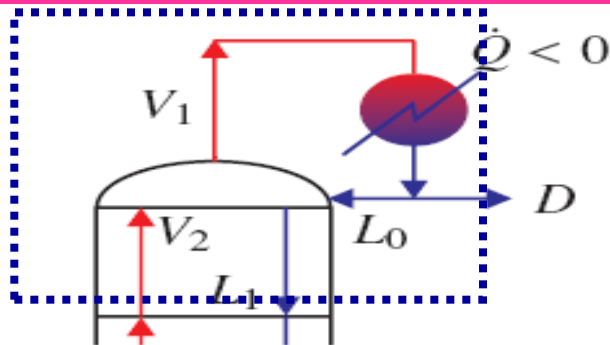


Distillation Operation

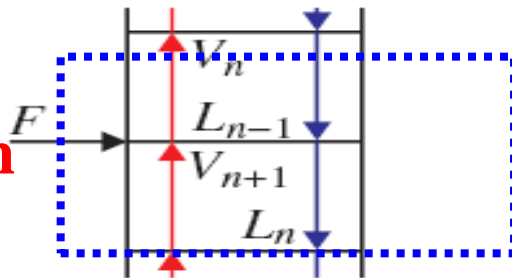
- **McCabe-Thiele Method**
- **Enthalpy-concentration Method**

McCabe-Thiele Method

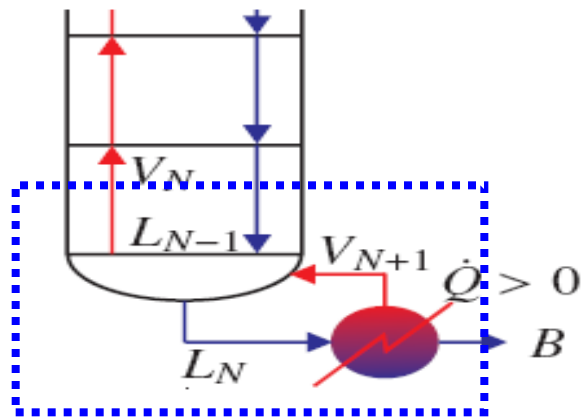
Rectifying section



Feed section



Stripping section



Counter-current distillation column

To calculate the solution of this separation problem, we need 3 sets of mass balances, (1) for the rectifying, (2) for the feed and (3) for the stripping section of the column. In addition there is an overall energy conservation assumption known as *constant molar overflow*.

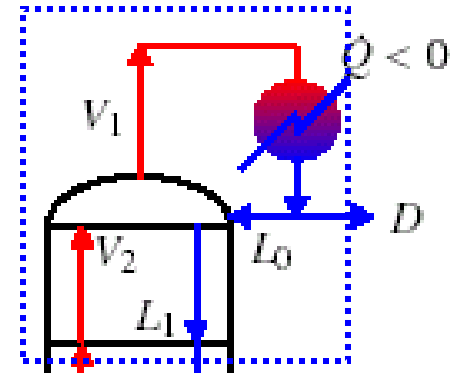
Operating Lines



The rectifying section

For the top section, the mass balances as one total balance and one component balance are

$$V_i = D + L_{i-1}$$
$$y_i V_i = x_0 D + x_{i-1} L_{i-1}$$



which means the heavier component is never considered explicitly. The equations are easily solved for the vapor composition:

$$y_i = x_0 \frac{D}{V_i} + x_{i-1} \frac{L_{i-1}}{V_i}$$
$$= x_0 \frac{D}{D + L_{i-1}} + x_{i-1} \frac{L_{i-1}}{D + L_{i-1}}$$

Operating Lines

The constant molar overflow assumption yields $L_0 = L_1 = \dots = L_{n-1} \equiv L$. Furthermore, it is customary to define the *external reflux ratio* of the column as $R \equiv L/D \in [0, \infty)$:

$$y_i = x_0 \frac{1}{1 + R} + x_{i-1} \frac{R}{1 + R}, \quad i \in [1, n]$$

This is the so-called *operating line* representing the combined mass and energy balances in the rectifying section of the column.

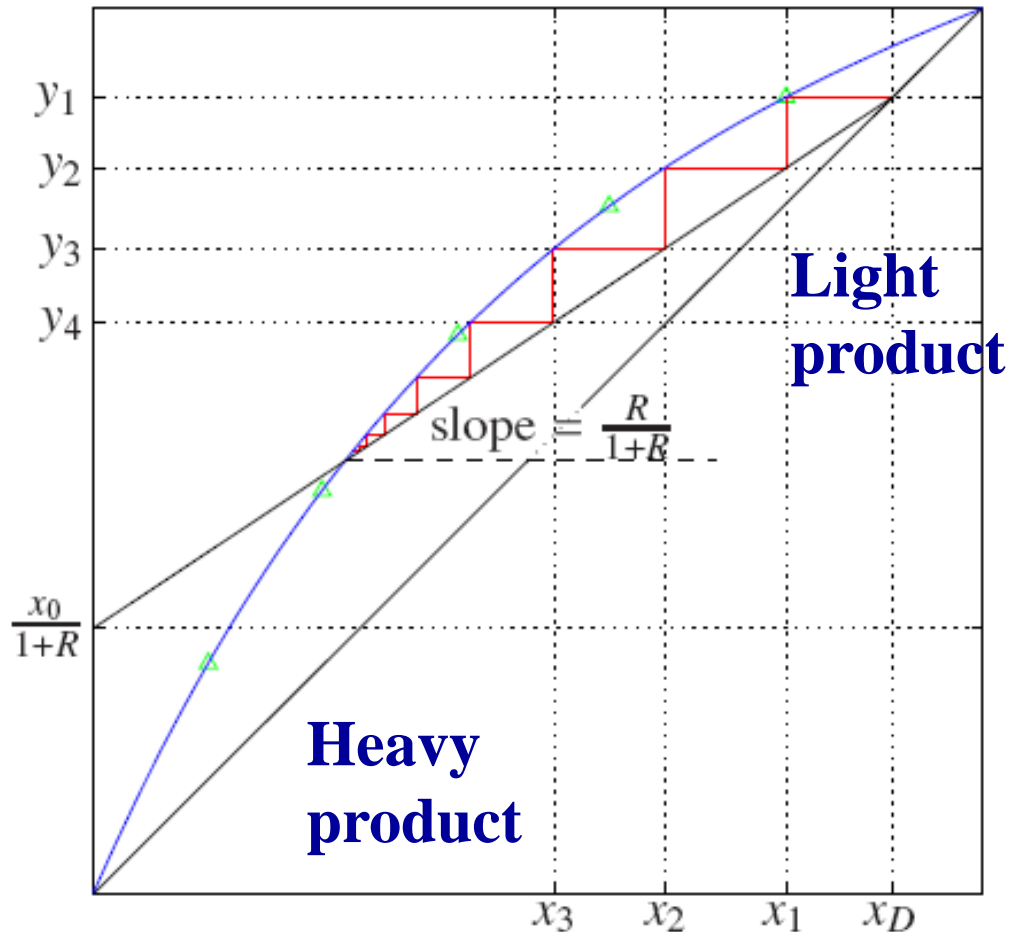
Notes:

- This equation is valid for all of the internal stages $i = 1, 2, \dots, n$ and in particular for $i = 1$ which yields $y_1 = x_0 = x_D$.

Operating Lines

- **Three ingredients of the McCabe–Thiele graphical method:**
 - (1) Constant molar overflow assumption
 - (2) Operating line
 - (3) Equilibrium curve
- The diagram is conventionally drawn with the heavier component to the left and the lighter component to the right. That means the equilibrium curve is located above the main 45° diagonal in the diagram.
- A typical example for an almost ideal mixture of benzene (light) and toluene (heavy), as show in below:

Operating Lines



Rectifying section of a benzene–toluene column ($R = 2$)

Operating Lines



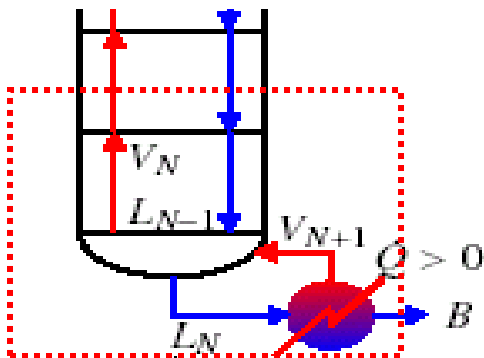
The stripping section

The operating line for the bottom section follows the same recipe as for the top section. The two mass balances are principally the same,

$$V_i + B = L_{i-1}$$

$$y_i V_i + x_B B = x_{i-1} L_{i-1}$$

For the vapor composition on the left hand side of the above balances,



$$\begin{aligned} y_i &= -x_B \frac{B}{V_i} + x_{i-1} \frac{L_{i-1}}{V_i} \\ &= -x_B \frac{B}{V_i} + x_{i-1} \frac{V_i + B}{V_i} \end{aligned}$$

Operating Lines

The constant molar overflow assumption yields $V_{n+1} = V_{n+2} = \dots = V_{N+1} \equiv V$. Furthermore, we may characterize the heat duty¹⁰ of the re-boiler as $S \equiv V/(V + B) \in [0, 1]$ and write

$$y_i = -x_B \frac{1 - S}{S} + x_{i-1} \frac{1}{S}, \quad i \in [n + 1, N + 1]$$

where S is the fraction of the down-coming liquid which is being evaporated. Alternatively we can define S as the heat duty of the re-boiler divided by the heat which is needed to evaporate all the down-coming liquid.

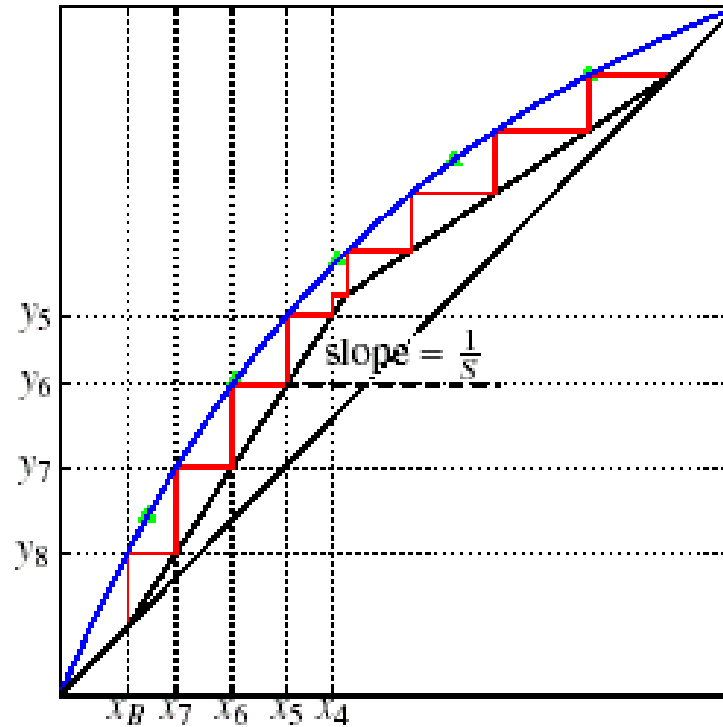
Notes:

- The operating line is valid for all the internal stages $i = n + 1, n + 2, \dots, N$ and also for the re-boiler $i = N + 1$.

Operating Lines

- The stripping section has therefore one external equilibrium stage in addition to the internal stages of the column (the situation is similar to that of a partial condenser in the rectifying section).
- The cross-over between the operating line and the main diagonal is given by $y_{N+2} = x_{N+1} = x_B$.
- The index $i = N + 2$ is strictly speaking outside the control volume but it does still serve as an easy-to-remember construction point of the diagram, as diagrammed as below:

Operating Lines



**Stripping section of a benzene–toluene column ($S = 2/3$).
Tray numbers are rounded to the nearest integer.**

Operating Lines

★ The feed tray

The operating line for the feed tray (q -line) requires four mass balances and two energy balances (including the constant molar overflow assumption). The extra mass and energy balances are needed to characterize the physical state of the feed stream. The component balances are

$$y_n V_n = x_D D + x_{n-1} L_{n-1}$$

$$x_n L_n = y_{n+1} V_{n+1} + x_B B$$

for the rectifying and stripping sections respectively.

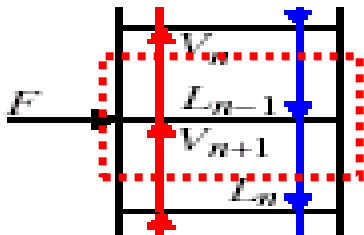
At the feed tray there will in general be sudden jumps in all the stream variables, but for an *optimal* placement of the feed tray the *intensive* state variables (temperature and composition) are *continuous*.

Operating Lines

Hence, it is required that $y_n = y_{n+1} \equiv y$ and that $x_n = x_{n-1} \equiv x$ in the equations above. Summation plus reorganization yields:

$$y(V_{n+1} - V_n) = x(L_n - L_{n-1}) - \underbrace{(x_D D + x_B B)}_{x_F F}$$

Note that the total mass balance $x_F F = x_D D + x_B B$ is substituted on the right side. The q -line is first written on the preliminary form:



$$y = x \frac{L_n - L_{n-1}}{V_{n+1} - V_n} - x_F \frac{F}{V_{n+1} - V_n}$$

The feed stream is subsequently replaced by the mass balance for the feed tray $F = (L_n - L_{n-1}) - (V_{n+1} - V_n)$. A little manipulation yields

Operating Lines

$$y = x \frac{L_n - L_{n-1}}{V_{n+1} - V_n} - x_F \left(\frac{L_n - L_{n-1}}{V_{n+1} - V_n} - 1 \right)$$
$$\equiv x \frac{\Delta L}{\Delta V} - x_F \left(\frac{\Delta L}{\Delta V} - 1 \right)$$

where ΔV and ΔL measure the differences in the vapor and liquid flows across the feed tray (top-down). This could serve as our final result, but it is customary to characterize the **feed quality** by

$$q \equiv \frac{\Delta L}{\Delta L - \Delta V}$$

where $q = 1 \Leftrightarrow \Delta V = 0$ (saturated liquid feed) and $q = 0 \Leftrightarrow \Delta L = 0$ (saturated vapor feed). Hence, the feed quality can be interpreted as the fraction of *saturated liquid* in the feed. The definition of the feed quality is easily inverted to give $\Delta L / \Delta V = q / (q - 1)$ which puts the q -line on the final form:

Operating Lines

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

Notes:

- This is the last of the three operating lines used in a McCabe-Thiele diagram, but it should be mentioned that the *optimal* feed tray location causes a slight redundancy in the calculation of the diagram: e.g. in most cases the composition specifications x_F and x_D are given in addition to the reflux ratio R and the feed quality q .
- This specifies the upper part of the column and the conditions of the stripper will be fixed once x_B or S is known (the other parameter is fixed by the common cross-over point of the operating lines).

Operating Lines

- Feed effects are important enough that a variable, q is assigned as a descriptor

(1) Sub-cooled Liquid , $q > 1$

$$q = 1 + c_{pL}(T_{bp} - T_f) / \lambda, \text{ where } \lambda \text{ is latent heat.}$$

(2) Saturated Liquid (bubble point feed), $q = 1$

(3) Partially Vaporized, $0 < q < 1$

$$q = (L/F) = (1 - V/F)$$

(4) Saturated Vapor (dew point feed), $q = 0$

(5) Superheated Vapor , $q < 0$

$$q = (-c_{pV}(T_f - T_{dp}) / \lambda)$$

Complete McCabe-Thiele Diagram

- The calculation is complete in the sense that it reveals all the significant figures of **a binary distillation column** for

(1) compositions of the top and bottom products;

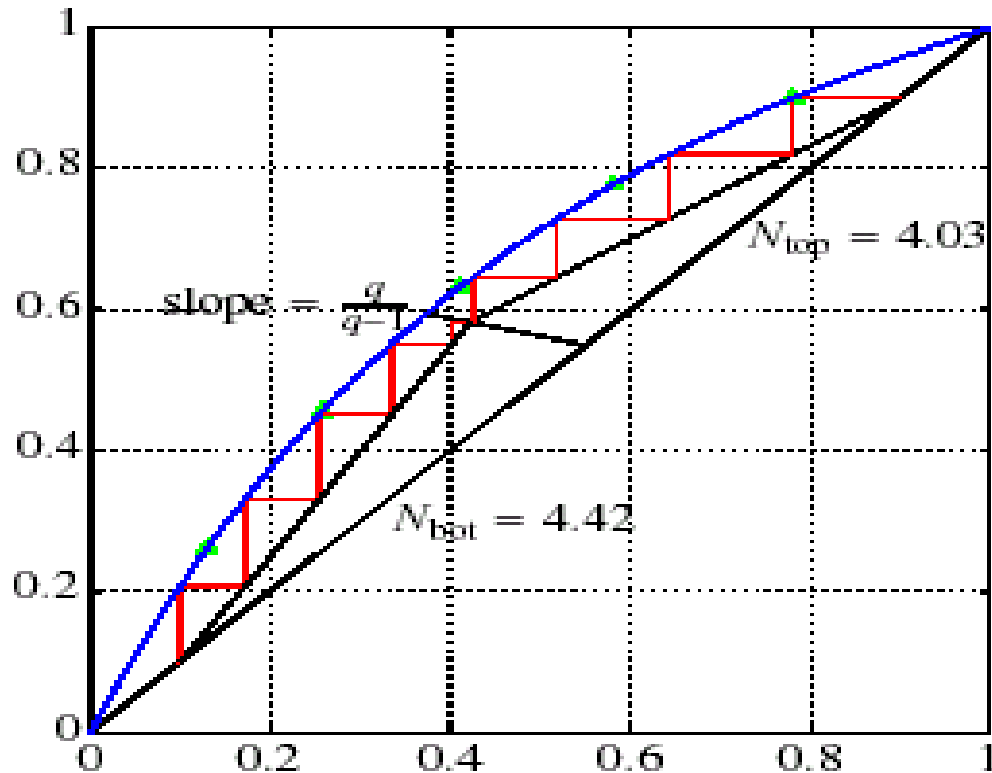
(2) composition and quality of the feed stream;

(3) reflux ratio (and condenser duty); and

(4) re-boiler duty,

as sketched in the figure below:

Complete McCabe-Thiele Diagram



Complete McCabe-Thiele diagram for a benzene–toluene column with parameters $x_D = 0.9$, $x_F = 0.55$, $x_B = 0.1$, $R = 2$ and $q = 0.2$ (consistent with $S = 2/3$).

Extreme Specifications

- The condition of *minimum reflux* is reached then
 - (1) the cross-over between the operating lines is located at the phase boundary; or
 - (2) the upper operating line is tangent to the equilibrium curve while the cross-over point is inside the phase diagram (applies to mixtures with concave equilibrium curves).

In both cases the number of theoretical stages approaches infinity.

- The other extreme is then the *reflux is infinite* and the operating lines for the column overlap with the main diagonal. **This yields the smallest number of theoretical stages for a given separation.**

Extreme Specifications

- The case ($q = \infty$) corresponds to a liquid feed so cold that it condenses all the vapor coming up from the re-boiler (ineffective rectifying section). The other case ($q = -\infty$) corresponds to a superheated vapor so hot that it evaporates all the liquid coming down from the condenser (ineffective stripping section).

Enthalpy-concentration Method

- McCabe Thiele method assumes constant molar flow rate because it considers equal latent heat of vaporization.
- Here we consider varying molar flow rate by solving simultaneous material and energy balances.
- In this case, the operating lines for the enriching and stripping section will be determined from simultaneous solution of mass and energy balance equations.
- To facilitate the solution of the heat balance equation, an enthalpy diagram can be constructed and used.

Column Design

Enriching Section

The mass balance:

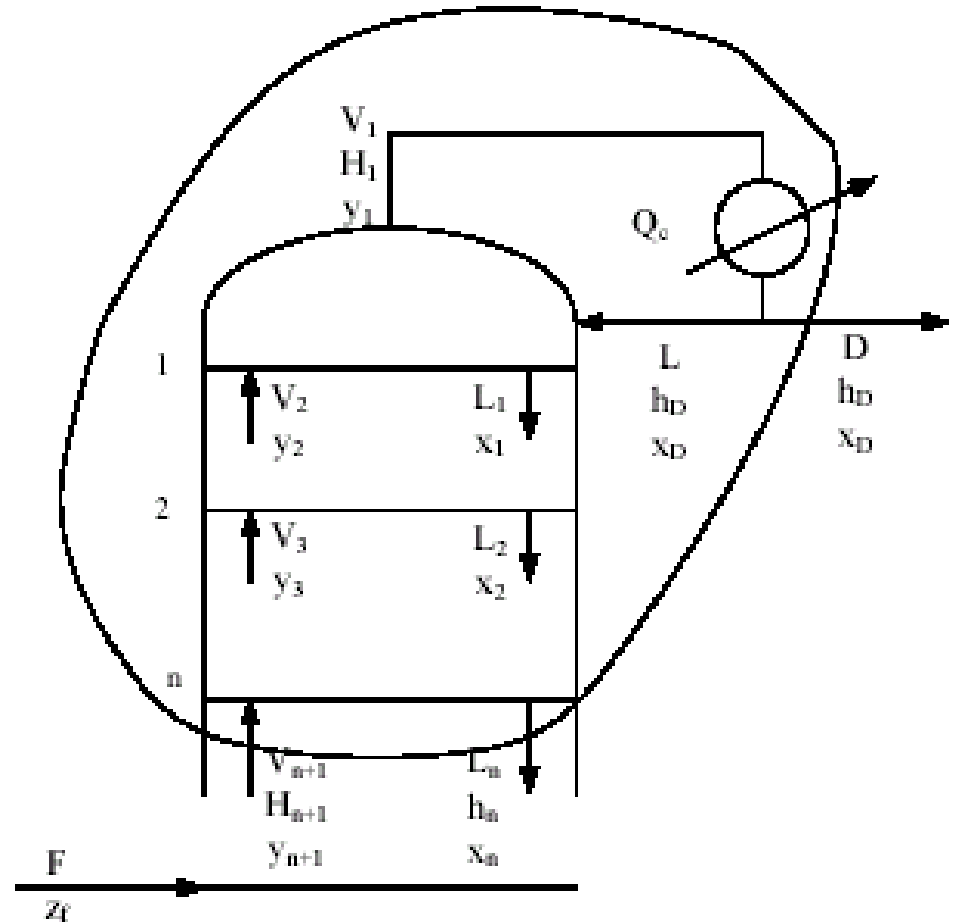
$$V_{n+1} = L_n + D$$

The component balance:

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

The enthalpy balance:

$$V_{n+1}H_{n+1} = L_n h_n + Dh_D + Q_c$$



Column Design

To eliminate the condenser duty is by heat balance around the condenser:

$$Q_c = V_1 H_1 - (L + D)h_D$$

Substituting for Q_c in equation

$$V_{n+1} H_{n+1} = L_n h_n + D h_D + Q_c$$

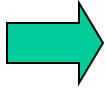


$$V_{n+1} H_{n+1} = L_n h_n + V_1 H_1 - L h_D$$

Inserting the mass balance equation

$$V_{n+1} = L_n + D$$

Column Design



$$V_{n+1}H_{n+1} = (V_{n+1} - D)h_n + V_1H_1 - Lh_D$$

Stripping section

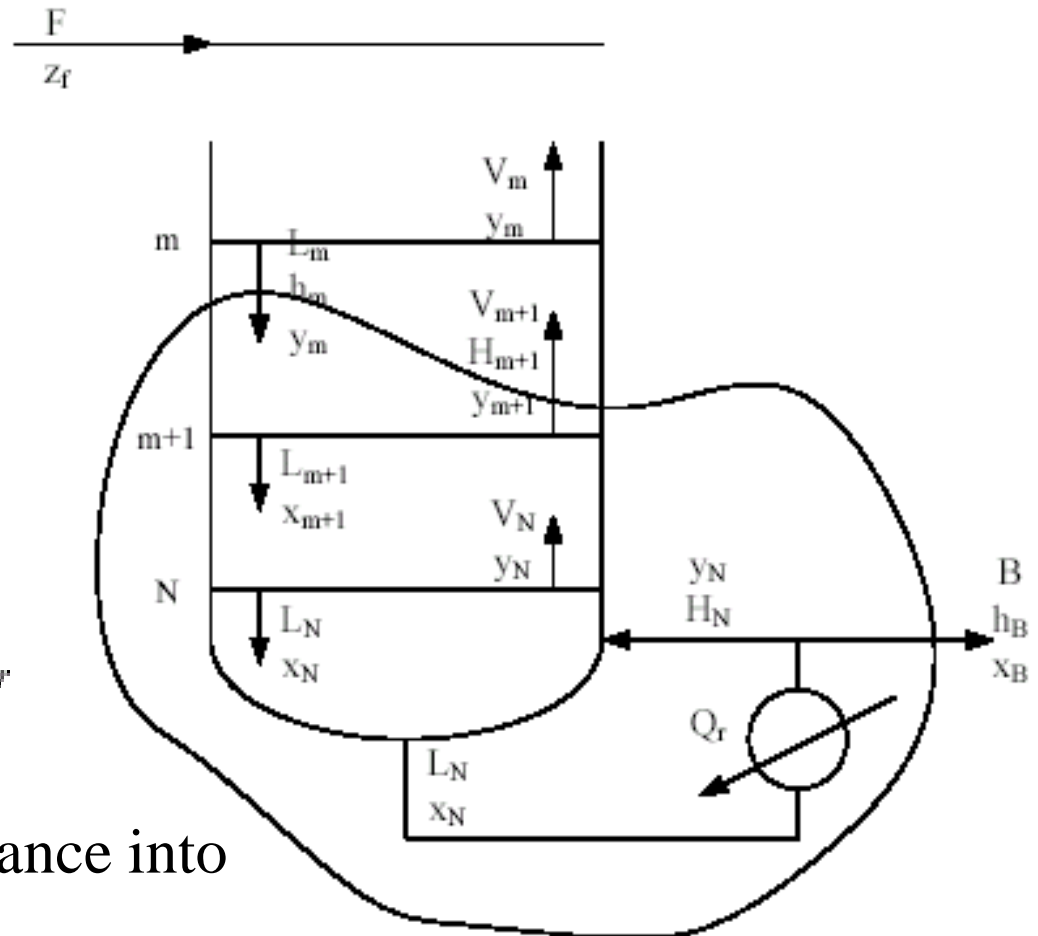
The mass balance:

$$L_m = V_{m+1} + B$$

The enthalpy balance:

$$V_{m+1}H_{m+1} = L_m h_m - B h_B + Q_r$$

Substituting the mass balance into this equation



Column Design

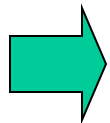

$$V_{m+1}H_{m+1} = (V_{m+1} + B)h_m - Bh_B + Q_r$$

Overall heat balance:

$$Q_r = Dh_D + Bh_B + Q_c - Fh_f$$

Substituting for Q_r into the heat balance equation

$$V_{m+1}H_{m+1} = (V_{m+1} + B)h_m - Bh_B + Q_r$$



$$V_{m+1}H_{m+1} = (V_{m+1} + B)h_m + Dh_D + Q_c - Fh_f$$

Column Design

The feed condition

The q line remain the same

Solution procedure

1. starting from x_D draw the **enriching operating line**:
 - (a) select a value for x between x_D and x_f
 - (b) assume a constant molar flow rate; $L_n = L$, $V_{n+1} = V$
 - (c) solve the component balance equation for y_{n+1}
 - (d) solve the heat balance for V_{n+1}
 - (e) solve the mass balance for L_n
 - (f) resolve the component balance for y_{n+1}
 - (g) if new value of y_{n+1} equals the old value go step(h)
else go back to step(c)
 - (h) repeat steps (a)-(g) for another value for x .

Tray Efficiency

Overall efficiency

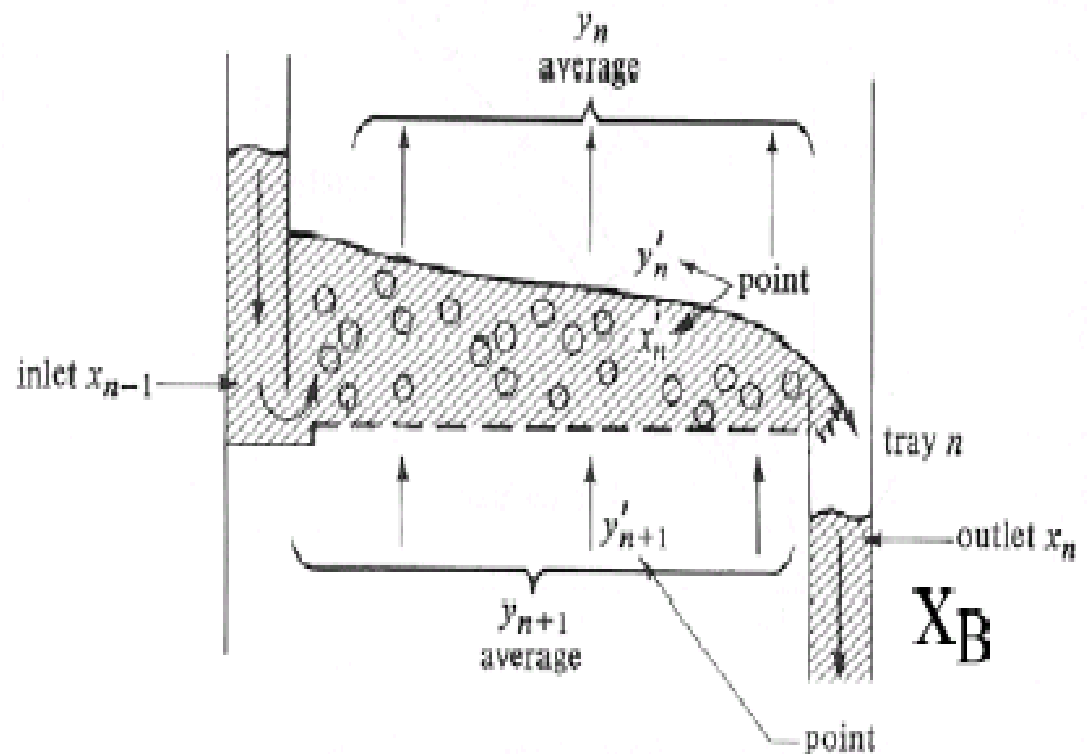
$$E_O = \frac{\text{Theroetical (ideal) numer of stages}}{\text{actual number of stages}}$$

Murphee Efficiency

$$E_M = \frac{y_n - y_{n+1}}{y_n^* - y_{n+1}}$$

Point Efficiency

$$E_{MP} = \frac{y_n' - y_{n+1}'}{y_n^* - y_{n+1}'}$$



Summary

- Distillation is not a new technique; it has been around for hundreds of years.
- In distillation, a mixture is separated into individual chemical compounds based on their various **boiling points**.

Example1: Separation of Water (H₂O) & Ethanol (C₂H₆O)

H₂O boils @ 100°C

Ethanol (C₂H₆O) boils @ 78°C

To distill a mixture of water & ethanol heat the mixture to around 85°C. At this temperature the ethanol becomes a gas and is collected in the apparatus overhead, leaving the water behind.

Remarks

Example 2: Industrial Distillation Tower at an Oil refinery

Q: What is crude oil?

A: Crude oil is a mixture of many different hydrocarbons, CH_4 to $\text{C}_{70}\text{H}_{142}$ with everything in between.

The hydrocarbons can be separated by their varying **boiling points**.

Reference Books

W.L. McCabe , J.C. Smith, and P. Harriott, *Unit Operations of Chemical Engineering* (6th Edition), McGraw-Hill, 2001,

Treybal, R.E., *Mass-Transfer Operations*, 3rd Edition (Reissue), McGraw-Hill, 1987