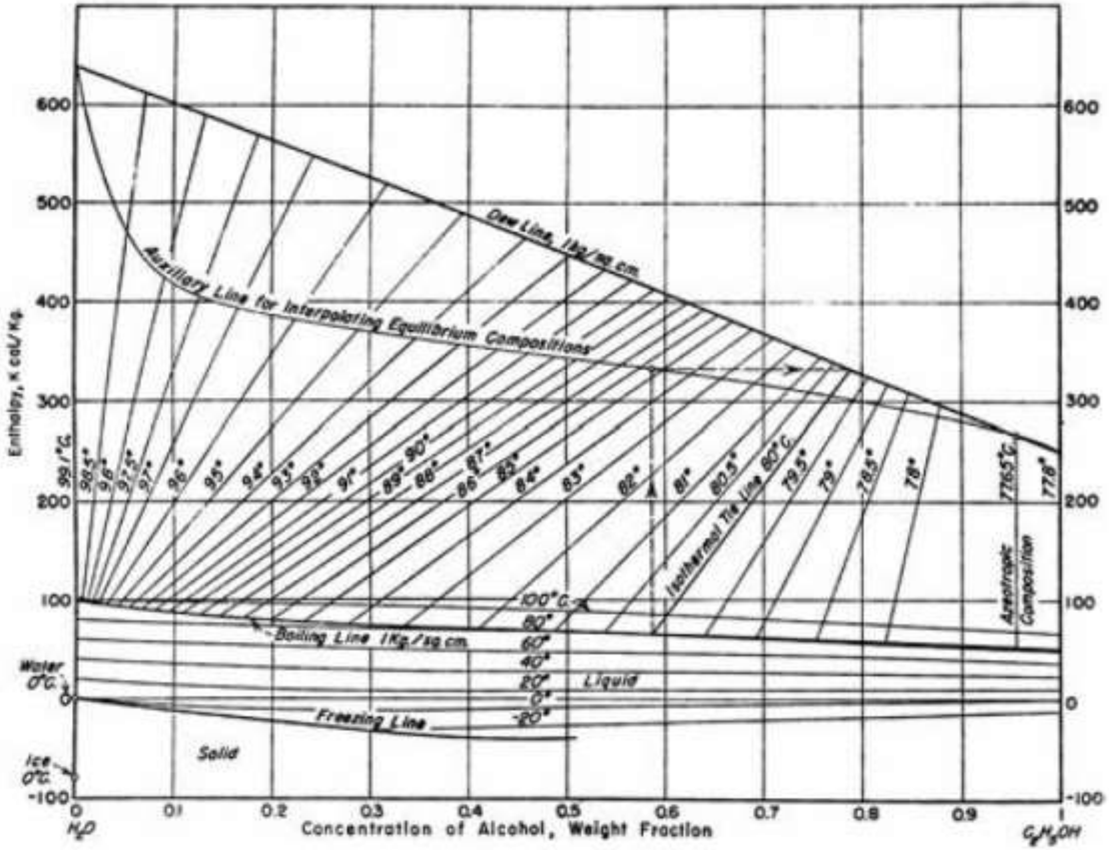
R. H. Perry, C. H. Chilton, and S.O. Kirkpatrick (Eds.), *Chemical Engineers Handbook*, 4th ed., New York, McGraw-Hill, p. 13–5, 1963.

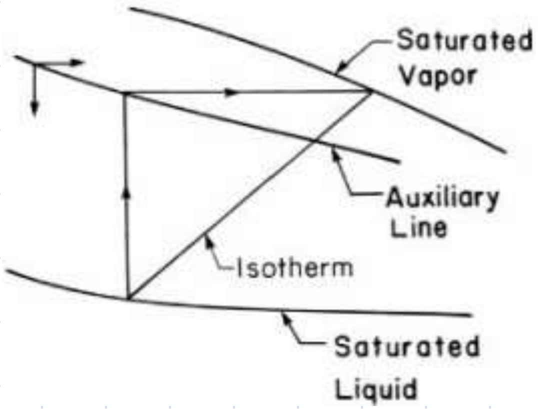




Example: McCabe Thiele

- Enthalpy – composition data at 1 atm





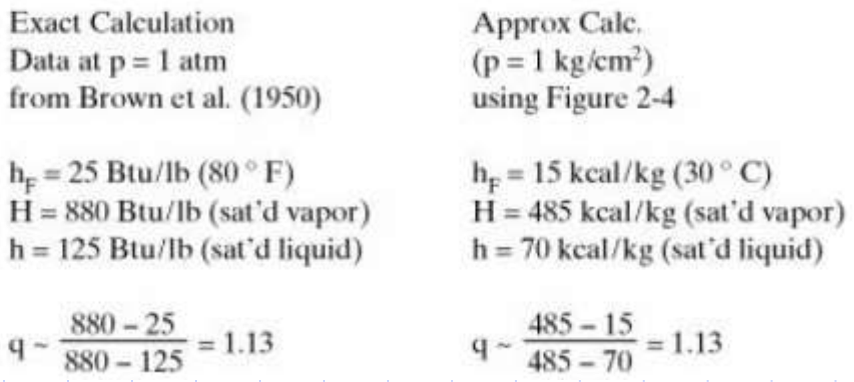
$$q \equiv \frac{\bar{L} - L}{F} \sim \frac{H - h_F}{H - h}$$

Example: McCabe Thiele

- Verify CMO by comparing the latent heat per mole of pure ethanol and pure water.
    - This checks the third and most important criterion for CMO.
    - The column is well insulated, the first criterion, adiabatic, will be satisfied.
    - The latent heats are: $\lambda_E = 9.22$ kcal/mol, $\lambda_W = 9.7171$ kcal/mol
    - The difference of roughly 5% is reasonable particularly since we always use the ratio of L/V or $\underline{L}/\underline{V}$
    - Using the ratio causes some of the change in L and V to divide out.
- Thus we will assume CMO

Example: McCabe Thiele

- *Feed Line:*
  - Convert feed concentration, 20 mol%, to wt % ethanol = 39 wt%.



Exact Calculation Data at p = 1 atm from Brown et al. (1950)	Approx Calc. (p = 1 kg/cm^2) using Figure 2-4
$h_F = 25$ Btu/lb (80 ° F)	$h_F = 15$ kcal/kg (30 ° C)
$H = 880$ Btu/lb (sat'd vapor)	$H = 485$ kcal/kg (sat'd vapor)
$h = 125$ Btu/lb (sat'd liquid)	$h = 70$ kcal/kg (sat'd liquid)
$q \sim \frac{880-25}{880-125} = 1.13$	$q \sim \frac{485-15}{485-70} = 1.13$

  - Slope of the feed line: $q/(q-1)= 8.7$
  - Feed line intersects $y=x$ line at feed concentration $z=0.2$

Top operating line

$$y = \frac{L}{V}x + \left(1-\frac{L}{V}\right)x_D$$

$$\text{Slope} = \frac{L}{V} = \frac{L/D}{1+L/D} = \frac{5/3}{1+5/3} = 5/8$$

$$\text{y intercept} = \left(1-\frac{L}{V}\right)x_D = (3/8)(0.8) = 0.3$$

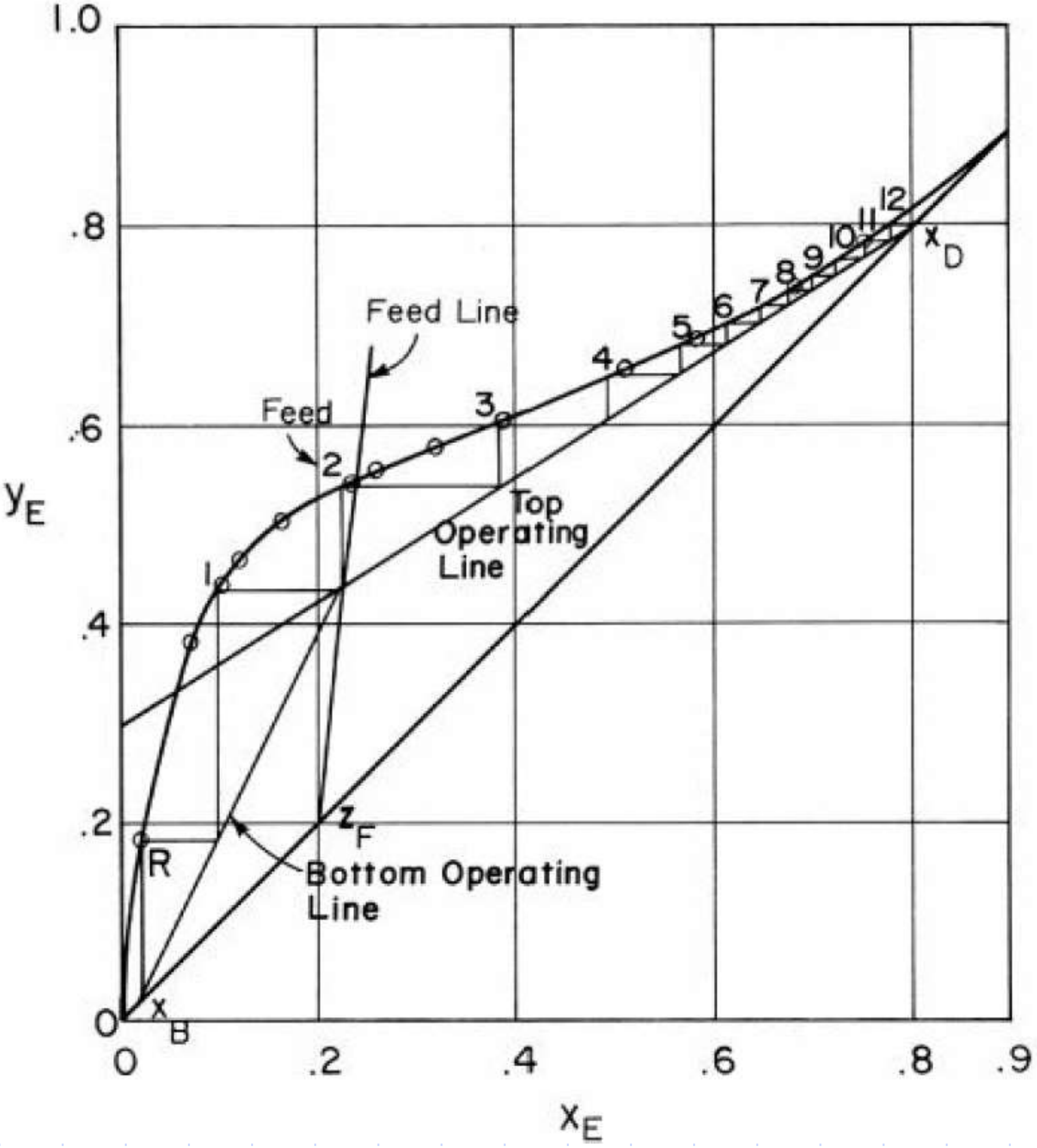
Bottom operating line

- It intersects the top OL at the feed line;
- Another point is the intersection of the bottom OL and the $y=x$ line at $y=x=x_B$
- Alternatively use mass balance

$$y = \frac{\bar{L}}{\bar{V}}x - \left(\frac{\bar{L}}{\bar{V}} - 1\right)x_B$$

Example: McCabe Thiele

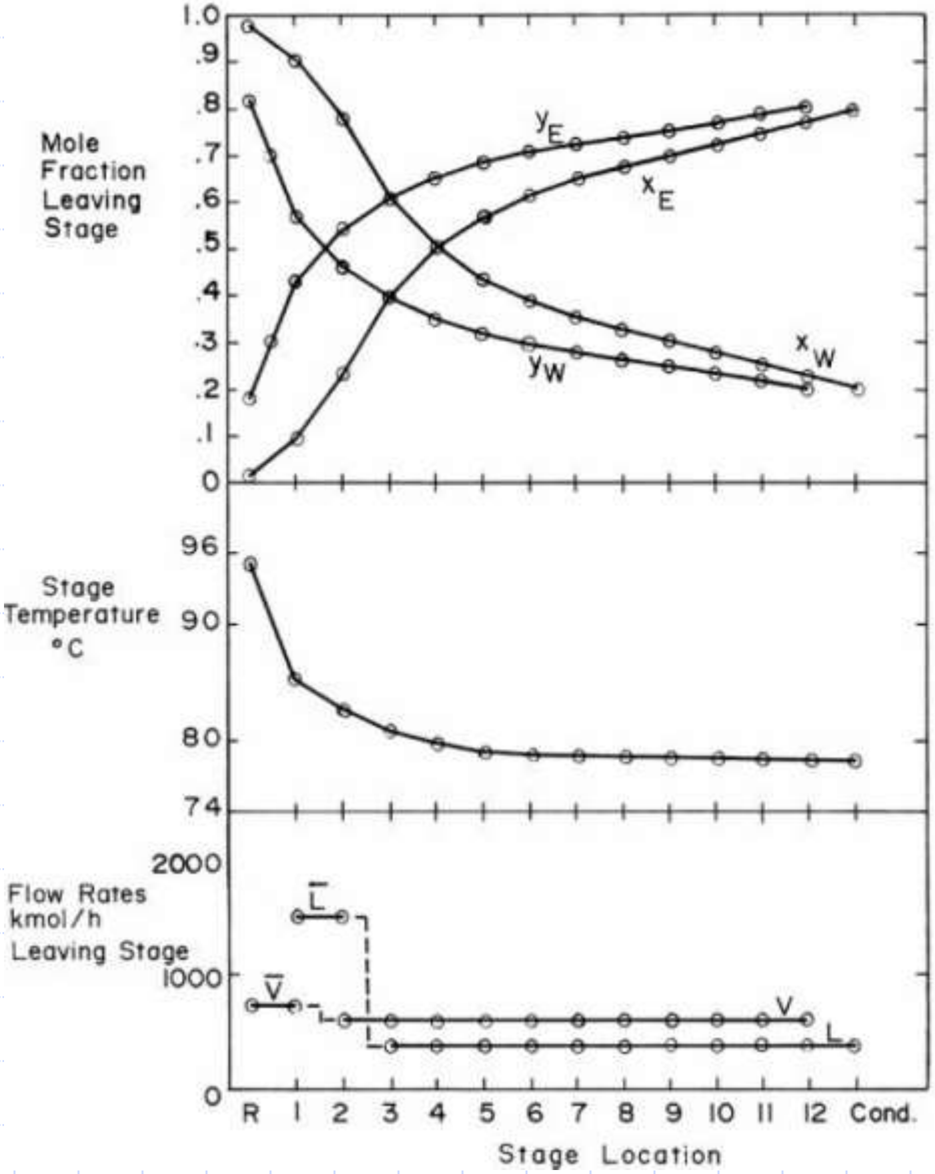
- Optimum feed stage
  - second above the partial reboiler.
- N. of stages
  - 12 equilibrium stages plus a partial reboiler.
- Checks
  - Slope of top OL L/V <1 and slope of bottom OL L/V >1 , and q > 1 as expected.
  - The most likely cause of error (and the hardest to check) is the equilibrium data.



Example: McCabe Thiele

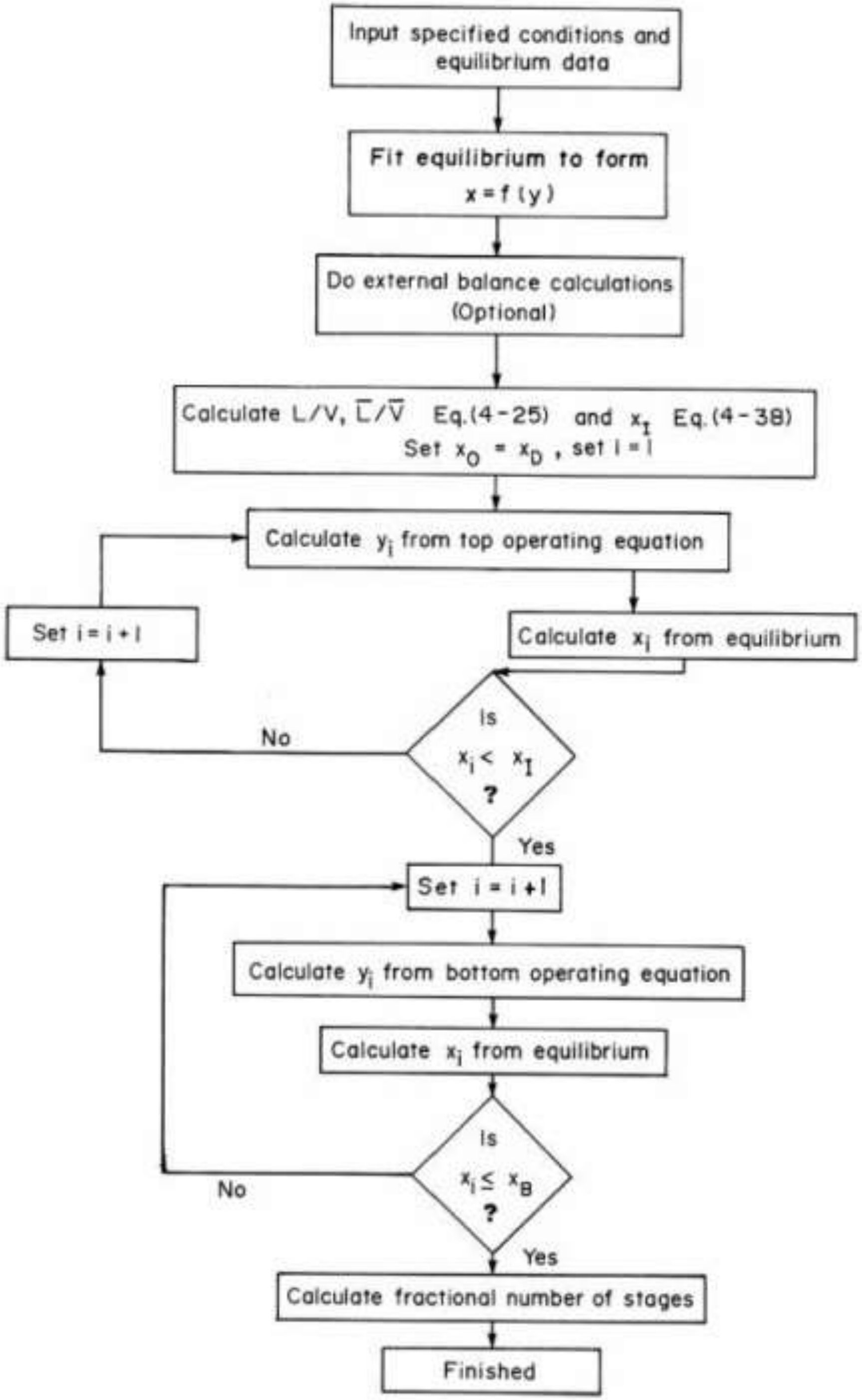
Column profiles

- where the operating line and equilibrium curve are close together we have a *pinch point.*
- Then the composition and temperature profiles will become almost horizontal and there will be very little change in composition from stage to stage.
- The location of a pinch point within the column depends on the system and the operating conditions.
- Flow profiles are flat in each section (CMO)
- As expected, $\underline{L}>\underline{V}$ and V>L.



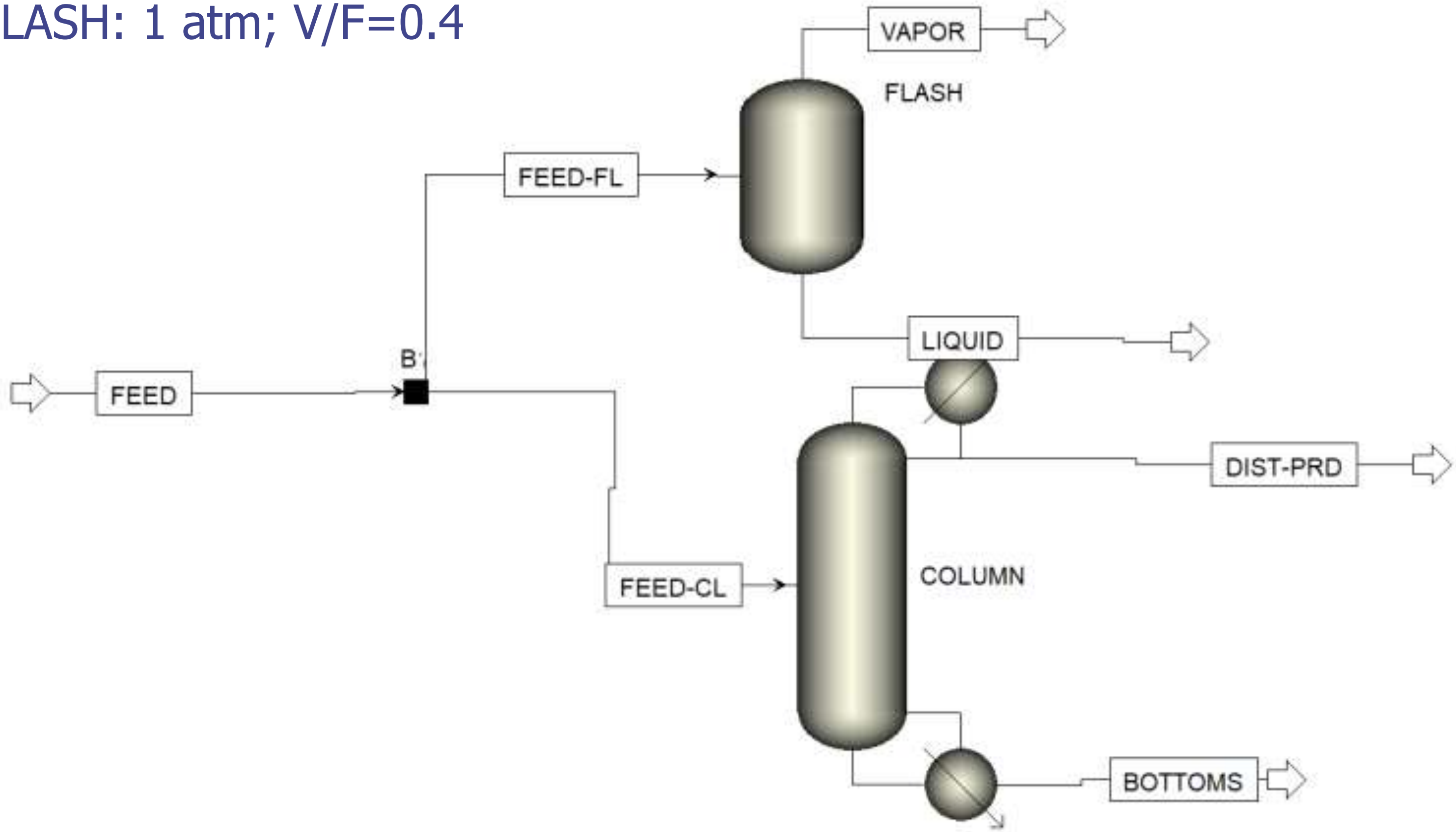
Flowsheet

- Assume that we decide to step off stages from the top down.
- If we step off stages from the bottom up, we will calculate y_i from equilibrium and x_i from the operating equation.
- For a more complex column the flowchart would be modified by:
  - Including equations for intermediate operating lines.
  - Including additional tests for optimum feeds.
  - Including side streams



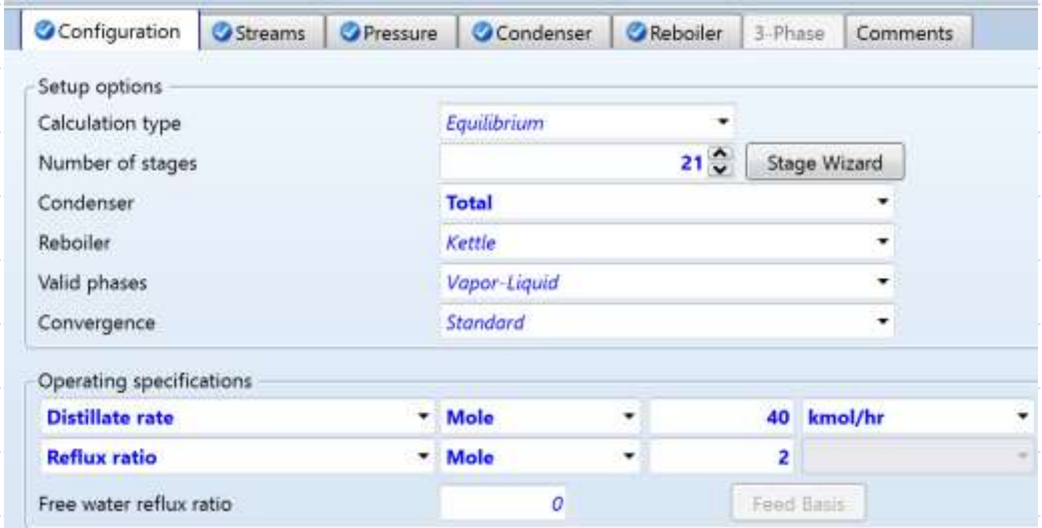
Binary distillation with Aspen+ Radfrac

- Binary distillation Ethanol – water: comparison with flash
  - Use of stream duplicator
  - FEED: 110 °C; 5 bar; 40 kmol/h ethanol, 60 kmol/h water
  - FLASH: 1 atm; V/F=0.4



Binary distillation with Aspen+ Radfrac

- Binary distillation Ethanol – water: comparison with flash
  - COLUMN:

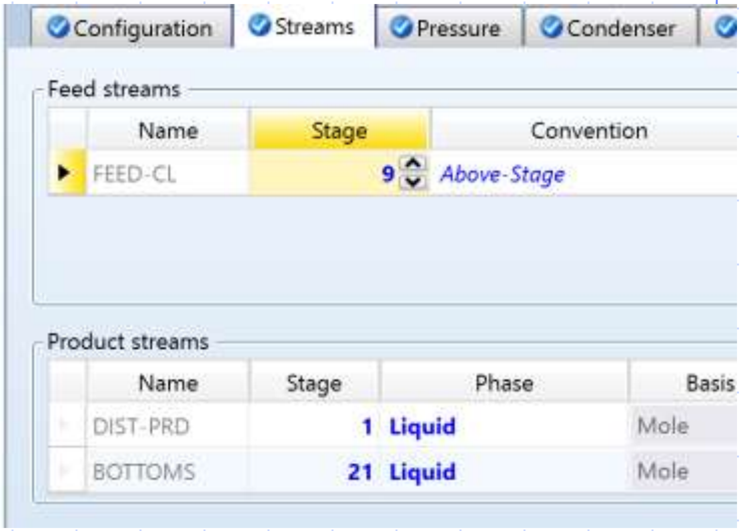


Setup options

Calculation type	*Equilibrium*
Number of stages	21
Condenser	**Total**
Reboiler	*Kettle*
Valid phases	*Vapor-Liquid*
Convergence	*Standard*

Operating specifications

Distillate rate	**Mole**	40	**kmol/hr**
Reflux ratio	**Mole**	2	
Free water reflux ratio		*0*	



Feed streams

Name	Stage	Convention
FEED-CL	9	*Above-Stage*

Product streams

Name	Stage	Phase	Basis
DIST-PRD	1	**Liquid**	Mole
BOTTOMS	21	**Liquid**	Mole

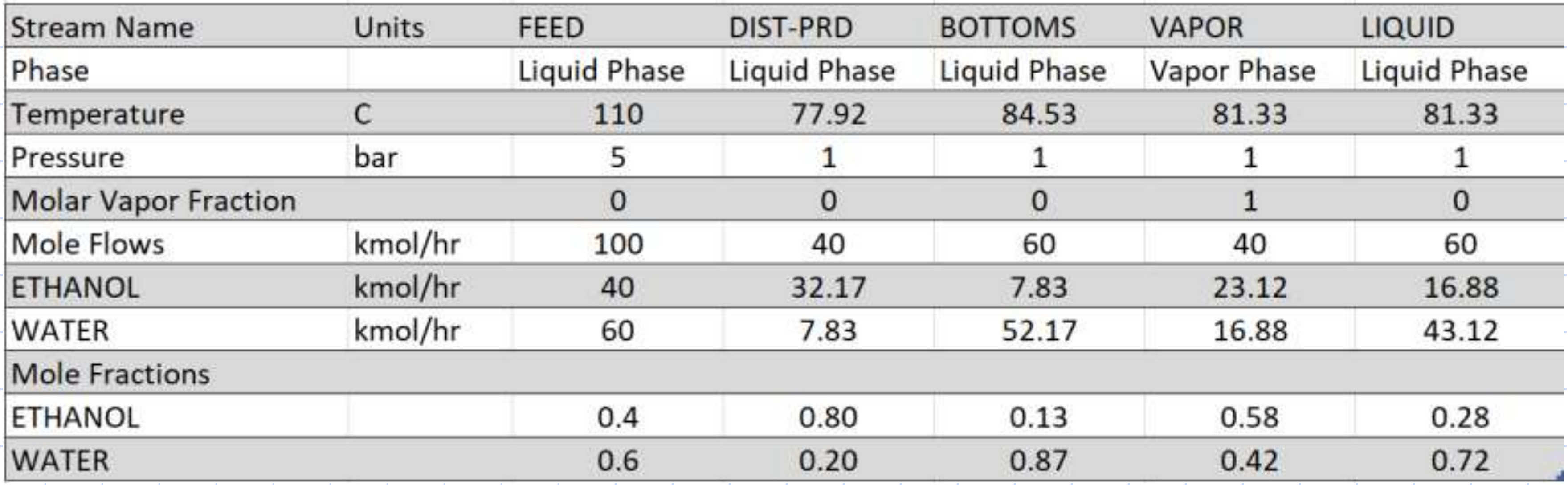
View: *Top / Bottom*

Top stage / Condenser pressure

Stage 1 / Condenser pressure: 1 **bar**

Binary distillation with Aspen+ Radfrac

- Binary distillation Ethanol – water: comparison with flash
  - Stream results



Stream Name	Units	FEED	DIST-PRD	BOTTOMS	VAPOR	LIQUID
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase	Liquid Phase
Temperature	C	110	77.92	84.53	81.33	81.33
Pressure	bar	5	1	1	1	1
Molar Vapor Fraction		0	0	0	1	0
Mole Flows	kmol/hr	100	40	60	40	60
ETHANOL	kmol/hr	40	32.17	7.83	23.12	16.88
WATER	kmol/hr	60	7.83	52.17	16.88	43.12
Mole Fractions						
ETHANOL		0.4	0.80	0.13	0.58	0.28
WATER		0.6	0.20	0.87	0.42	0.72

Home exercise

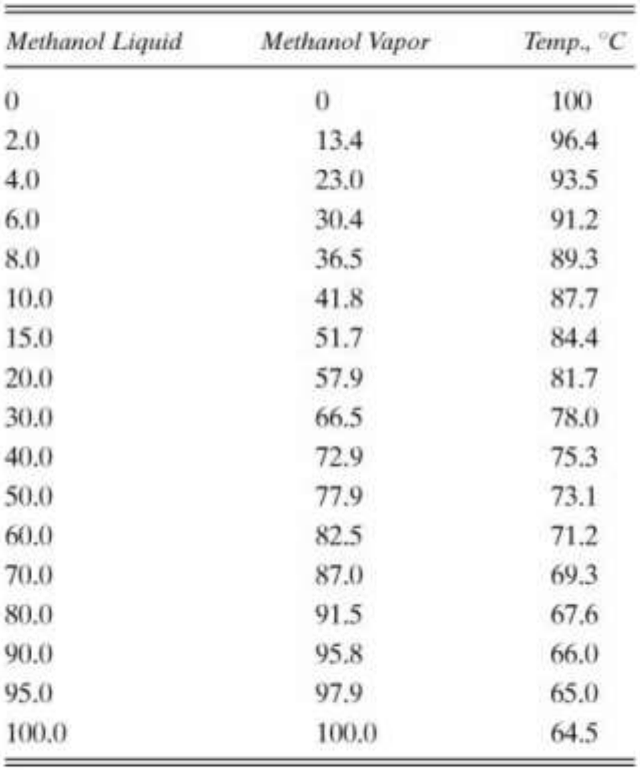
- Methanol water
  - hands and graphical calculations
  - Aspen+ solution and comparison with hands calculations
- Separation of 1,2-dichloroethane from 1,1,2-trichloroethane.
  - Aspen+ simulation (see text)

Home exercise: binary distillation

- A continuous, steady-state distillation column with a total condenser and a partial reboiler is separating methanol from water at one atmosphere (see Table for data). The feed rate is 100 kmol/h. The feed is 55 mol% methanol and 45 mol% water. We desire a distillate product that is 90 mol% methanol and a bottoms product that is 5 mol% methanol. Assume CMO.
  - **a.** If the external reflux ratio L/D = 1.25 plot the top operating line.
  - **b.** If the boilup ratio $\underline{V}/B = 2.0$ plot the bottom operating line.
  - **c.** Step off stages starting at the bottom with the partial reboiler. Use the optimum feed stage. Report the optimum feed stage and the total number of stages.
  - **d.** Plot the feed line. Calculate its slope. Calculate q. What type of feed is this?
  - **e.** Simulation of items a-d with Aspen+ RADFRAC

Home exercise: binary distillation

- Simulation of the same system with Aspen+ RADFRAC: base case
  - Feed: 1 atm, flow rates 55 and 65 kmol/hr; Feed q from hands calculations
  - N stages and Feed location from hands calculations, P = 1atm
  - Radfrac specifications:
    RR = 1.25;
    B/F = 0.50 (from material balance)
  - Plot profiles
- Add design specifications
  - Xdistillate 90% methanol
  - Xbottom 0.05% methanol



Methanol Liquid	*Methanol Vapor*	*Temp., °C*
0	0	100
2.0	13.4	96.4
4.0	23.0	93.5
6.0	30.4	91.2
8.0	36.5	89.3
10.0	41.8	87.7
15.0	51.7	84.4
20.0	57.9	81.7
30.0	66.5	78.0
40.0	72.9	75.3
50.0	77.9	73.1
60.0	82.5	71.2
70.0	87.0	69.3
80.0	91.5	67.6
90.0	95.8	66.0
95.0	97.9	65.0
100.0	100.0	64.5

Binary distillation with Aspen+ Radfrac

- Separate 1,2-dichloroethane from 1,1,2-trichloroethane.
  - Feed is 100 kmol/h of 60% dichloroethane.
  - Operation is at 1.0 atm.
  - Column has a total condenser and a kettle type reboiler.
  - Peng-Robinson is a reasonable VLE package.
  - Be sure to select the correct components from the AspenPlus menu. Note that 1,1,1-trichloroethane should not be used since it has very different properties.

Home exercise: Radfrac binary distillation

- Separate 1-2dichloroethane from 1-1-2 tricholoroethane.
  - Feed is 100 kmol/h of 60% dichloroethane.
  - Pressure is 1 atm.
  - Use Peng-Robinson EOS.

1. Equilibrium data.
   - Plot the x-y diagram from Aspen Plus and compare to an approximate plot with a constant α relative volatility of 2.24 (an over-simplification, but close).
2. Column simulation
   - The feed is 100% vapor at 1.0 atm. (vapor fraction in feed = 1)
   - Column has a total condenser and a kettle reboiler

Binary distillation with Aspen+ Radfrac

- We want a distillate product that is 92 mol% dichloroethane and a bottoms that is 8 mol% dichloroethane.
  - Since Aspen Plus is a simulator program, it will not allow you to specify these concentrations directly. You need to try different columns (change number of stages and feed location) to find some that work.
- Use L/D = 2.0. Set Distillate flow rate that will satisfy the mass balance.
  - Find D and B from mass balances. Do this calculation *accurately* or you may never get the solution you want.
  - Pick a reasonable number of stages and a reasonable feed stage (Try N = 21 and feed at 9 [vapor] to start).
  - Simulate the column and check the distillate and bottoms mole fractions. This is easiest to do with the *liquid* composition profiles for stage 1 and N.
  - They should be purer than you want.
  - Also, check the K values and calculate the relative volatility at the top, feed stage, and bottom of the column to see how much it varies.

Home exercise: Radfrac binary distillation

3. Column simulation (continue)
   - Find the optimum feed stage by trying different feed stages to see which one gives the greatest separation
     - Use sensitivity analysis
     - highest dichloroethane mole fraction in distillate and lowest in bottoms
   - Then decrease the total number of stages
     - using optimum feed stage each time until you have the lowest total number of stages that still satisfies the specifications for distillate and bottoms.
     - Use sensitivity analysis (same as above)
     - Note that the ratio (optimum feed stage)/(total number) is approximately constant.
4. Triple the pressure, and repeat steps 1 and 2. Determine the effect of higher pressure on the relative volatility.
5. Return to P = 1 atm and simulation in part 3
   4. Find the Reflux ratio (with N=21 and NF= 9)
   5. Use design specification
6. Return to P = 1 atm and simulations in part 3.
   - Increase the temperature of the feed instead of specifying a vapor fraction of 1

Home exercise: Radfrac binary distillation

7. Return to part 2, but aim for a distillate product that is 99% dichloro and a bottoms that is 2% dichloro.
   - Do the mass balances and determine settings for Distillate flow rate.
   - Find N and feed location that achieves this separation with an L/D = 2.
   - Note that separation should not be possible since the external reflux ratio (L/D) is too low.
   - See what happens as you increase L/D (try 4 and 8).
8. Try varying different settings for Operating Specifications in the Radfrac Setup-DataBrowser.
   - For example, pick a condenser duty instead of distillate flow rate that will give the same specification.
9. Add 1,1,1 trichloroethane to your component list.
   - Run analysis for 1,2-dichloroethane and 1,1,1 trichloroethane.

Binary distillation with Aspen+ Radfrac: tips

- Use L/D = 2.0.
  - Set Distillate flow rate that will satisfy the mass balance: find D and B from mass balances.
  - F=D+B → F=100 → D=100-B
  - 0.6 100 =0.92 D + 0.08 B = 0.92 D + 8 - 0.08 D
  - → D =(60-8)/(.92-.08) = 62; B=100 – 62 = 38
  - Try N = 21 and feed at 9 [vapor] to start.
  - Simulate the column and check the distillate and bottoms mole fractions.
  - They should be purer than you want. (xD = .928; xB = .027)
  - Also, check the K values and calculate the relative volatility at the top, feed stage, and bottom of the column to see how much it varies. Not much (top = 2.206, feed = 2.23; bottom = 2.24
- Optimum feed stage (N=21): use sensitivity on feed stage location
  - Tabulate XxD and xB → Optimal feed location: 11
- Optimal number of stages: keep the sensitivity and change the total number of stages (tabulate xD, xB) → N=14 NF=10
- Triple pressure: Alfa goes down to 2.0 (see xy graphs)
- Optimal RR = 1.778 (from Des Spec).
- Sensitivity (S-2) on Tfeed gives the best condition for T