Single stage thermal separation: flash

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Agenda

- Definitions
- Degrees of freedom, material and energy balances
- Vapor liquid equilibrium, relative volatility
- Bubble point and dew point calculations
- Flash calculations
- Binary systems: McCabe - Thiele diagram
- Quench process
- Flash in enthalpy concentration diagram
- Multi component flash: Rachford-Rice Equation
- Three phase flash
- Examples: hand calculations, EXCEL, Aspen+
- Flash drum design
- Differential vaporization process

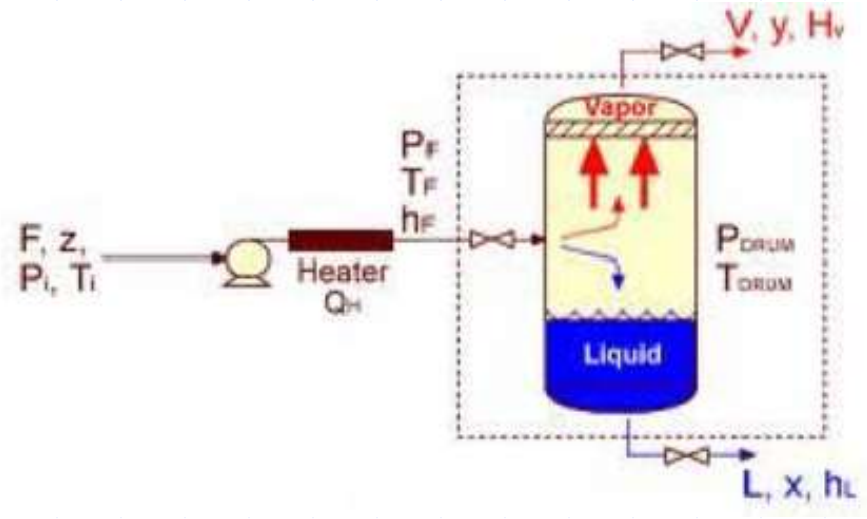
Separation problem definition

- A separation problem is defined when, starting from a feed with known flow rate F and composition z_i, the desired product specifications are set.
- Product specification may be
  - Flow rate
  - Purity of product
  - Recovery of one component
- For a vaporization process:
  - Vapor flow rate V and purity of one vapor component y_i
  - Purity and recovery of one component in the vapor phase.
- Recovery is defined as:

$$R_i = \frac{V y_i}{F z_{F,i}}$$

Single stage thermal separation unit

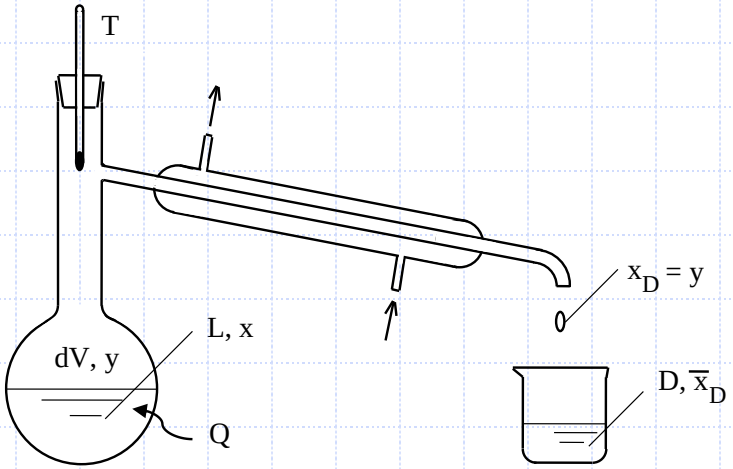
- Continuous operation at steady state:



- Semi-batch operation:

@ t=0 → L=F

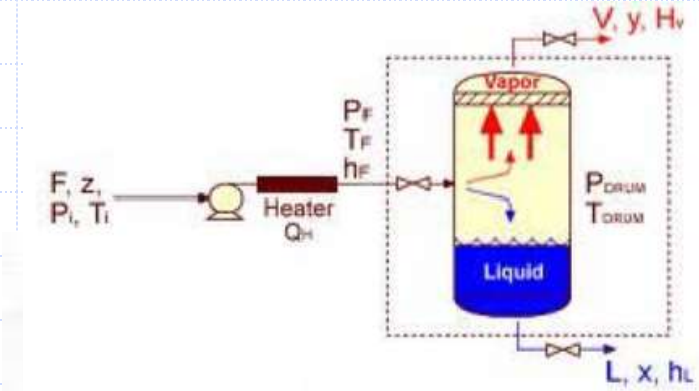
→ $x=z_F$

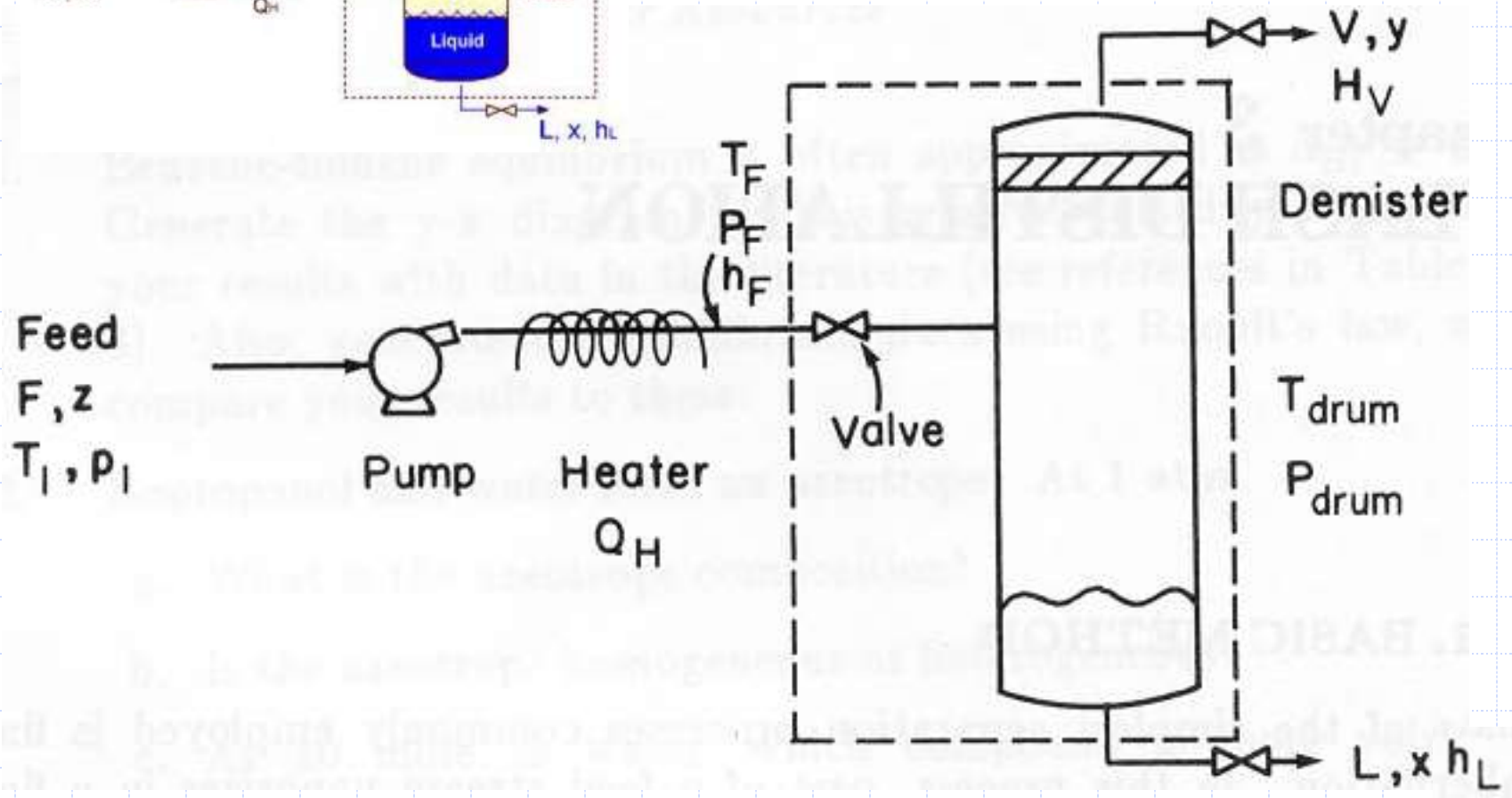


Flash Distillation

- Flash distillation is the simplest method of separation.
- A feed stream is "flashed" into a chamber or "flash drum"
  - the liquid and vapor are allowed to separate under equilibrium.
- It is "flashed" by throttling the feed stream through a nozzle or valve into the chamber – the pressure drops through the valve.
  - The drum pressure must be below the critical pressure for the mixture
- The more volatile component will be concentrated in the vapor stream – the less volatile in the liquid stream.
- The system is very close to a single "equilibrium stage".
- Separation is usually not very high for a single equilibrium stage.

Flash Distillation system





Degrees of Freedom (DoF)

- Intensive variables:
  - Temperature, Pressure, concentration, …
- Extensive variables
  - mass flow, energy flow, …
- Iterative variables
  - n° of stages in a distillation column

$$N_i = N_v - N_r$$

N_i = independent variables

N_v = total variables

N_r = independent equations

- Inherent relations (specific of the system)
- Mass balance relations
- Energy balance relations
- Phase equilibria relations
- Chemical equilibria relations

- $N\_i > 0$: "problem is underspecified and additional variables must be specified in order to determine the remaining variables"
- $N\_i = 0$: problem can be solved
- $N\_i < 0$: problem is overdetermined with redundant and possibly inconsistent relations

Flash: degrees of freedom

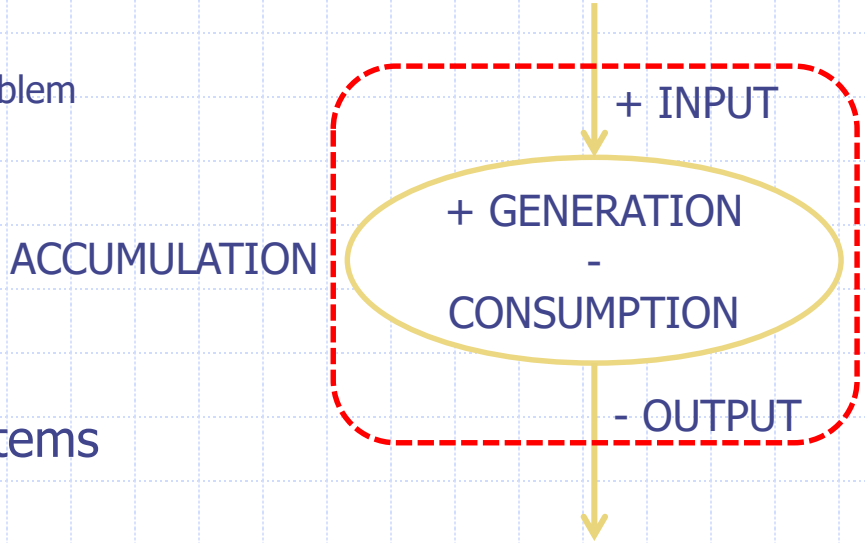
- Independent variables:
  - (NC+2) + 2 (NC+2) + 1 = (3 NC+7)
    Feed L+V Q
- Independent equations:
  - NC mass balances + 1 energy balance + NC equilibrium relations + 2 (T_L=T_V and P_L=P_V) = 2 NC+3
- Degrees of freedom (Operating Variables):
  - OV = (3 NC+7) – (2 NC+3) = NC+4
- … but in normal conditions the feed is specified
  - (NC+2) variables are subtracted form the degrees of freedom
- Flash process has ***2 degrees of freedom, i.e. operating variables***
  - Usually: flash pressure (P_F) and heat (Q).
  - Flash temperature and compositions are not used as operating variables since they are not easy to control.

Material and energy Balances

- The general balance equation

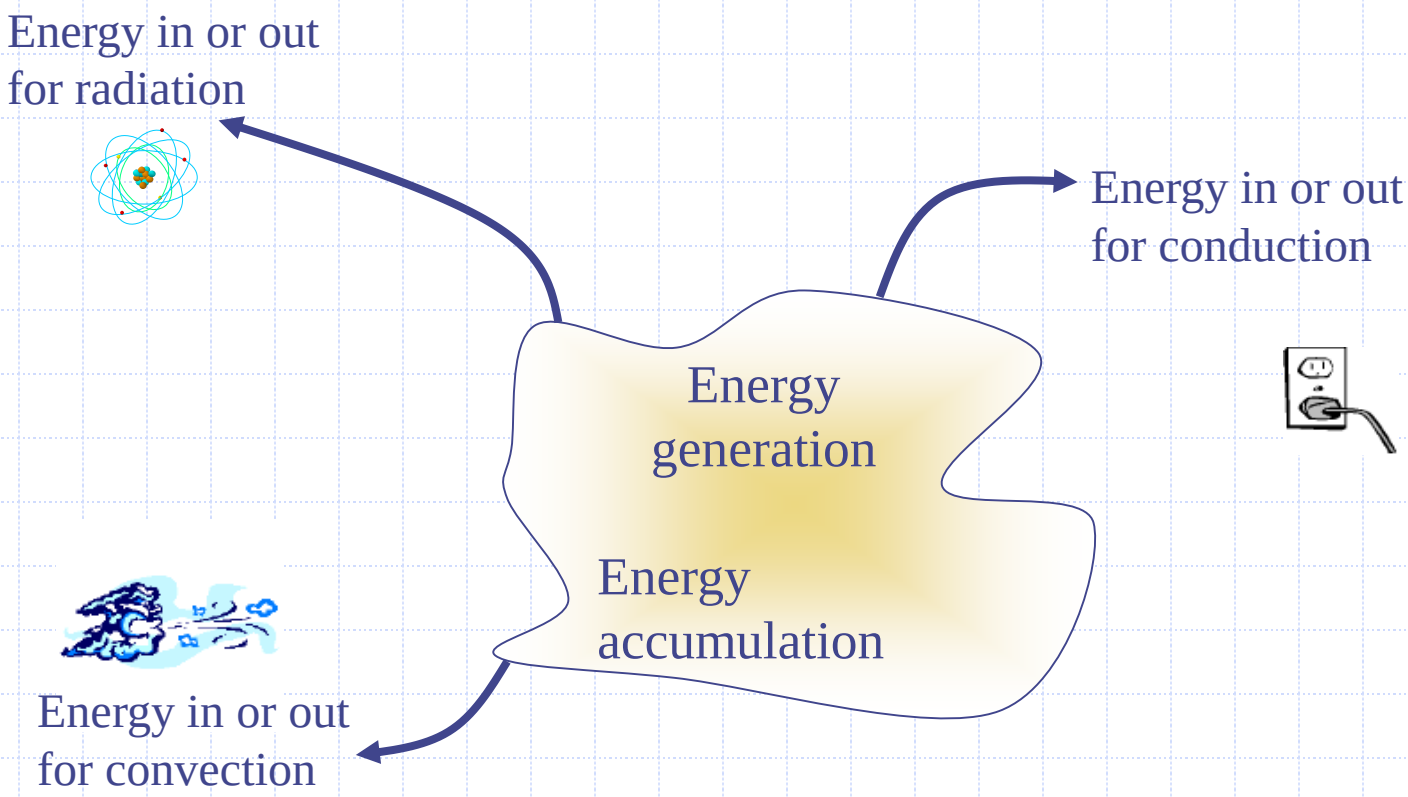
$$input + generation - output - consumption = accumulation$$

- Valid for Batch, Continuous and Semi batch
- The procedure for a single unit
  - Define the basis
  - Write the flowchart ... write all the known variables, label unknowns
  - Convert all the data in consistent units
  - Perform the degree of freedom analysis
  - Write the equations in an efficient solver and solve the system
  - Calculate the quantities requested in the problem statement
- Balances on multiple-unit processes (recycle – bypass)
- Balances on reactive processes
  - Molecular or atomic species
  - Extent of reaction
- Single phase and multiple phase systems



Energy balance

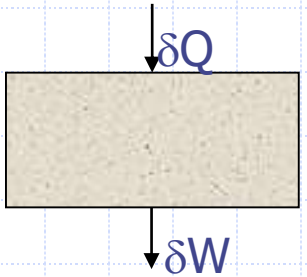
$$input + generation - output = accumulation$$



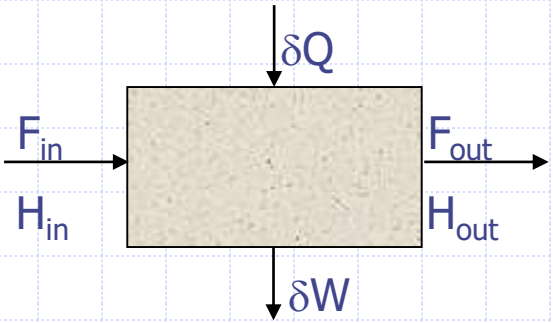
Thermodynamics fundamentals

- Closed system (First principle)

$$\Delta E = \delta Q - \delta W$$



- Open System



Rate of flow of heat to the system from the surroundings

Rate of accumulation of energy in the system

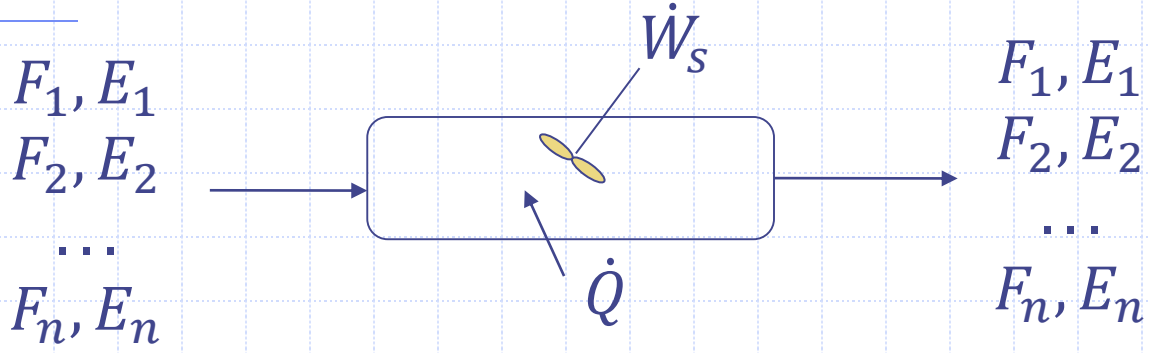
$$\frac{dE}{dt} = \dot{Q} - \dot{W} + \sum_{i=1}^{n} F_i E_{i_{in}} - \sum_{i=1}^{n} F_i E_{i_{out}}$$

Rate of work done by the system on the surroundings

Rate of energy added to the system by **mass** flow into the system

Rate of energy leaving the system by **mass** flow out the system

Evaluation of E and W terms



$$\dot{W} = \dot{W}_s + \textit{Rate of Flow Work}$$

Work spent to take mass in and out of the system

$$= -\sum_{i=1}^{n} F_i PV_i\Big|_{in} + \sum_{i=1}^{n} F_i PV_i\Big|_{out}$$

$$E_i = U_i + \frac{u^2{}_i}{2} + g\,z + \ldots$$

E_i is the sum of internal, kinetic, potential energy + other energies (magnetic, electric, light,…)

For the majority of unit operations in chemical engineering only Internal Energy is important

$$E_i \cong U_i$$

Energy balances in terms of Enthalpy

$$\dot{Q} - \dot{W} + \sum_{i=1}^{n} F_i E_i|_{in} - \sum_{i=1}^{n} F_i E_i|_{out} = \frac{d\hat{E}}{dt}$$

Substituting E_i and W

$$\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_i PV_i|_{in} - \sum_{i=1}^{n} F_i PV_i|_{out} + \sum_{i=1}^{n} F_i U_i|_{in} - \sum_{i=1}^{n} F_i U_i|_{out} = \frac{d\hat{E}}{dt}$$

Now $H = U + PV$

Energy balance equation in terms of Enthalpy is obtained:

$$\dot{Q} - \dot{W}_s + \sum_{i=1}^{n} F_i H_i|_{in} - \sum_{i=1}^{n} F_i H_i|_{out} = \frac{d\hat{E}}{dt}$$

Now, let's focus on enthalpy

Internal Energy U

- Macroscopic measure of subatomic and molecular energies
  - It is NOT directly measurable
  - It is a state function – only differences in U are calculated
  - Consequently, it is an exact differential
  - It can be expressed (for a pure component) in terms of two intensive variables (phase rule)
    - Temperature
    - Specific volume
  - U = U(T,V)

$$d\hat{U} = \left(\frac{\partial \hat{U}}{\partial T}\right)_{\hat{V}} dT + \left(\frac{\partial \hat{U}}{\partial \hat{V}}\right)_{T} d\hat{V}$$

  - At constant volume:

$$\hat{U}_2 - \hat{U}_1 = \int_1^2 C_v \, dT$$

Enthalpy H

- Defined as a combination of variables: → H=U +pV
  - It is NOT directly measurable
  - It is a state function – only differences in H are calculated
  - Consequently, it is an exact differential
  - It can be expressed (for a pure component) in terms of two intensive variables (phase rule)
    - Temperature
    - Pressure
  - H = H(T,p)

$$d\hat{H} = \left(\frac{\partial \hat{H}}{\partial T}\right)_p dT + \left(\frac{\partial \hat{H}}{\partial p}\right)_T dp$$

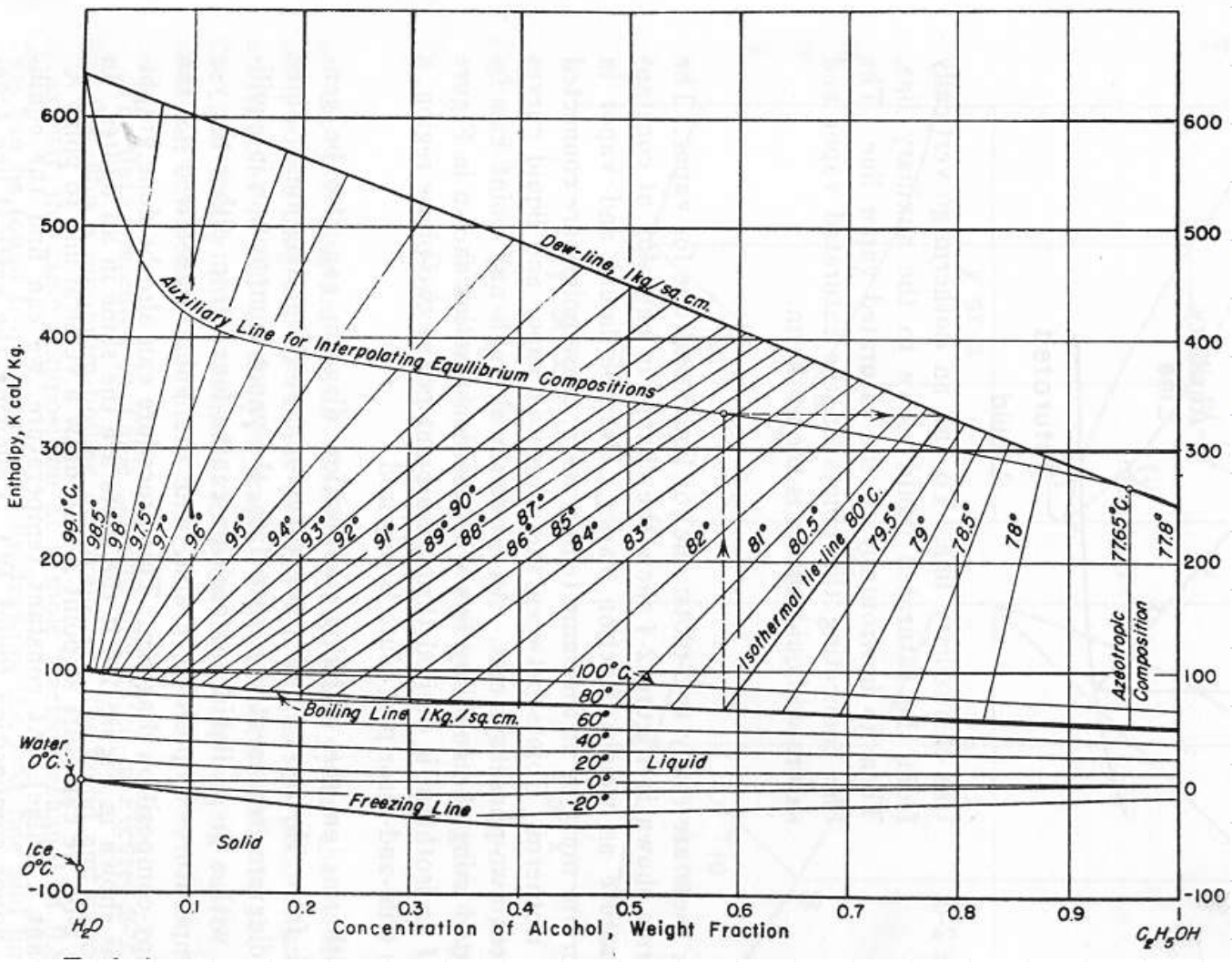
$$\hat{H}_2 - \hat{H}_1 = \int_1^2 C_p \, dT$$

  - At constant pressure:

Enthalpy vs. Composition: Ponchon-Savarit Plot

- We have begun to employ mass balances, both total and component.
- We will also need to employ energy balances, based on enthalpy, for certain separation problems.
- We can use the Enthalpy vs. composition plot to obtain this information.

Enthalpy vs. Composition: Ponchon-Savarit Plot



Flash process in enthalpy composition diagram

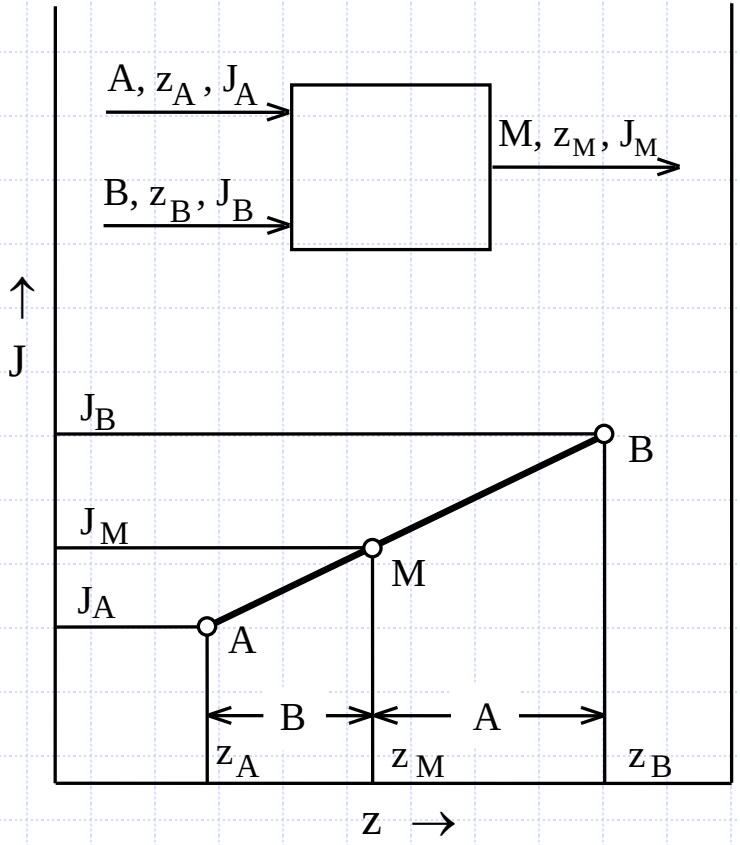
1) Adiabatic Mixing is represented by a straight line

$$M = A + B$$

$$Mz_M = Az_A + Bz_B$$

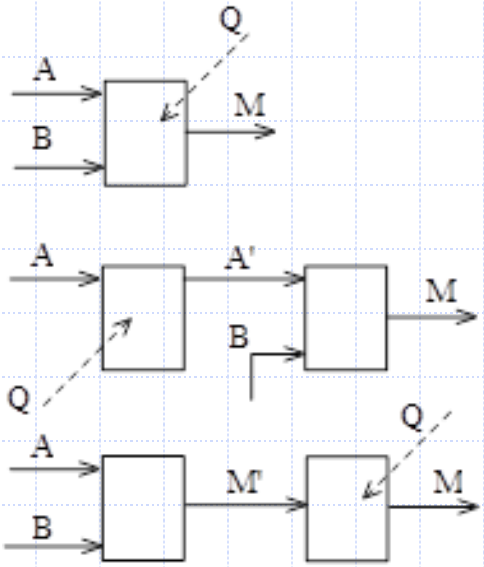
$$MJ_M = AJ_A + BJ_B$$

$$\frac{J_M - J_B}{J_A - J_M} = \frac{z_M - z_B}{z_A - z_M} = \frac{A}{B}$$



Flash process in enthalpy composition diagram

2) Mixing with heat exchange



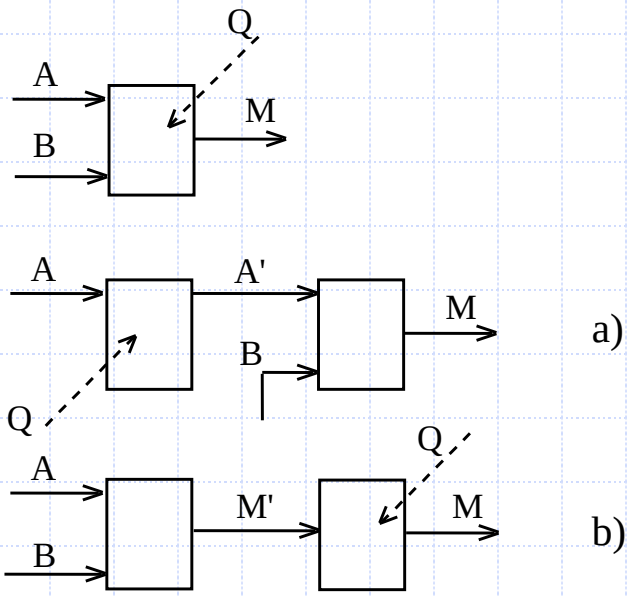
$$AJ_A + BJ_B + Q = MJ_M$$

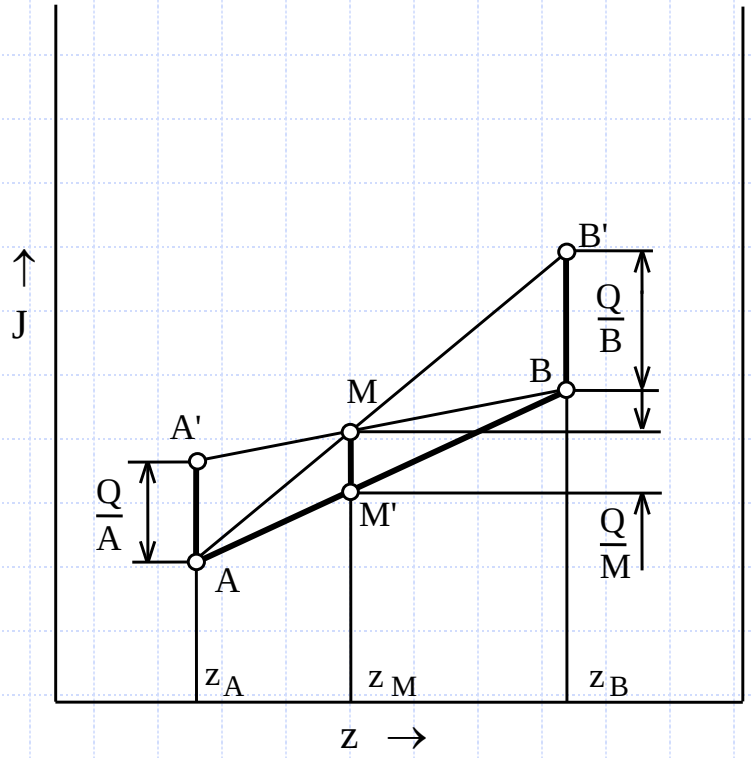
a) $AJ_{A'} + BJ_B = MJ_M$ $\qquad J_{A'} = J_A + \frac{Q}{A}$

b) $AJ_A + BJ_B = MJ_M$ $\qquad J_M = J_{M'} + \frac{Q}{M}$

Flash process in enthalpy composition diagram

2) Mixing with heat exchange





Enthalpy vs. Composition: Enthalpy Determination

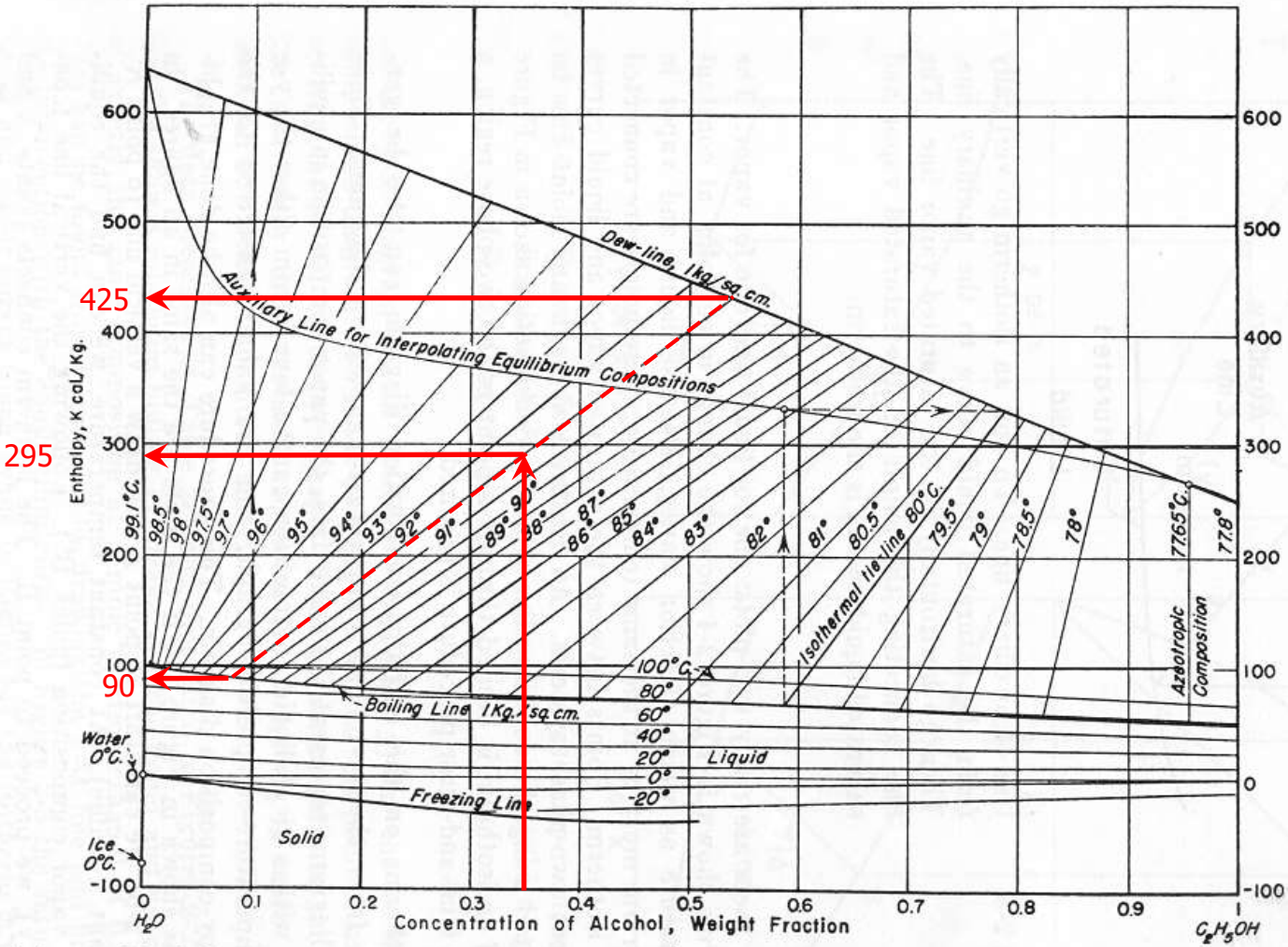
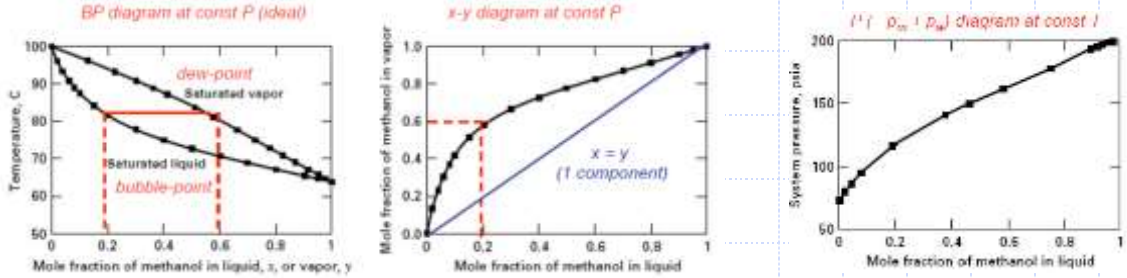


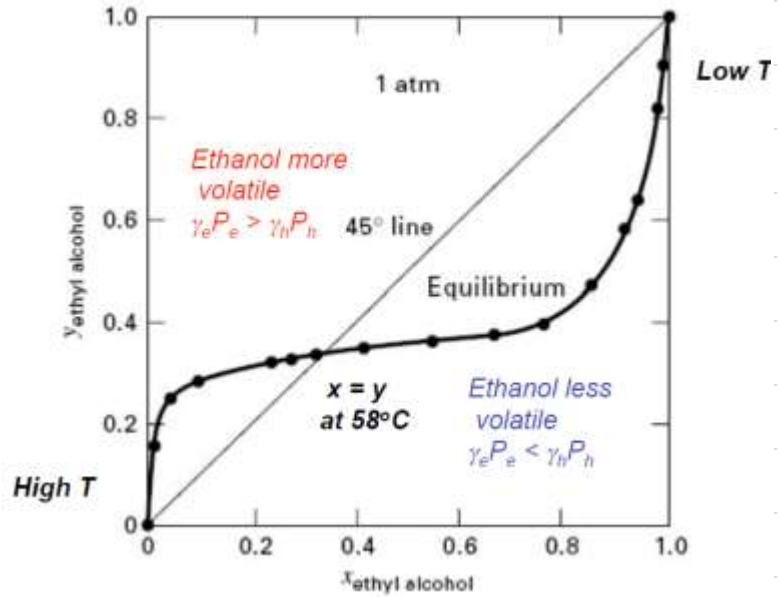
Figure 2-4. Enthalpy-composition diagram for ethanol-water at a pressure of 1 kg/cm^2. (Bosnjakovic, *Technische Thermodynamik*, T. Steinkopff, Leipzig, 1935)

Vapor – liquid equilibria (near ideal and non ideal systems)

- Methanol – water
  - (methanol more volatile Pm > Pw, Pm > 1 atm)



- n-hexane-ethanol system
  - (ethanol less volatile)



- Summarizing:

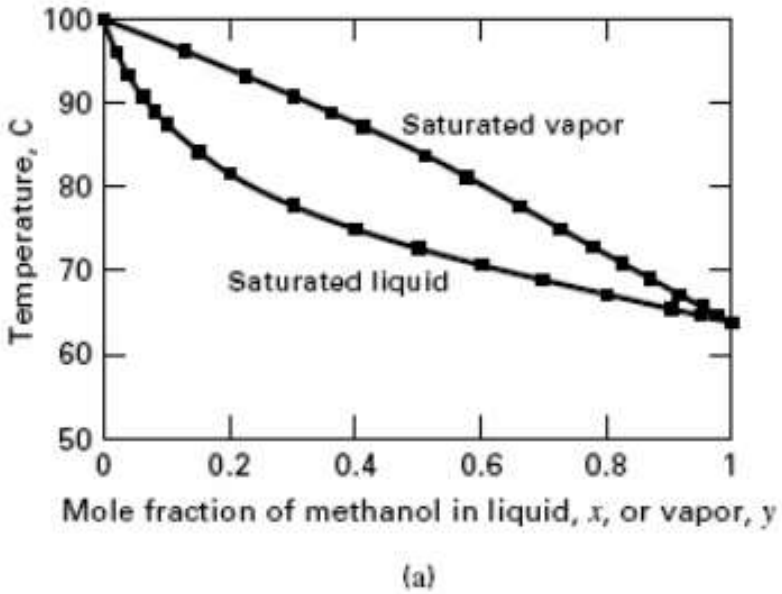
0 < P < 2 bar $Py_i = P_i^{sat}\gamma_i x_i$

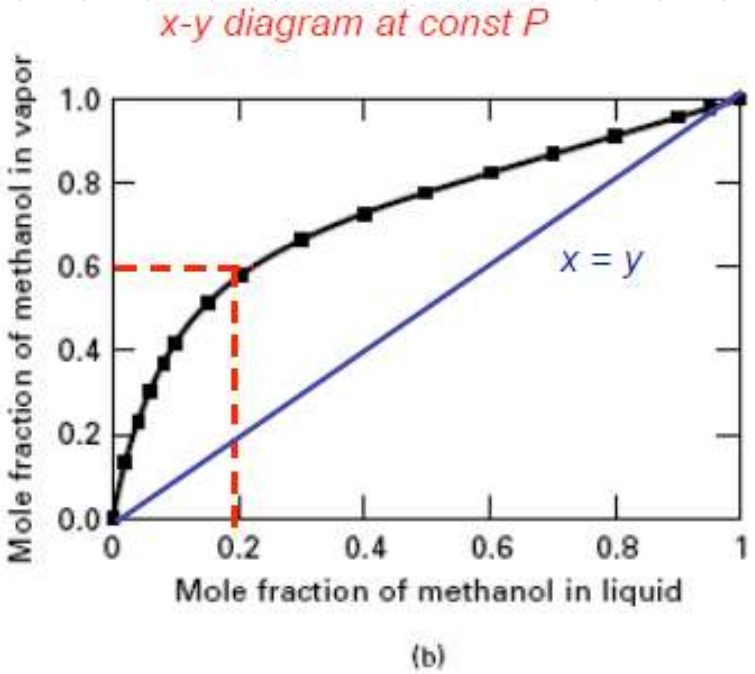
2 < P < 40 bar $\varphi_i^V P y_i = \varphi_i^{*V,sat} P_i^{sat} \gamma_i x_i$

P > 40 bar $\varphi_i^V y_i = \varphi_i^L x_i$

Flash Distillation – Equilibrium

- The equilibrium relationships that we have been using can be applied to flash distillation problems.
- Equilibrium data or a valid equilibrium relationship must be available at the flash drum pressure.





The greater the separation between the equilibrium and 45° line, the easier the separation

Equilibrium ratio and relative volatility

1. Equilibrium ratio (capacity factor): $K_i = \frac{y_i}{x_i}$

2. Relative volatility (selectivity): $\alpha_{i,j} = S_{i,j} = \frac{K_i}{K_j}$

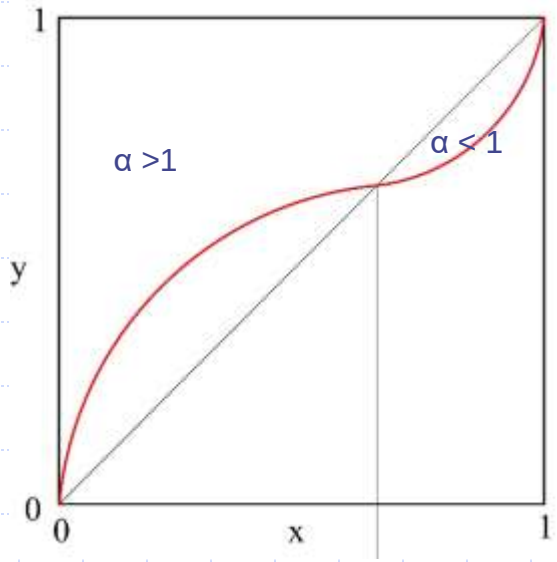
3. For a binary system: $\alpha = \alpha_{1,2} = \frac{y/x}{(1-y)/(1-x)}$

Equilibrium ratio and relative volatility

- At low pressure

$$Py_i = P_i^{sat}\gamma_i x_i \qquad K_i = \frac{P_i^{sat}\gamma_i}{P} \qquad \alpha_{i,j} = \frac{K_i}{K_j} = \frac{P_i^{sat}(T)\gamma_i(T,x)}{P_j^{sat}(T)\gamma_j(T,x)}$$

- Relative volatility is NOT constant, depends on composition
  - *For ideal solution is nearly constant



At the azeotrope: $x = y \longrightarrow \alpha = 1$

Binary systems: Brown's equation

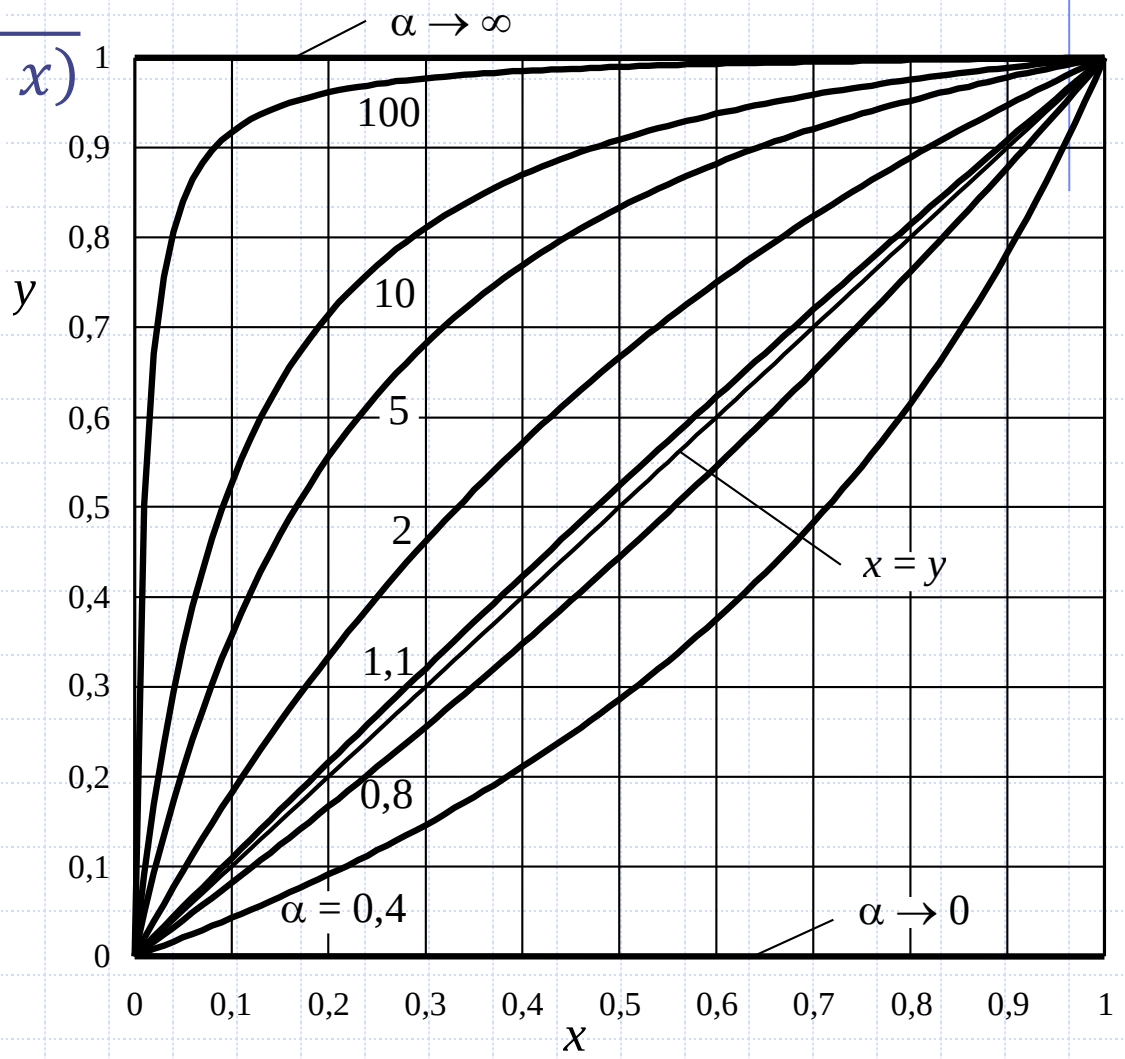
$$\alpha = \alpha_{1,2} = \frac{y/x}{(1-y)/(1-x)}$$

- Rearranging

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

- Limit for thermal separation processes

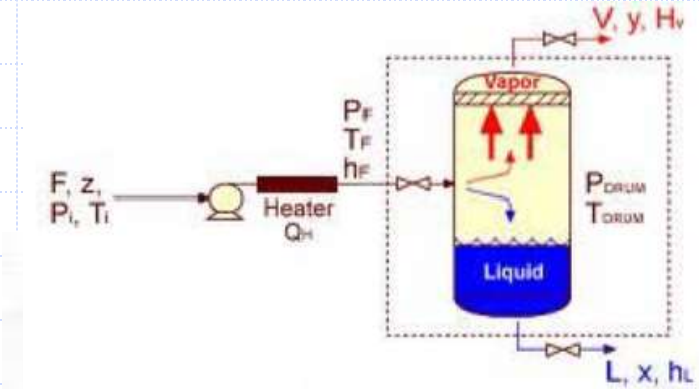
$$|\alpha_{i,j} - 1| \geq 0.05$$

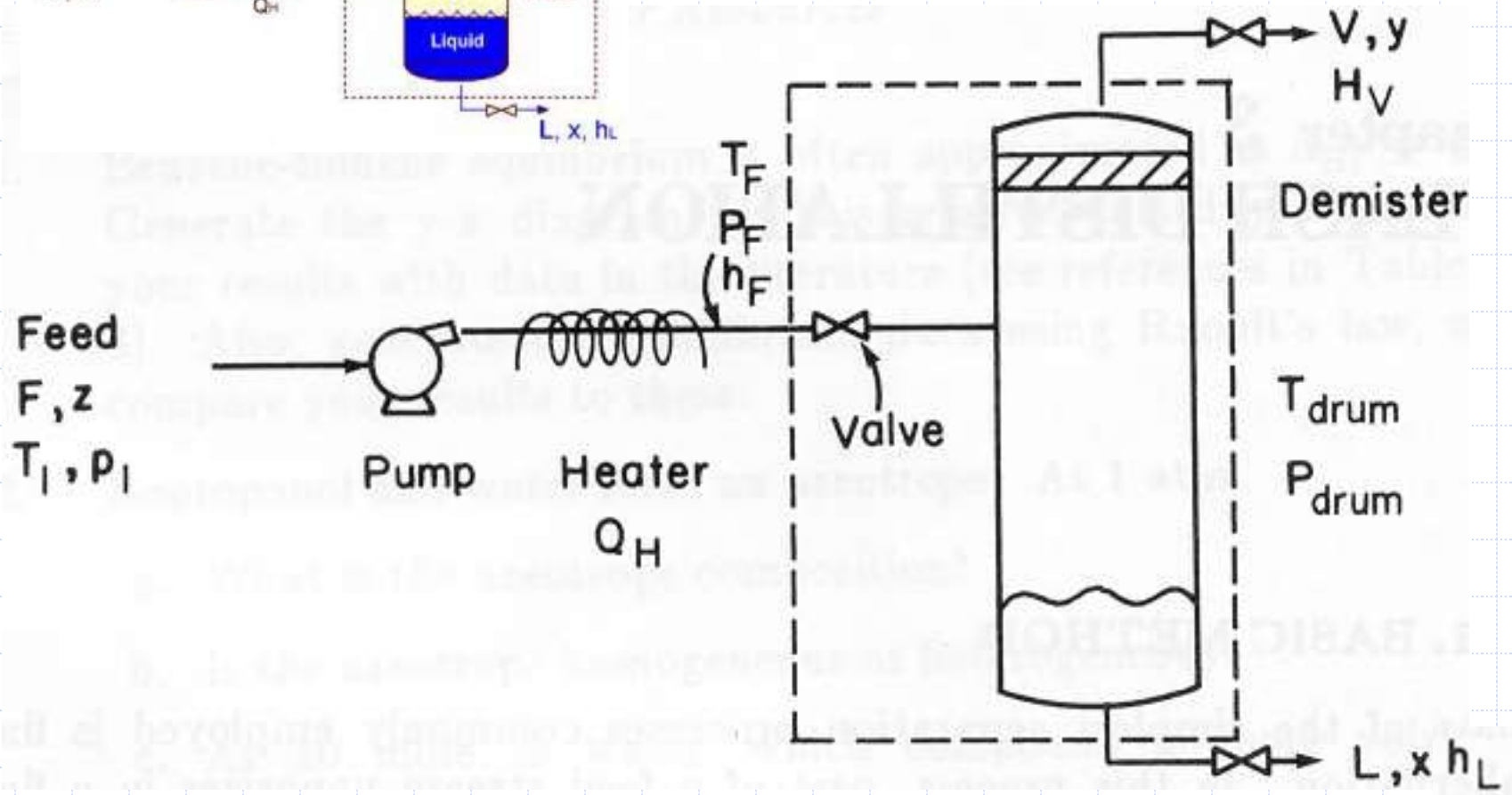


Vapor liquid equilibrium calculation types

- Bubble point calculation,
  - *Given:* the liquid composition (x) and equilibrium T or P
  - *Calculate*: the vapor composition (y) and equilibrium P or T
- Dew point calculations
  - *Given:* the vapor composition (y) and equilibrium T or P
  - *Calculate*: the liquid composition (x) and equilibrium P or T
- Flash calculation
  - *Given:* the global composition (z) and equilibrium T and P
  - *Calculate*: the liquid (x) and vapor (y) compositions

Flash Distillation system



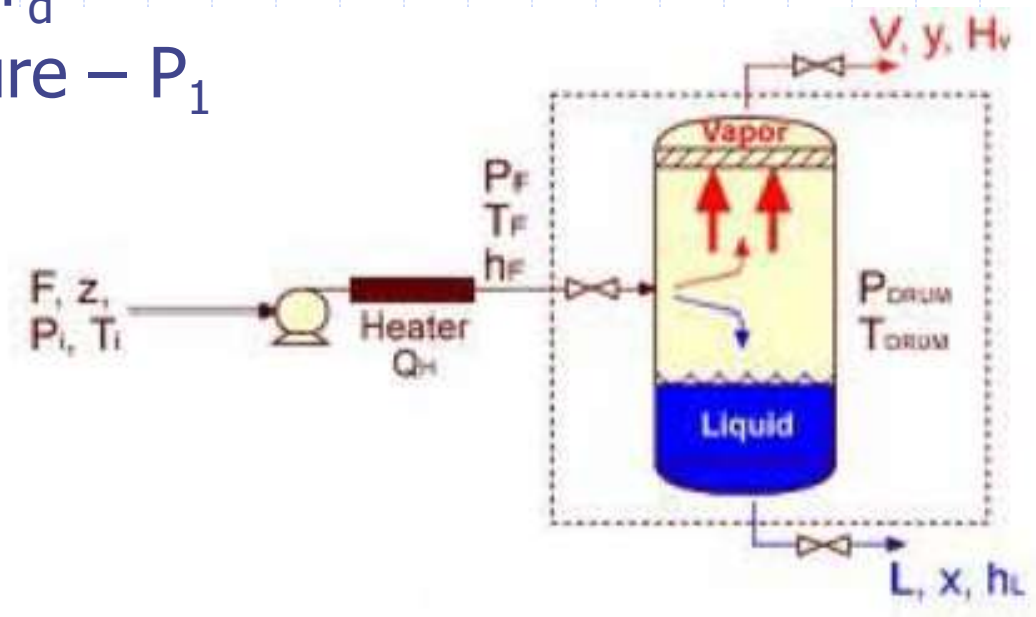


Flash Distillation – Solution

- Flash distillation problems can be solved using three sets of equations:
  - Equilibrium relationship
  - Mass balance
  - Energy balance
- The equilibrium relationships that we have been using can be applied to flash distillation problems.
- Equilibrium data or a valid equilibrium relationship must be available at the flash drum pressure.

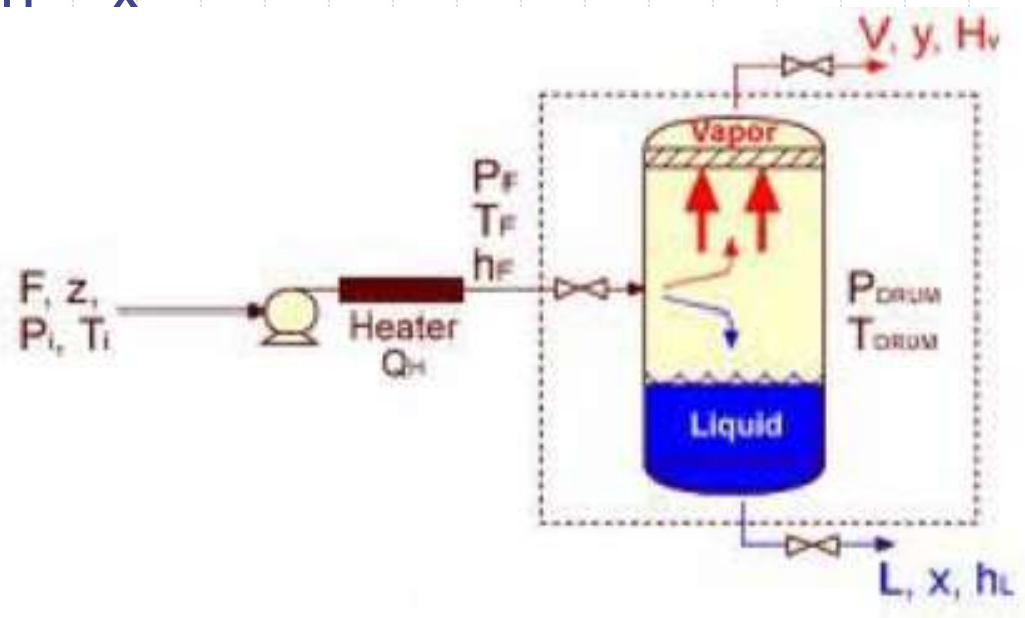
Flash Distillation – Equilibrium Parameters

- Feed Composition – z
- Vapor-Phase Composition – y
- Liquid-Phase Composition – x
- Upstream Feed Temperature – T_1
- Feed Temperature – T_F
- Drum Temperature – T_d
- Upstream Feed Pressure – P_1
- Feed Pressure – P_F
- Drum Pressure – P_d



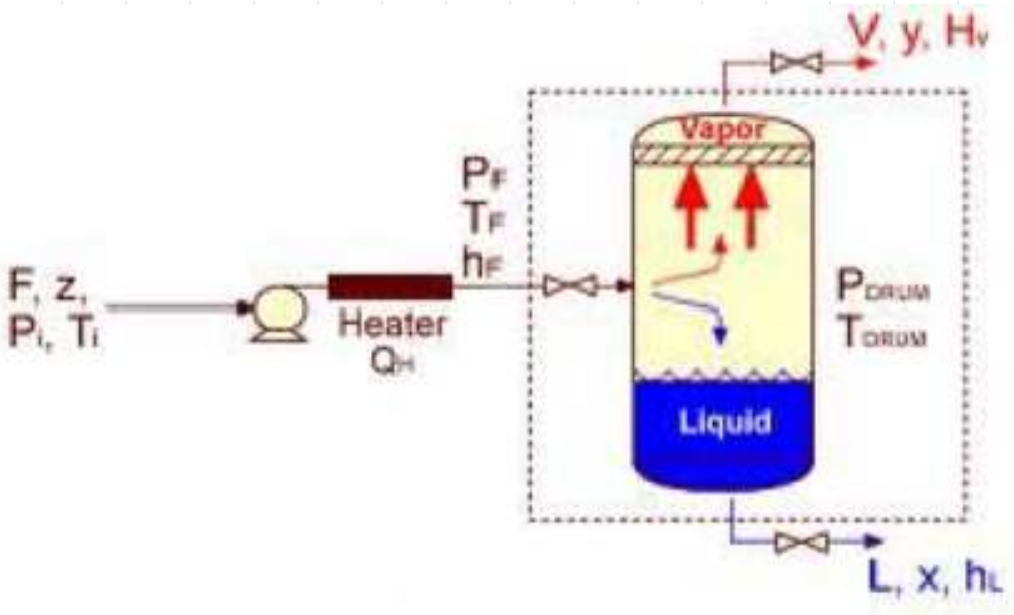
Flash Distillation – Mass Parameters

- Feed Flow Rate – F
- Vapor Flow Rate – V
- Liquid Flow Rate – L
- Feed Composition – z
- Vapor-Phase Composition – y
- Liquid-Phase Composition – x



Flash Distillation – Energy Parameters

- Heater Input – Q_H
- Flash Drum Heat Input – Q_{flash}
- Feed Enthalpy– h_F
- Vapor Enthalpy – H_V
- Liquid Enthalpy – h_L
- Upstream Feed Temperature – T_1
- Feed Temperature – T_F
- Drum Temperature – T_d



Material balances for flash

- Total balance $F = V + L$
- NC balances $F z_i = V y_i + L x_i$

$$f = \frac{V}{F};$$

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

$$z_i = f y_i + (1 - f) x_i$$

- For a binary system:
  - For more volatile component $z = f y + (1 - f) x$
- NC equilibrium relations $y_i = K_i x_i$ $K_i = K_i(\bar{x}, \bar{y}, P, T)$
- For a binary systems:

$$y = K_1 x$$

$$1 - y = K_2 (1 - x)$$

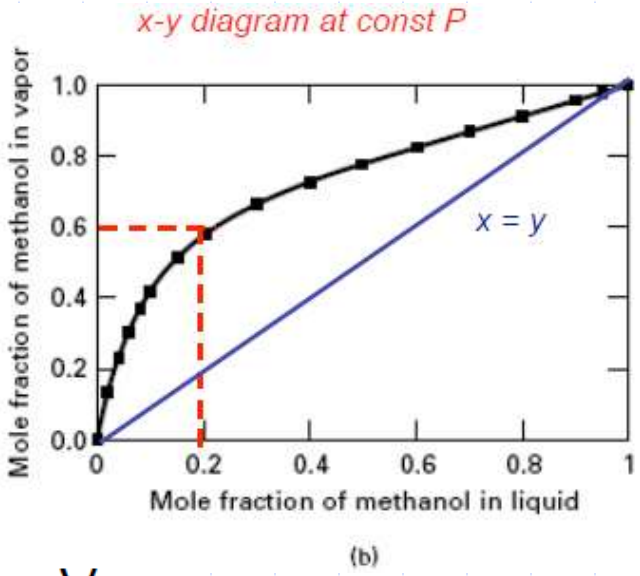
Simple flash distillation (single stage; heated to T, phase split)

- Overall mass balance

$$F = V + L$$

- Component mass balance

$$Fz = Vy + Lx$$



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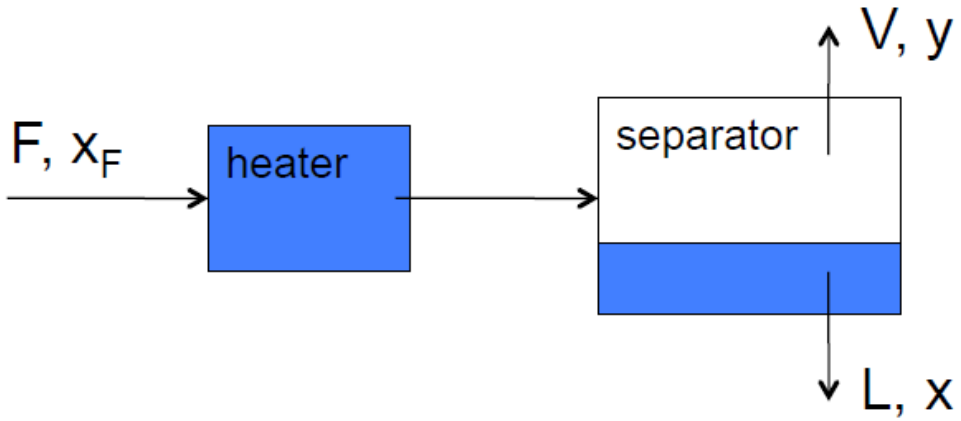


Flash Distillation – Operating Line

Solving the overall mass balance for y yields

$$y = -\frac{L}{V}x + \frac{F}{V}z$$

which is termed the operating line. It relates the composition of the streams leaving the stage or drum.

Problem specifications.

- Common problem specifications
  - Liquid to vapor ratio → L / V
  - Fraction of feed vaporized → f = V / F
  - Fraction of feed remaining as liquid → q = L / F
- Operating Line Form – Fraction Vaporized
  - From the overall mass balance

$$\frac{L}{V} = \frac{F - V}{V} = \frac{1 - V/F}{V/F} = \frac{1 - f}{f}$$

  - Then

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

- Operating Line Form - Fraction Remaining as Liquid
  - or

$$\frac{L}{V} = \frac{L}{F-L} = \frac{L/F}{1-L/F} = \frac{q}{1-q}$$

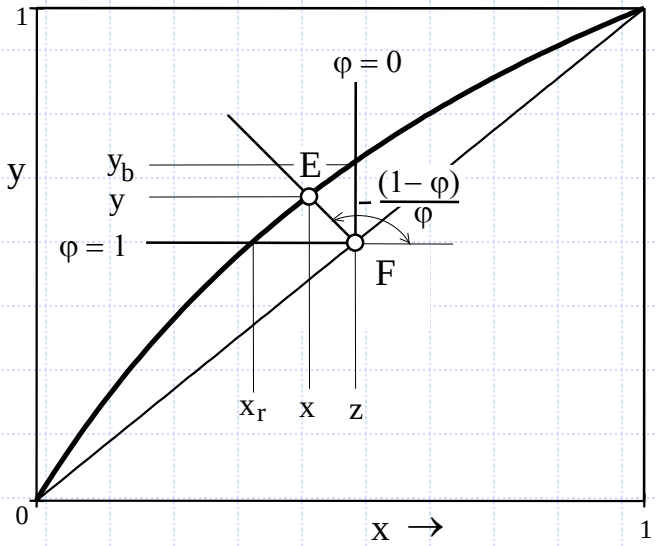
  - and

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

Operating Lines – Linear!

- Slope $$-\frac{L}{V} = -\frac{1-f}{f} = -\frac{q}{1-q}$$
- y Intercept $$\frac{F}{V} z = \frac{1}{f} z = \frac{1}{1-q} z$$
- x intercept $$\frac{F}{L} z = \frac{1}{1-f} z = \frac{1}{q} z$$
- How to solve it?
  - We often know all of the system parameters except the compositions of the vapor and liquid leaving the flash drum (2 unknowns, y and x)
  - We have two equations: Equilibrium Relationship and Mass Balance (Operating Line)
  - With two equations and two unknowns we can solve the problem!

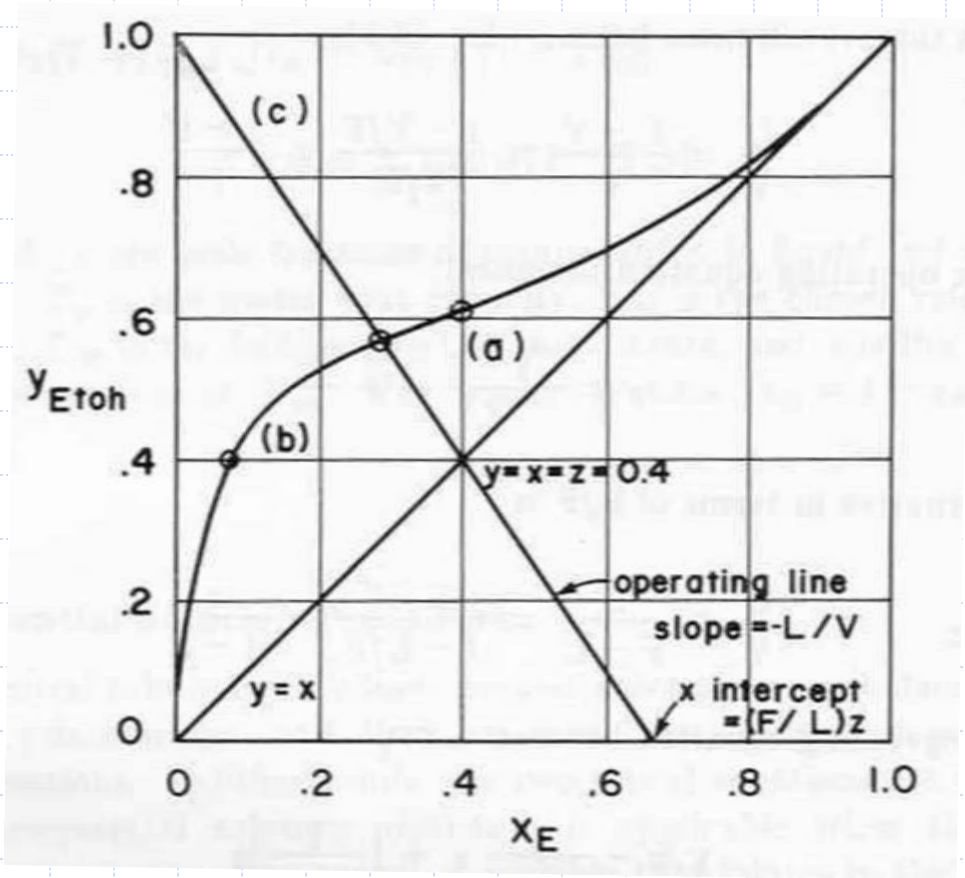
Binary systems: McCabe-Thiele Analysis



- Feed line

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

  - 2 limit conditions:
  - Max vapor composistion
  - Min. liquid composistion



Energy balance for flash

- Balance equations

$$F h_F + Q_{flash} - L h_L - V H_V = 0$$

h_F = feed enthalpy
h_L = saturated liquid enthalpy
H_V = saturated vapor enthalpy
Q_{flash} = heat flash chamber

- Introducing
  - F=L+V
  - $\lambda = H_v - h_L$
  - f = V/F
- One obtains:

$$f = \frac{Q}{\lambda F} + \frac{h_F - h_L}{\lambda}$$

- Energy consumption is closely related to the degree of vaporization

$$\frac{Q}{F} \cong \lambda f$$

- Operating cost of a thermal separation process is directly proportional to its energy consumption

Energy balance for flash

h_F = feed enthalpy
h_L = saturated liquid enthalpy
H_V = saturated vapor enthalpy
Q_{flash} = heat flash chamber
Q_h = heat supplied by heater

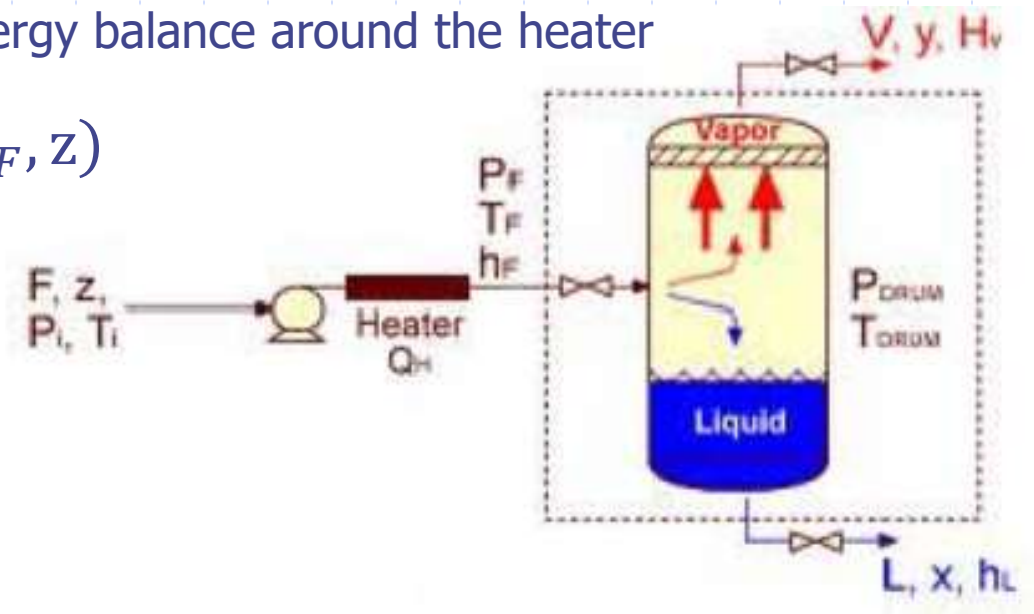
- Balance equations

$$Fh_F + Q_{flash} - Lh_L - VH_V = 0$$

  - With h = f (T, conc)
  - Enthalpies are known if T and compositions are given,
  - Q_{flash} = 0 (adiabatic flash)
  - The only unknown in the energy balance equation is the feed enthalpy h_F
  - Once is known, TF can be obtain from enthalpy equation
  - Q_h = is calculated from an energy balance around the heater

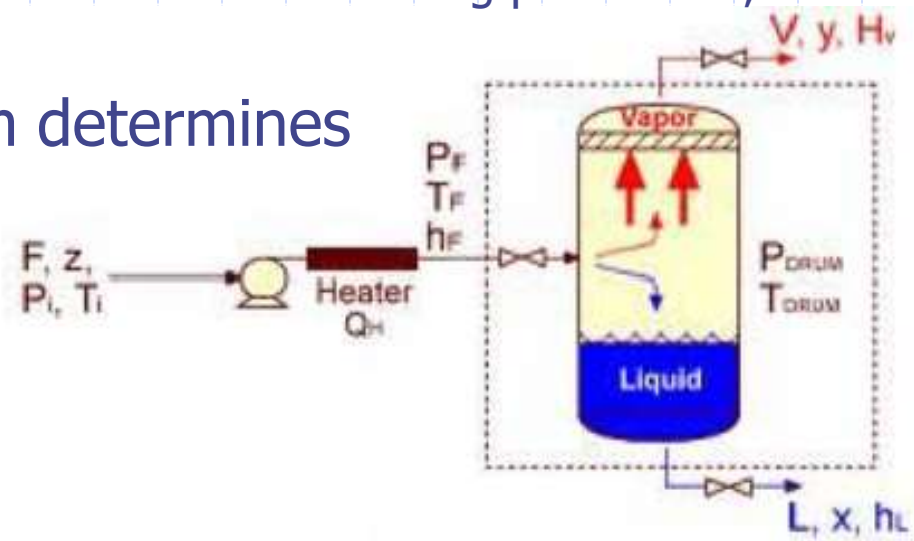
$$Fh_L(T_I, z) + Q_h = Fh_F(T_F, z)$$

  - The feed pressure P_F is semi arbitrary (any P high enough to prevent boiling at temperature T_F)



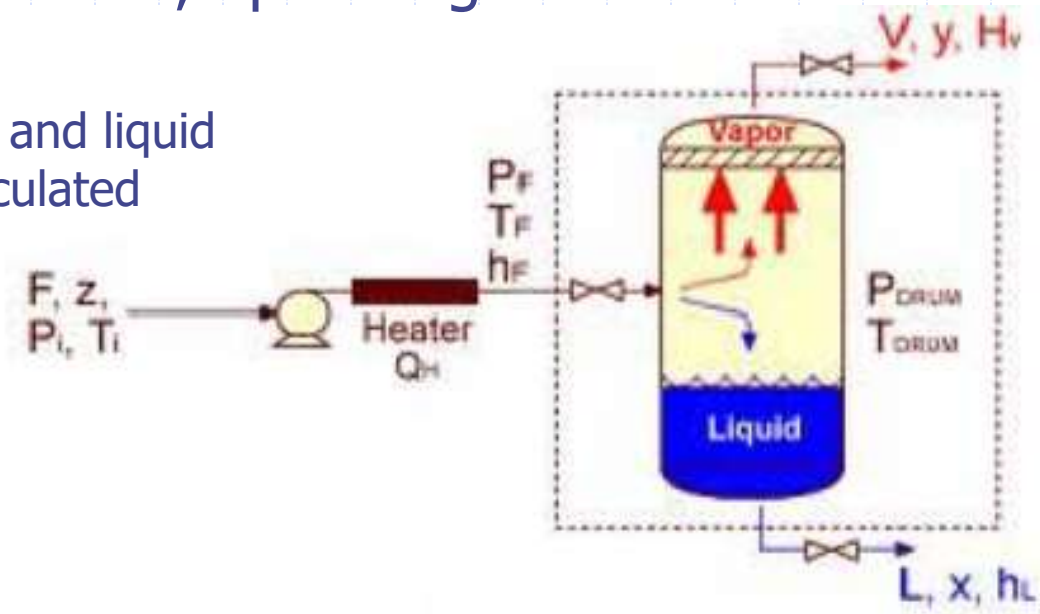
Flash Distillation – Typical Problem

- One will usually be given
  - the feed stream, F, or it can be assumed.
  - the feed composition, z, in mole or weight fraction.
- One will also typically be given one of the following:
  - x, y, T_d, f = V/F, q = L/F, L/V, or T_F.
- One will usually be given
  - the pressure, P_d, in the flash drum,
  - or it will be chosen such that the feed is above its boiling point at Td, so that some of it vaporizes.
- What is given in the problem determines the type of problem and the method of solution.

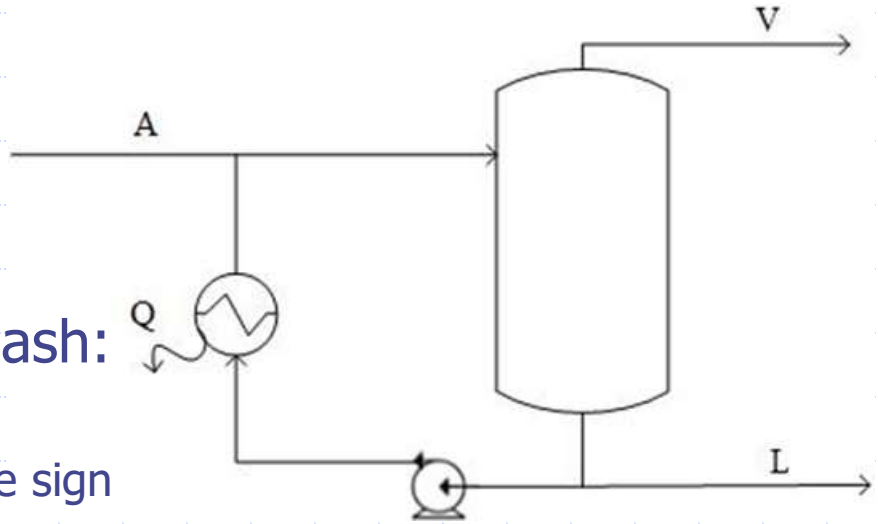


Flash problem: binary system

- If fixed P_D and Q (and consequently f)
  - x and y compositions are calculated if VLE is known
  - Flash T is calculated as bubble T of the liquid out from the flash
- If fixed P_D e T_D
  - x and y compositions are calculated if VLE is known
  - f and Q are calculated from the slope of the feed line
- Since it is difficult to control T, operating variables are usually P_D and Q:
  - Temperature, compositions and liquid and vapor flow rate are calculated



The quench process



- It is an equilibrium partial condensation process.
- Differences from traditional Flash:
  - Feed is vapor
  - Thermal consumption has opposite sign
  - Not necessary to use different pressures
- Material and energy balances are the same, if one uses the same definition of f (or 1-f = degree of condensation)
- Calculation procedure is the same
- For a binary system graphical representation is the same
- P_F value may be >= to atmospheric pressure, while it could be necessary a lower T_F value than the atmospheric one.

Flash Distillation – Problem Type 1a: Sequential Solution

- If one of the equilibrium conditions (x, y, or T_d) in the drum is specified, then the other two can be found from the equilibrium relationships using:
  - Equilibrium data and plots or
  - K values or
  - Relative volatility relationships
- With x and y, we can solve for the streams (F, V, and L) using:
  - Overall mass balance and
  - Component mass balance
- We can then solve the energy balances to determine Q_H, T_F, and T_1 (Q_{flash} = 0, since we typically assume an adiabatic drum) using enthalpies from:
  - Heat capacities and latent heats of vaporization or
  - Enthalpy-composition plots
- This method of solution is known as a sequential solution method since the energy balance is decoupled from the equilibrium and mass balances.

Flash Distillation – Problem Type 1b: Sequential Solution

- If the stream parameters are specified, usually as fraction of feed vaporized (f = V/F) or the fraction of feed remaining as liquid (q = L/F), then the problem can be solved for x, y, T_d, F, V, and L by a simultaneous solution using:
  - Equilibrium relationships and
  - Mass balances
- We can then solve the energy balances to determine Q_H, T_F, and T_1 using enthalpies from:
  - Heat capacities and latent heats of vaporization or
  - Enthalpy-composition plots
- This method of solution is also known as a sequential solution method since the energy balance is still decoupled from the equilibrium and mass balances.

Flash Distillation – Problem Type 2: Simultaneous Solution

- If the temperature, T_F, of the feed is given, then the problem requires a simultaneous solution for all of the other parameters using:
  - Equilibrium relationship and
  - Mass balance and
  - Energy balance
- This method of solution is known as a simultaneous solution method since the energy balance is not decoupled from the equilibrium and mass balances.

Flash Distillation – Pressures

- The pressure, $\mathbf{P_d}$, in the flash drum is chosen such that the **feed is above its boiling point at T_d**, so that some of it vaporizes.
- The pressure, $\mathbf{P_1}$, is chosen such that the **upstream feed is below its boiling point and remains liquid at T_1**.
- Likewise, the feed pressure, $\mathbf{P_F}$, must be chosen so that the **feed is below its boiling point and remains liquid**.
- The pump and heater assist in adjusting the required pressures and temperatures of the system.
- If the **feed is already hot enough**, the heater may not be needed, and **if the pressure of the flash drum is low enough**, the pump may not be needed.

Multi-Component Flash Distillation

- One handles the solution of multi-component flash distillation systems similarly to that of binary flash distillation
  - the methods for solving Type 1a, Type 1b, and Type 2 problems will be the same based upon the information that is given in the problem.
- One difference is that one cannot typically solve multi-component systems graphically
  - we will need to use numerical methods.
- Another difference is that we usually express the equilibrium equation using K values.
- A final difference is the number of equations involved...

Multi-Component Flash Distillation – How many unknowns?

- Suppose we have 10 components:
- For a 10 component problem,
  - C = 10, assuming that F, z_i's for C-1 components, P_d, and T_d or one of the x_i's or y_i's are specified (a Type 1a Problem),
  - we can solve the equilibrium and mass balances first and then the energy balance (a sequential solution)
- However,
  - we still need to determine 10 K's, 10 x's, 10 y's, 1 L, and 1 V, or 32 variables!

Multi-Component Flash Distillation – How many equations?

- 32 Equations for mass balance only

Equilibrium Relationship:

$$y_i = K_i x_i \qquad \text{10 equations}$$

$$K_i = K_i(T_d, P_d, \text{all } x_i) \qquad \text{10 equations}$$

Stoichiometric (mole fraction) Relationships:

$$\sum_{i=1}^{C} x_i = 1.0 \qquad \sum_{i=1}^{C} y_i = 1.0 \qquad \text{2 equations}$$

Mass Balance Equations:

$$Fz_i = Vy_i + Lx_i \qquad \text{10 equations}$$

$$F = V + L$$

Energy Balance:

$$Fh_F + Q_{flash} = VH_V + Lh_L$$

Multi-Component Flash Distillation – How do we readily handle?

- We could define all 32 equations, and solve the 32 simultaneous equations simultaneously.
- This may or may not be possible
  - we are dealing with a large number of simultaneous equations,
  - and one may experience convergence problems in a numerical solution.
- How can we "help" the convergence?
  - One method is to partially solve the set of equations for a parameter which is tightly bounded
  - that is its values cannot vary widely.
- A convenient choice is the fraction of feed vaporized,
  - f = V/F, which varies between 0 and 1.

Multi-Component Flash Distillation – Combining Equilibrium Relationship and Mass Balances

- Substituting the equilibrium relationship for y_i, into the component mass balance we obtain

$$Fz_i = Lx_i + VK_i x_i \qquad i = 1, 2, \ldots, C$$

- Substituting the overall mass balance for L in eq. above, solving for x_i, and dividing through by F/F yields

$$x_i = \frac{z_i}{1 + (K_i - 1)\frac{V}{F}} \qquad i = 1, 2, \ldots, C$$

- Since $y_i = K_i x_i$ we also obtain

$$y_i = \frac{K_i z_i}{1 + (K_i - 1)\frac{V}{F}} \qquad i = 1, 2, \ldots, C$$

Multi-Component Flash Distillation – Rachford-Rice Equation

- Substituting into the mole fraction ($\sum x=1$) relationships yields:

$$\sum \frac{z_i}{1+(K_i-1)\frac{V}{F}} = 1 \qquad \sum \frac{K_i z_i}{1+(K_i-1)\frac{V}{F}} = 1$$

- Subtracting the two above equations one obtains:

$$\sum \frac{(K_i-1)z_i}{1+(K_i-1)\frac{V}{F}} = 0 = f(V/F)$$

- Eq. above is known as the **Rachford-Rice equation.**
  - It has excellent conversion properties for use in numerical solutions of multi-component flash distillations.
  - Newton Raphson convergence is fast

Multi-Component Flash Distillation – Energy Balances

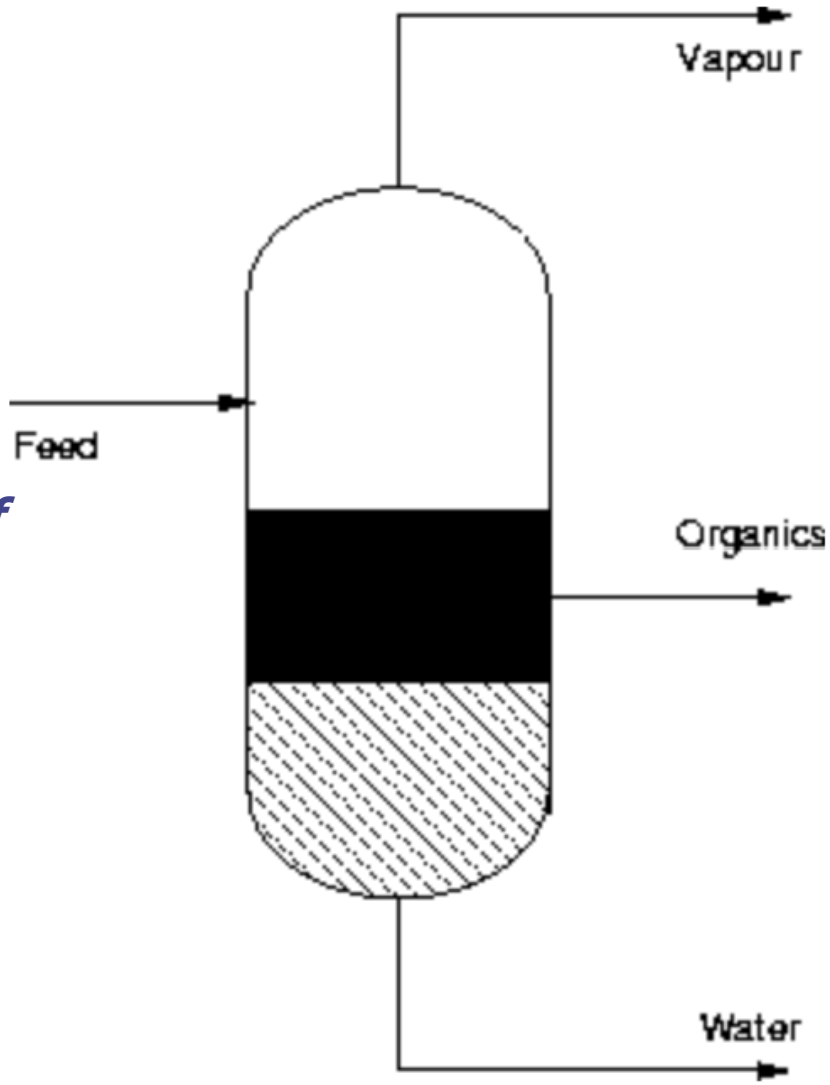
- Once one solves the Rachford-Rice equation and determines all of the vapor and liquid mole fractions, the accompanying energy balances can then solved.
- For ideal solutions enthalpies may be determined from the sum of the pure component enthalpies multiplied by the corresponding mole fractions:

$$H_V = \sum_{i=1}^{C} y_i \tilde{H}_{V_i}(T_d, P_d) \qquad h_L = \sum_{i=1}^{C} x_i \tilde{h}_{L_i}(T_d, P_d)$$

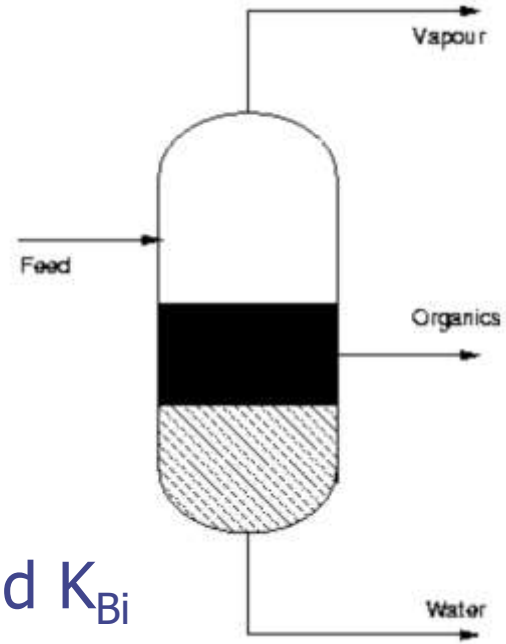
- Then energy balance may be calculated

3 phase flash

- 2 liquid phases and 1 vapor phase
  - Example: primary separation of light organics, heavy organics and water
- degrees of freedom:
  - ***C.D.F = no. of streams - no. of interfaces***
  - Number of streams = 4
  - Number of interfaces = 2
  - Hence ***C.D.F = 4 - 2 = 2***
- Typical control specifications would be feed rate and pressure



3 phase flash: solution



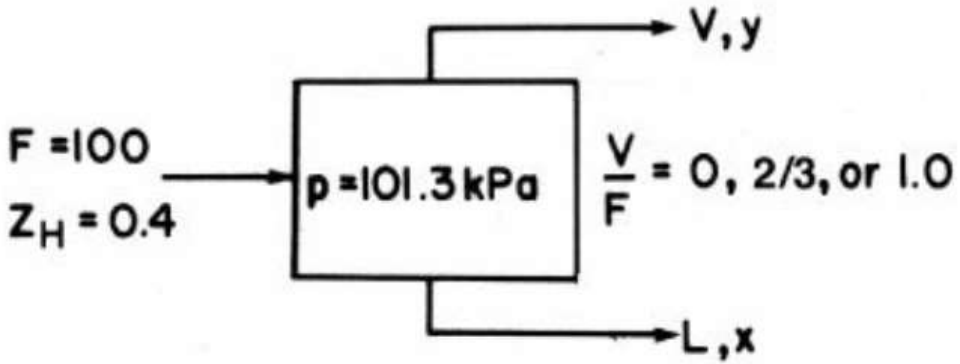
- Material balances around the flash tank:
  - $F = L_A + L_B + V$
  - $F_{zi} = L_A x_{Ai} + L_B x_{Bi} + V y_i$
- Mole fraction summation to one
- Equilibrium relations of each phase K_{ai} and K_{Bi}
- Following the same procedure used for Rachford-Rice equation, we obtain:

$$0 = \sum_{i=1}^{C} \frac{\left(K_{i,vapor-liquid\_2} - 1\right) z_i}{\left[1 + \left(K_{i,liquid\_1-liquid2} - 1\right)\frac{L_{liquid\_1}}{F} + \left(K_{i,vapor-liquid\_2} - 1\right)\frac{V}{F}\right]}$$

$$0 = \sum_{i=1}^{C} \frac{\left(K_{i,liquid\_1-liquid\_2} - 1\right) z_i}{\left[1 + \left(K_{i,liquid\_1-liquid2} - 1\right)\frac{L_{liquid\_1}}{F} + \left(K_{i,vapor-liquid\_2} - 1\right)\frac{V}{F}\right]}$$

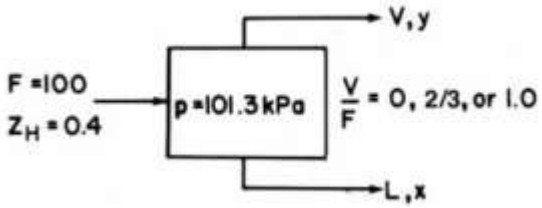
Example: ethanol – water flash

- A flash distillation chamber operating at 101.3 kPa is separating an ethanol-water mixture. The feed mixture is 40 mol% ethanol and F = 100 kmol/h.
  - (a) What is the maximum vapor composition and
  - (b)what is the minimum liquid composition that can be obtained if V/F is allowed to vary?
  - (c) If V/F = 2/3, what are the liquid and vapor compositions?
  - (d) Repeat step c, given that F is specified as 1000kmol/h



Example: ethanol – water flash solution

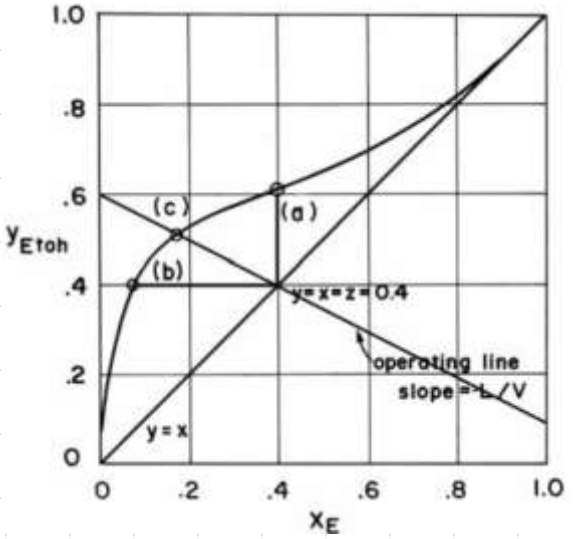
- From the overall balance, L = F – V:
  - when V/F=0.0, V=0, L=F, and L/V=F/0=∞
  - when V/F=2/3, V=(2/3)F, L=(1/3)F, and L/V=(1/3)F/[(2/3)F] = ½
  - when V/F=1.0, V=F, L=0, and L/V=0/F=0
- Slopes (–L/V) are –∞, –1/2, and –0.
  - Solve for y=x interception → at y=x=z=.4 for 3 cases.
- 3 operating lines through y=x=z=.4, with slopes of –∞, –1/2 and –0.
  a) Highest y is for V/F = 0: y = 0.61 [x = 0.4]
  b) Lowest x is for V/F = 1.0: x = 0.075 [y = 0.4]
  c) When V/F is 2/3, y = 0.52 and x = 0.17
  d) When F = 1,000 with V/F = 2/3, the answer is exactly the same as in part c. ***The feed rate will affect the drum diameter and the energy needed in the preheater.***



$$F = V + L$$

$$Fz = Vy + Lx$$

$$y = -\frac{L}{V}x + \frac{F}{V}z$$

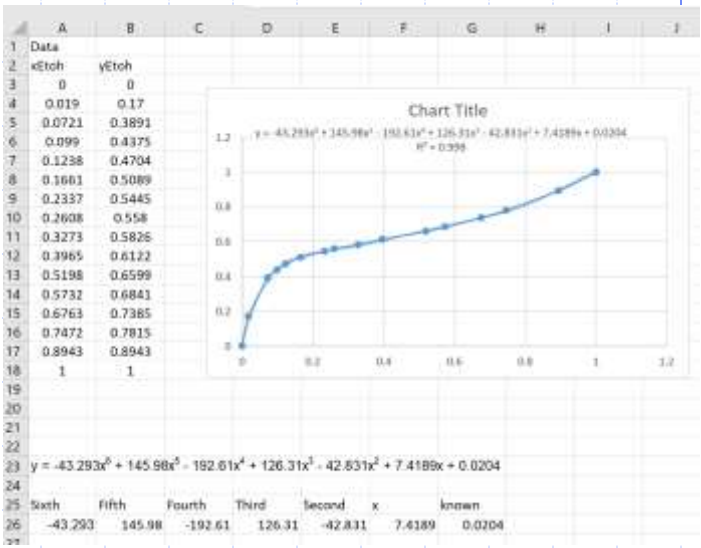


Example: ethanol – water flash solution

- Check.
  - We can check the solutions with the mass balance, Fz = Vy + Lx.
  - a. (100)(0.4) = 0(0.61) + (100)(0.4) checks
  - b. (100)(0.4) = 100(0.4) + (0)(0.075) checks
  - c. 100(0.4) = (66.6)(0.52) + (33.3)(0.17)
    - Note V = (2/3)F and L = (1/3)F
    - This is 40 = 39.9, which checks within the accuracy of the graph
  - d. Check is similar to c : 400 = 399
  - We can also check by fitting the equilibrium data to a polynomial equation and then simultaneously solve equilibrium and operating equations by minimizing the residual.
- Generalization.
  - The method for obtaining bounds for the answer (setting the V/F equation to its extreme values of 0.0 and 1.0) can be used in a variety of other situations. In general, the feed rate will not affect the compositions obtained in the design of stage separators. Feed rate does affect heat requirement and equipment diameters.

Flash with EXCEL

- Regress equilibrium Ethanol - water y-x data
  - With Excel or Polymath
- Construct the Excel formula



	A	B
1	Z	0.3
2	f = V/F	0.4
3		
4	x0	0.157000796491326
5	Yeq	= -43.293*B4^6 + 145.98*B4^5 - 192.61*B4^4 + 126.31*B4^3 - 42.831*B4^2 + 7.4189*B4 + 0.0204
6	Yeq	=D2*B4^6+E2*B4^5+F2*B4^4+G2*B4^3+H2*B4^2+I2*B4+J2
7	yeq (polymath)	=F5+F6*B4+F7*B4^2+F8*B4^3+F9*B4^4+F10*B4^5+F11*B4^6
8	Yop	=-((1-B2)/B2)*B4+B1/B2
9		
10	eq	=1000*(B7-B8)
11		

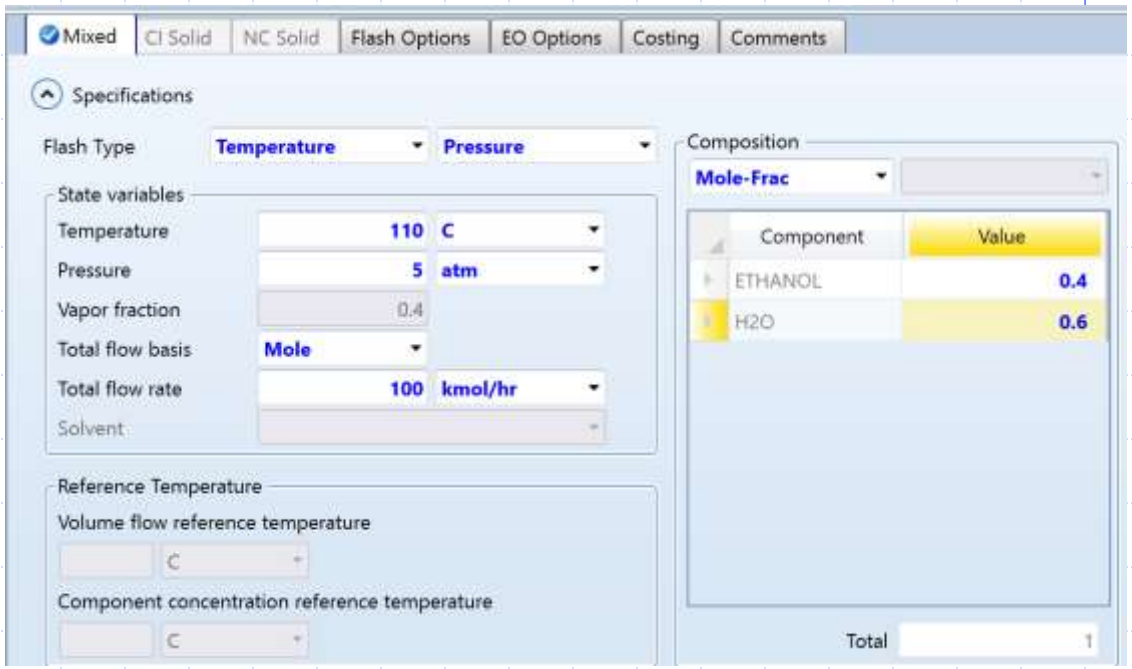
Variable	Value	95% confidence
a0	0.02043	0.027381
a1	7.418852	0.93753
a2	-42.8311	9.653953
a3	126.3078	40.08928
a4	-192.607	77.51905
a5	145.9821	69.81639
a6	-43.2928	23.66327

	A	B
1	Z	0.3
2	f = V/F	0.4
3		
4	x0	0.157000796
5	Yeq	0.514484613
6	Yeq	0.514484613
7	yeq (poly	0.514498871
8	Yop	0.514498805
9		
10	eq	6.56012E-05
11		

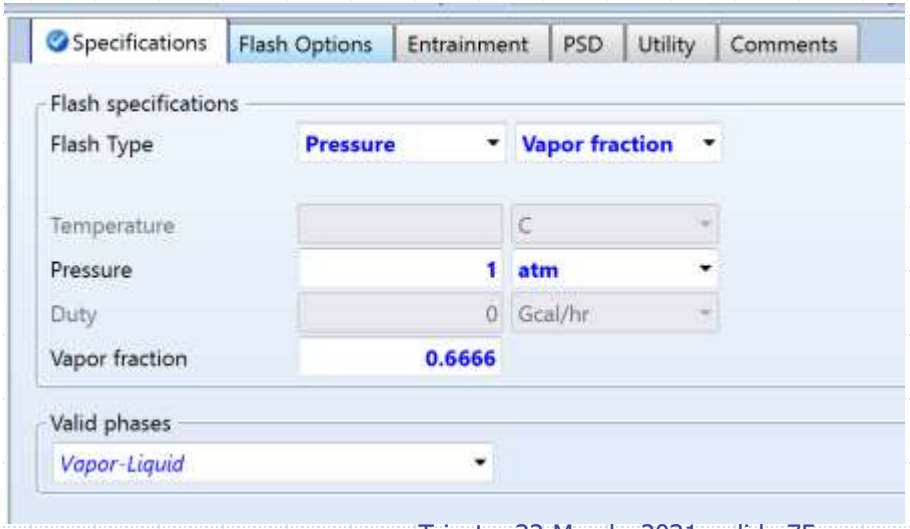
- Use Goal seek to set cell B10 to zero by changing cell B4

Flash in Aspen+

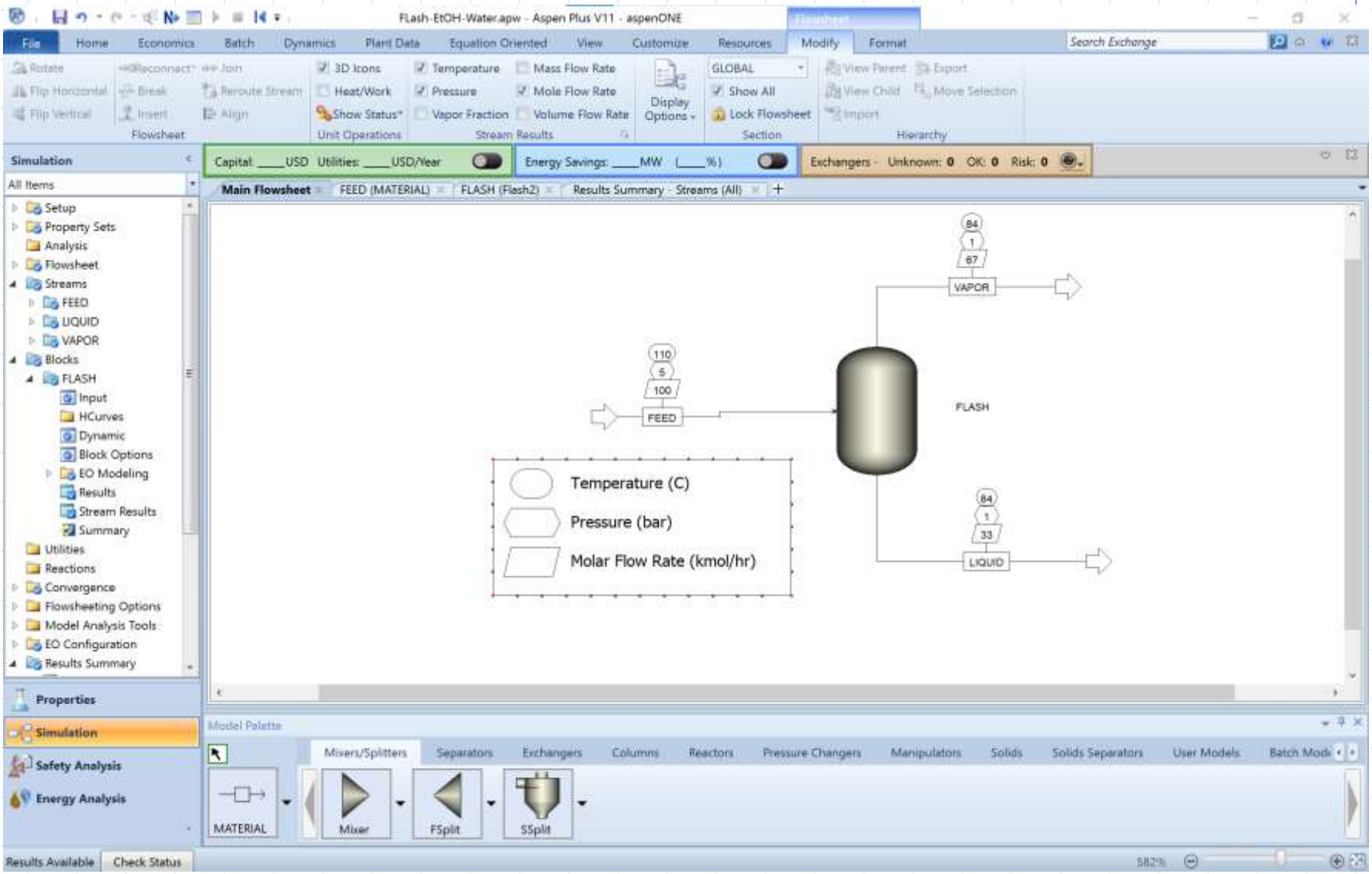
- Input stream FEED:
  - Ethanol - water
  - T= 110°
  - P= 5 atm
  - Total flow: 100 kmol/hr
  - Mole frac .4 EtOH – 0.6 water



- Block Flash input
  - Pressure = 1 atm
  - Vapor fraction = 0.666
- Other specifications
  - Duty =0

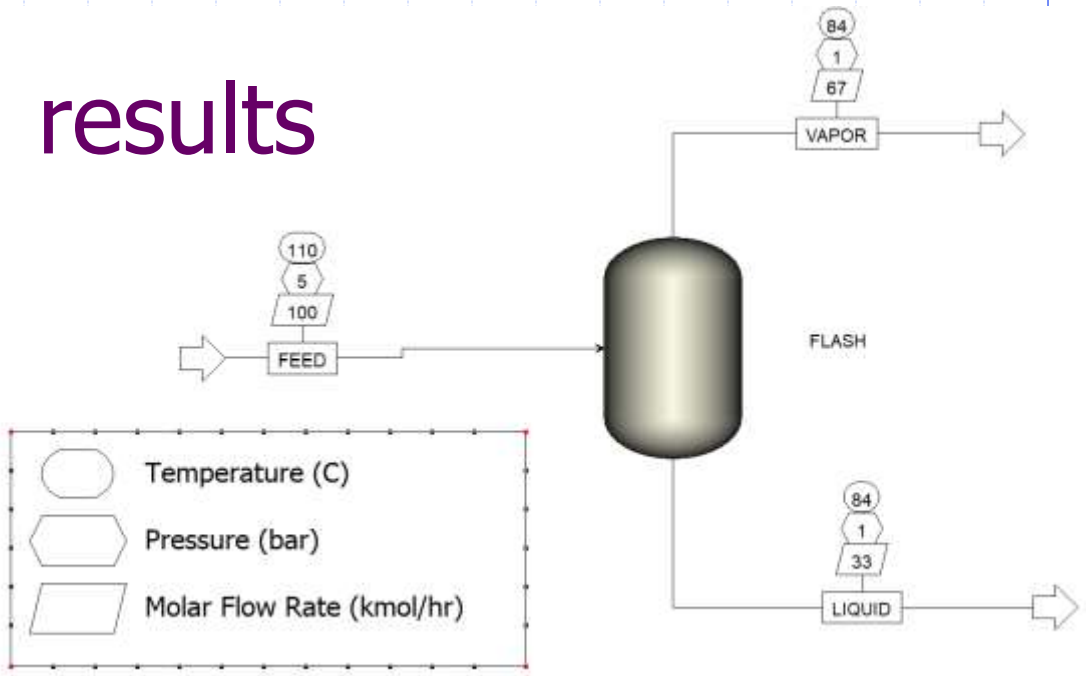


Flash in Aspen+: results



Flash in Aspen+: results

- Note (& compare)
  - T = 84°C
  - V/F = 2/3
  - X etoh = 0.17
  - Y etoh = 0.52
  - V = 66.66 kmol/hr
  - L = 33.34 kmol/hr

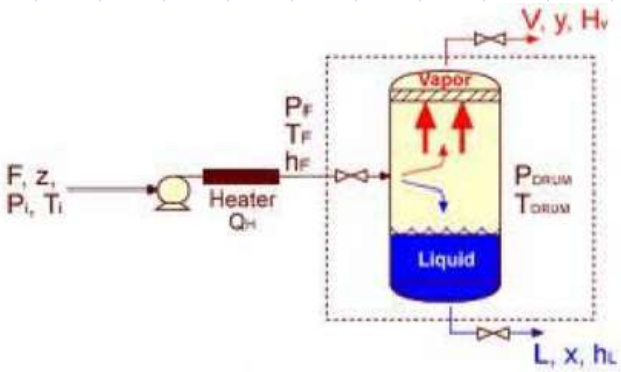


	Units	FEED	LIQUID	VAPOR
Molar Entropy	cal/mol-K	-49.7347	-42.2391	-29.2947
Mass Entropy	cal/gm-K	-1.7011	-1.86317	-0.900796
Molar Density	mol/cc	0.0260003	0.0377331	3.41496e-05
Mass Density	kg/cum	760.166	855.432	1.11057
Enthalpy Flow	Gcal/hr	-6.53799	-2.22631	-3.74453
Average MW		29.2368	22.6706	32.5209
+ Mole Flows	**kmol/hr**	**100**	**33.34**	**66.66**
− Mole Fractions				
ETHANOL		0.4	0.165943	0.517064
H2O		0.6	0.834057	0.482936

Flash drum design

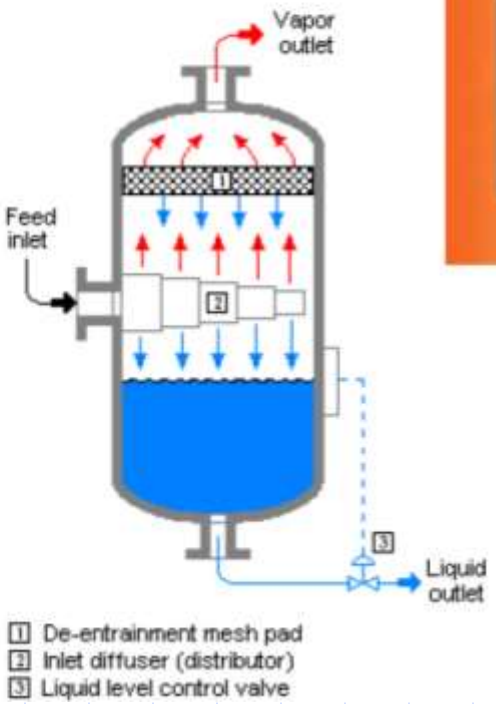
Vertical vessel

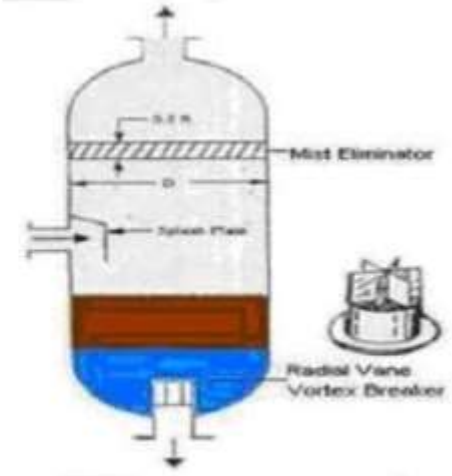
Horizontal Vessel



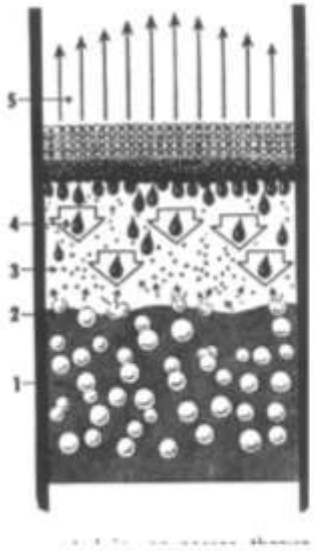
Installed Units

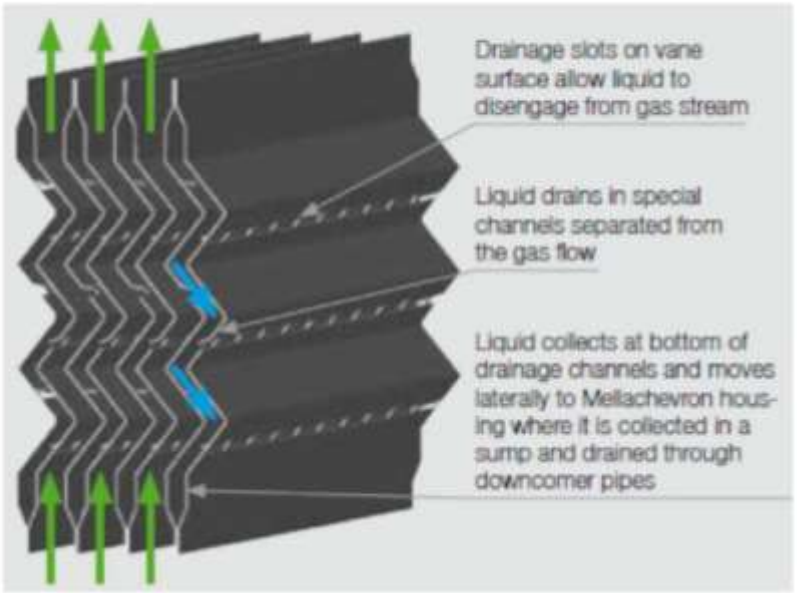
Flash drum design: deflectors and diffusers





Flash drum design: demisters



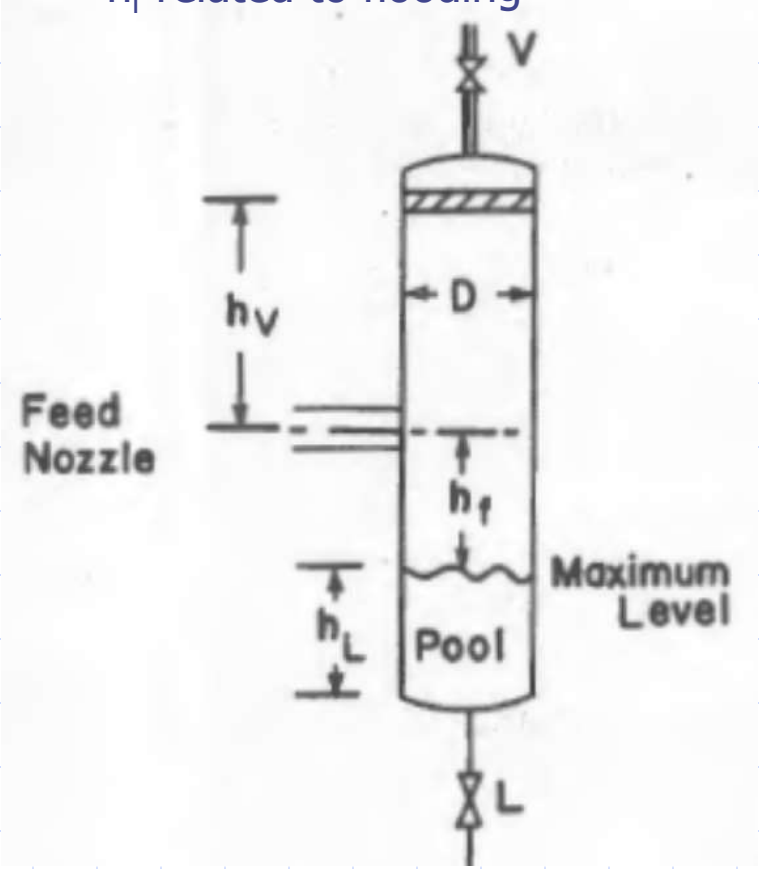


Flash drum design

- Once vapor and liquid compositions and flow rates are known, the flash drum can be sized.
  - Flash drums can be vertical or horizontal
  - Diameter calculation is based on hydrodynamic phenomena
- The main variable is the maximum vapor velocity.
  - In drums without demister it is set to avoid flood of liquid in the exit vapor stream
- The approach is empirical, based on experimental data of different systems in different conditions
  - Key parameters are K_{drum}, vapor velocity and flux $F_{l,v}$

Flash drum design

- Dimension to decide: D, h_v, h_l, h_f,
  - D related to vapor velocity
  - h_v related to vapor velocity
  - h_l related to level control
  - h_f related to flooding



$$F = L + V$$

$$Fz_i = Lx_i + Vy_i$$

$$y_i = K_i x_i$$

$$\sum_i x_i = 1$$

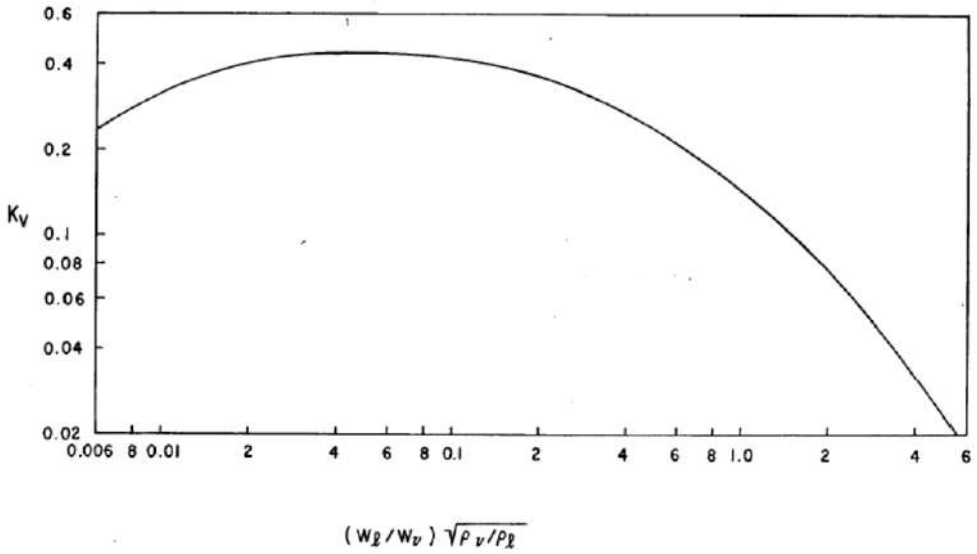
$$\sum_i y_i = 1$$

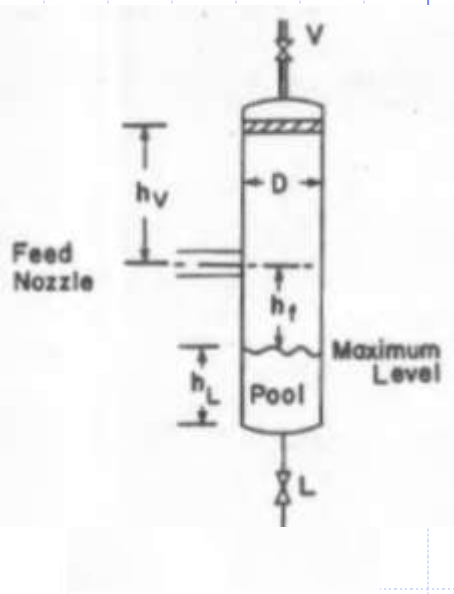
$$\Rightarrow \begin{cases} x_i = \dfrac{z_i}{\left[1 + {V}/{F}\,(K_i - 1)\right]} \\ y_i = \dfrac{K_i z_i}{\left[1 + {V}/{F}\,(K_i - 1)\right]} \end{cases}$$

D is related to vapor velocity

Permitted velocity

$$v_{perm} = K\sqrt{\frac{(\rho_L - \rho_V)}{\rho_V}}$$





$$K = e^{A+B\ln F_{lv}+C(\ln F_{lv})^2+d(\ln F_{lv})^3+E(\ln F_{lv})^4}$$

$$F_{lv} = \frac{W_L}{W_V}\sqrt{\frac{\rho_L}{\rho_V}}$$

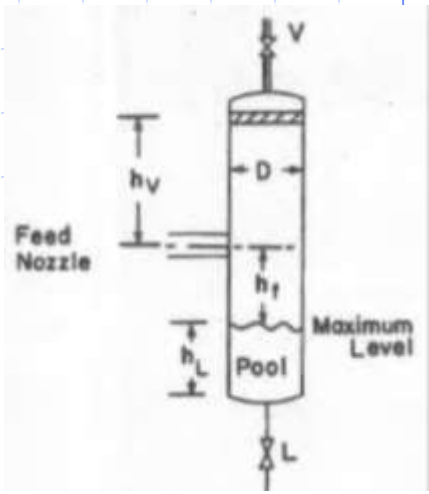
$$A = -1.877478$$
$$B = -0.814580$$
$$C = -0.187074$$
$$D = -0.014523$$
$$E = -0.001015$$

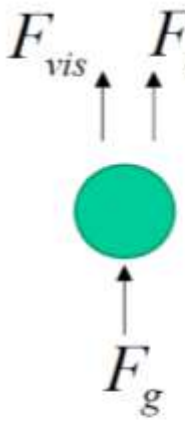
Where do these come from ?

Liquid and vapor flow rate

K is related to drop diameters: force balances on liquid drop

- Max velocity is calculated to avoid flooding





$$F_{vis} = 6\pi\mu R_d v_d \qquad \text{Stokes}$$

$$F_{drag} = C_D \frac{1}{2} A \rho_V v_d^2 \qquad \text{drag}$$

$$F_g = (\rho_L - \rho_V) g \frac{4}{3} \pi R_d^3 \qquad \text{gravity-Buoyancy}$$

$$F_{drag} + F_{vis} \approx F_{drag} = F_g \Rightarrow C_D \frac{1}{2}\left(\pi R_D^2\right) \rho_V v_d^2 = (\rho_L - \rho_V) g \frac{4}{3} \pi R_d^3$$

$F_{drag} >> F_{vis}$

$$\Rightarrow v_{perm} = K \sqrt{\frac{(\rho_L - \rho_V)}{\rho_V}} \qquad K = \sqrt{\frac{8 g R_d}{3 C_D}}$$

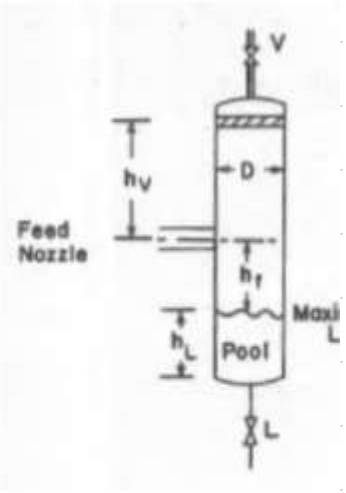
What about C_D?

- Dimensional analysis for drag
  - Force is dependent on velocity, cross sectional area, density and viscosity

$$f_a\left(F_{drag}, v_d, A, \rho_V, \mu\right) = 0$$

Two nondimensional numbers:

$$\mathrm{Re} = \frac{v_d \sqrt{A/\pi}}{\mu} \qquad C_D = \frac{F_{drag}}{\frac{1}{2}\rho_V A v_d^2}$$



Therefore

$$f_b\left(\mathrm{Re}, C_D\right) = 0 \quad \rightarrow \quad C_D = \frac{F_D}{\frac{1}{2}\rho_V A v_d^2} = f_c\left(\mathrm{Re}\right)$$

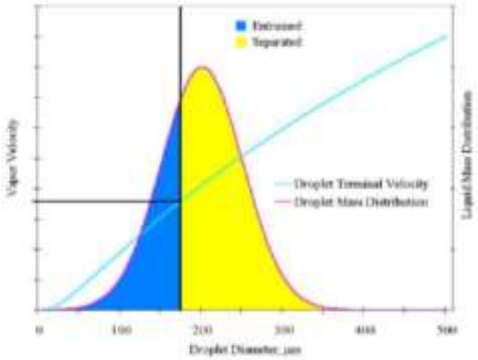
Thus C_D is a function of the particle Reynolds number. →

$$K = \sqrt{\frac{8gR_d}{3f_c\left(\mathrm{Re}\right)}}$$

What about C_D?

- C_D is a function of the particle Reynolds number
- Fluid dynamics in the drum should avoid liquid entrainment

But, what R_d should be used? The criteria is that 5% of the liquid is entrained.

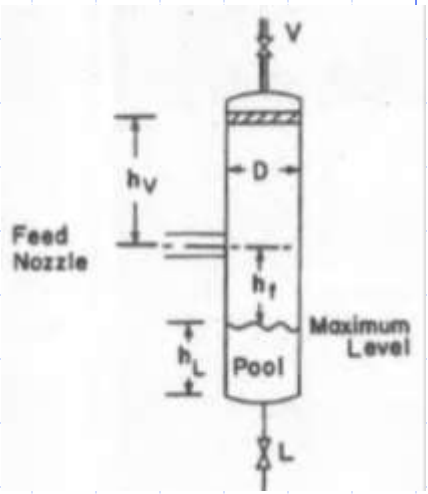


Thus

$$K = e^{A+B\ln F_{lv}+C(\ln F_{lv})^2+d(\ln F_{lv})^3+E(\ln F_{lv})^4} \quad ; \quad F_{lv} = \frac{W_L}{W_v}\sqrt{\frac{\rho_L}{\rho_v}}$$ were obtained

fitting experimental data.

Flash drum dimensions



- Using the known vapor rate V, convert v_{perm} into an horizontal area

$$D = \sqrt{\frac{4}{\pi} A_D} = \sqrt{\frac{4}{\pi} \frac{V}{v_{perm} \rho_V}}$$

  - Demister should take care of the 4% (or less) of the 5%.
- Dimensions:
  - Depth of the liquid pool is defined by experience from liquid surge thanks
  - $h_v = 36" + 1/2\ D$ – minimum 48”
  - 36” is the room for demister
  - $h_f = 12" + 1/2\ D$
  - $h_L = \frac{V_{surge}}{\pi D^2/4}$ where V_{surge} is the desired surge volume
- Finally H total is:

$$H = h_v + h_f + h_L$$ should be 3 < H/D < 5

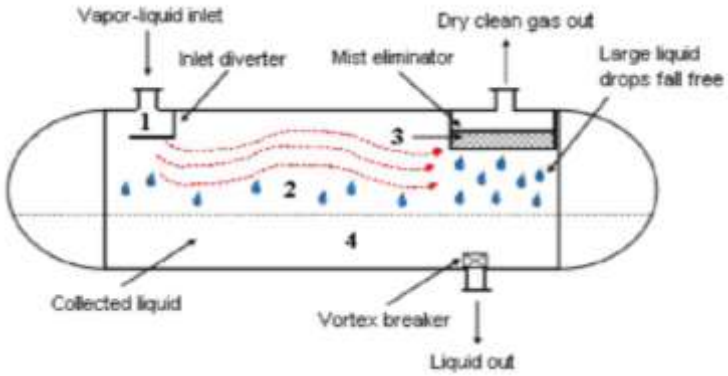
Nozzle size $(u_{max})_{nozzle} = 100/\sqrt{\rho_{mix}}$, ft./sec.

$(u_{min})_{nozzle} = 60\sqrt{\rho_{mix}}$, ft./sec.

Flash drum design: final considerations

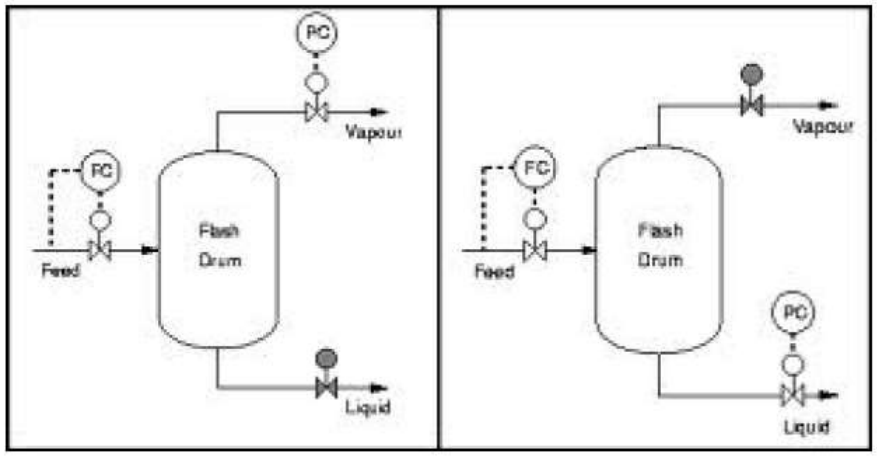
- If H/D < 3 use a larger liquid surge volume
- If H/D > 5 (large flow rates) use an horizontal drum
  - Horizontal drum has a different design protocol
  - Horizontal drums are particularly useful when large liquid surge capacities are needed
- Using existing flash drum
  - Verify that

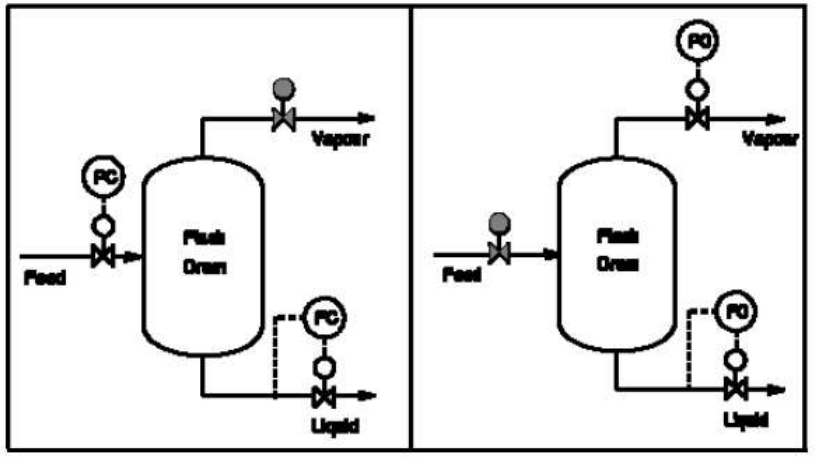
$$V_V \leq u_{V,\max} A, \quad A = \frac{\pi D^2}{4}$$

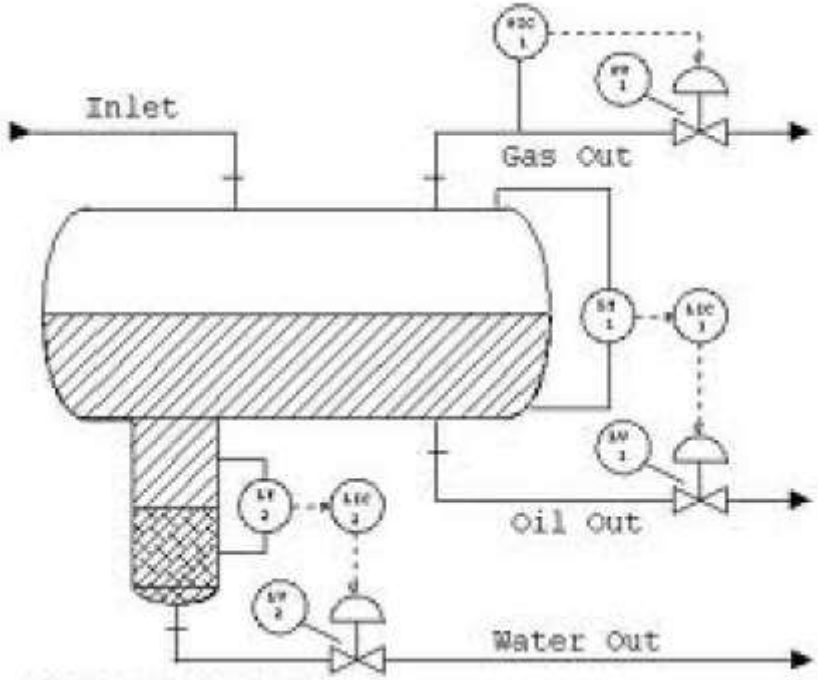


N.B: use a security factor of 0.85 relative to the calculated velocity

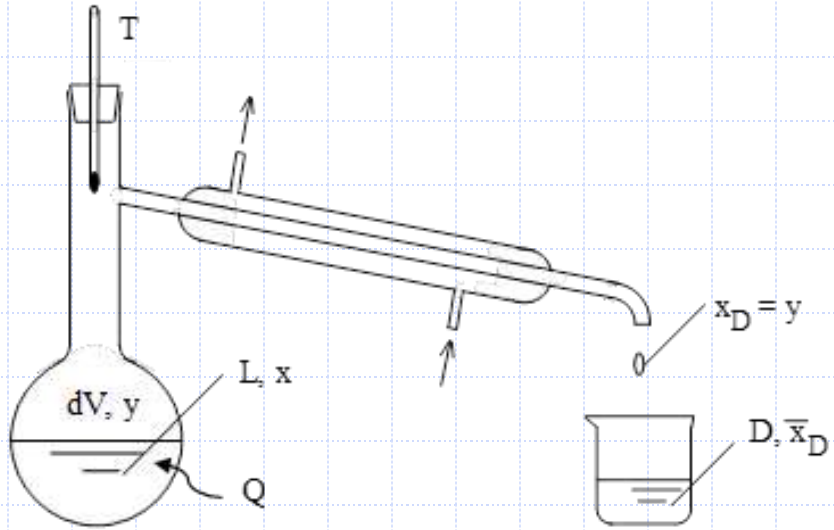
Flash drum design: control schemes







Differential vaporization process



Molar balance valid at each time t:

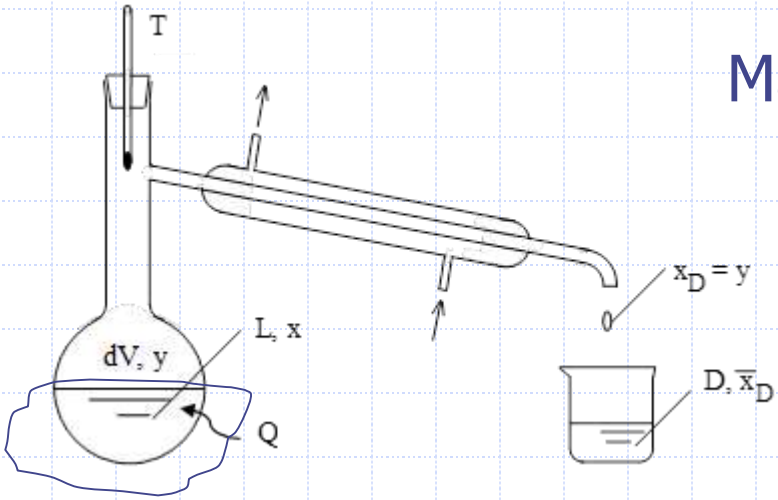
$$F = L + D$$

$$F z_F = L x + D \bar{x}_D$$

At each time t there is a variation of: $x, y, \bar{x}_D, L, D$

The distillate composition decreases with time

Differential vaporization process



Material balance around the liquid:

$$\frac{dL}{dt} = -\frac{dV}{dt} = -\frac{dD}{dt}$$

$$\frac{d(Lx)}{dt} = -y\frac{dV}{dt}$$

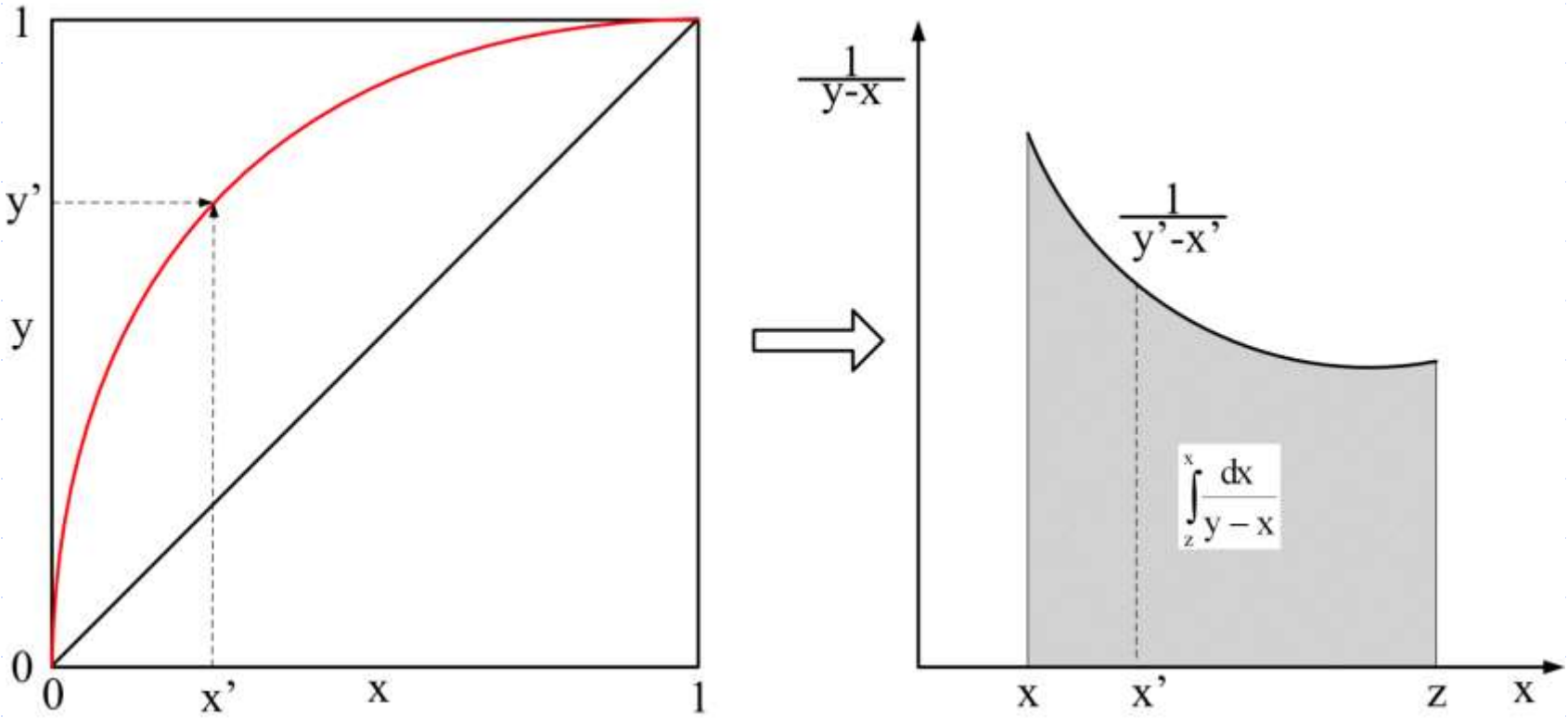
$$\frac{dL}{L} = \frac{dx}{y-x}$$

$$\ln\frac{L}{F} = \int_{z_F}^{x} \frac{dx}{y-x}$$

Rayleigh Equation

Differential vaporization process

Graphical integration:



Differential vaporization process: concentration profiles

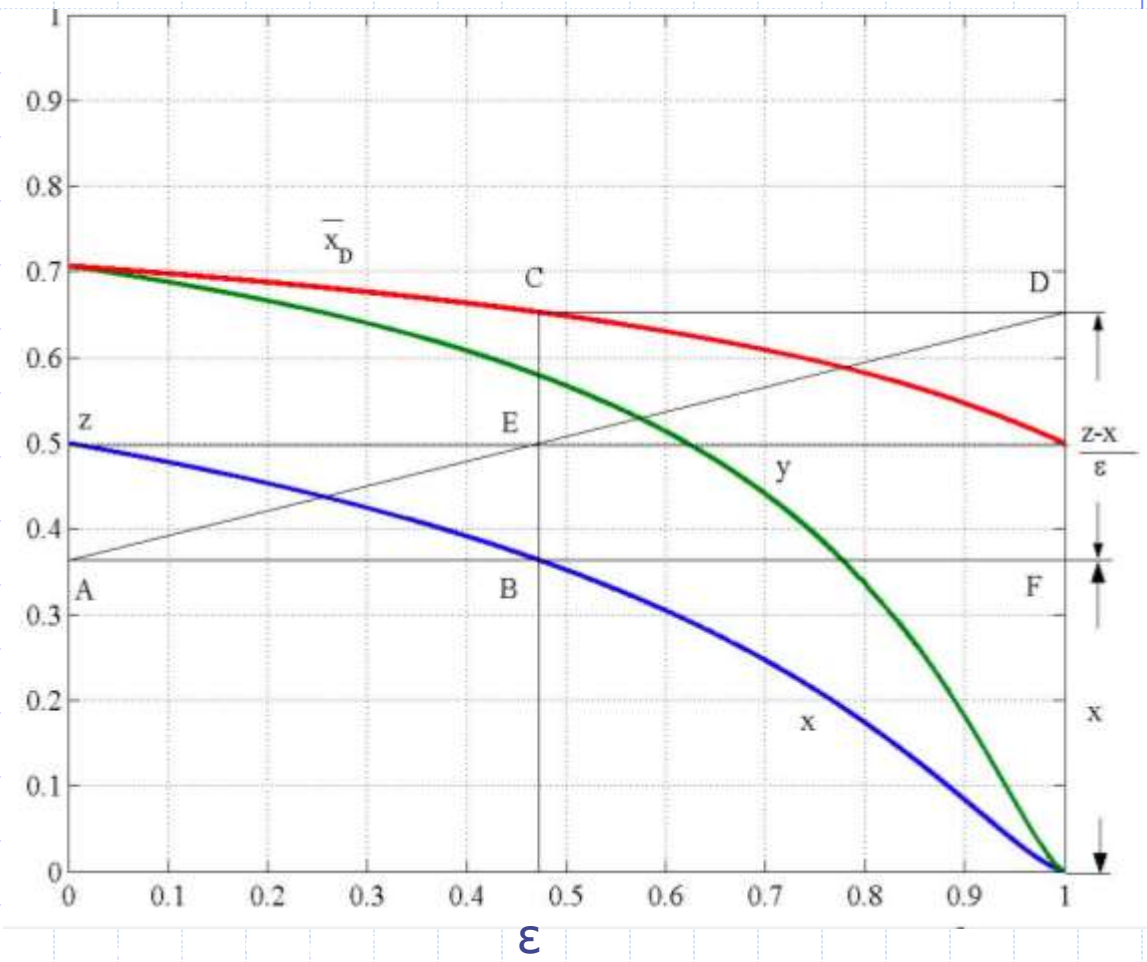
$$\varepsilon = \frac{D}{A}$$

$$1 - \varepsilon = \frac{L}{A}$$

$$\frac{\bar{x_D} - x}{1} = \frac{z - x}{\varepsilon}$$

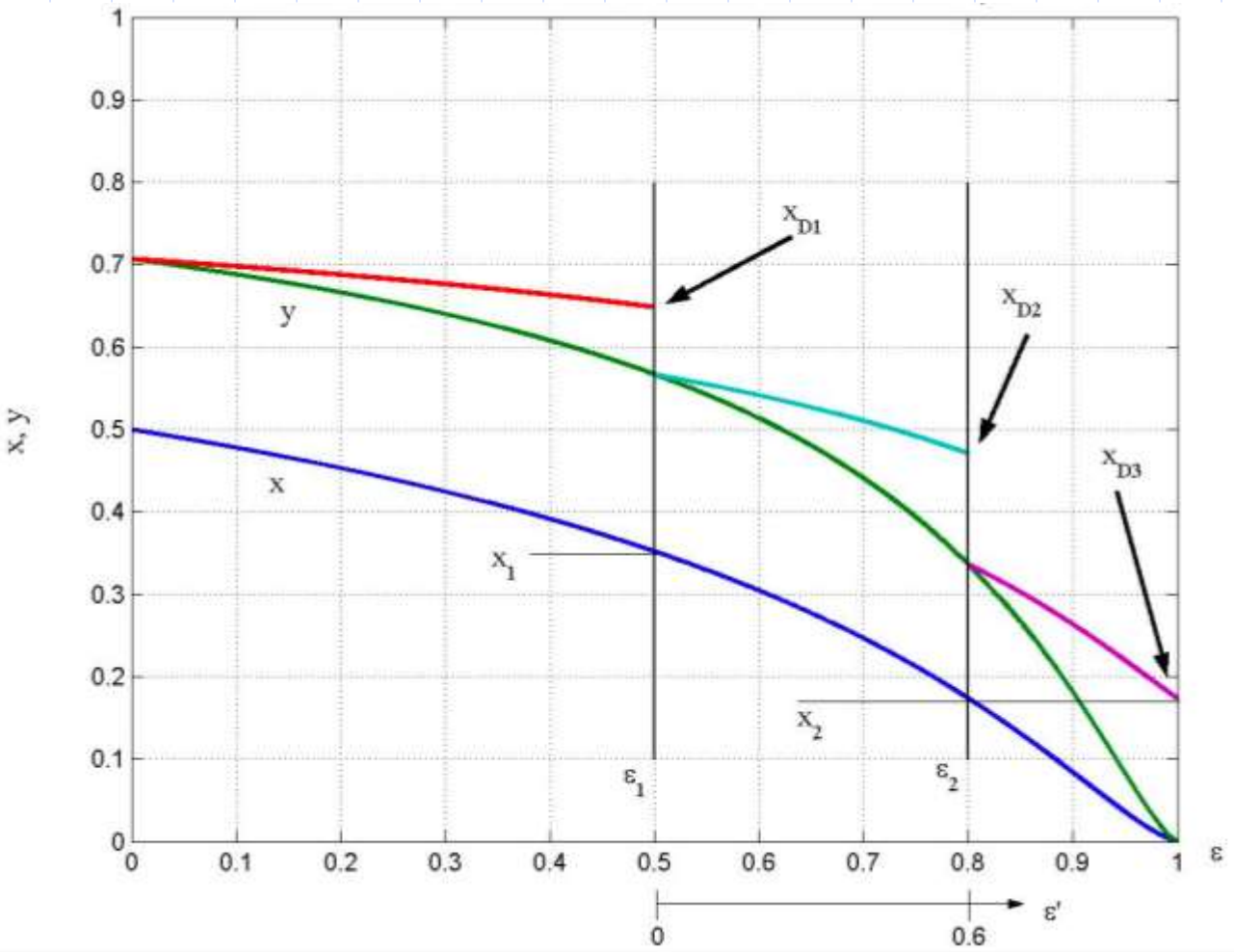
$$\frac{DF}{AF} = \frac{EB}{AB}$$

Differential vaporization for the system n-Hexane / n-heptane

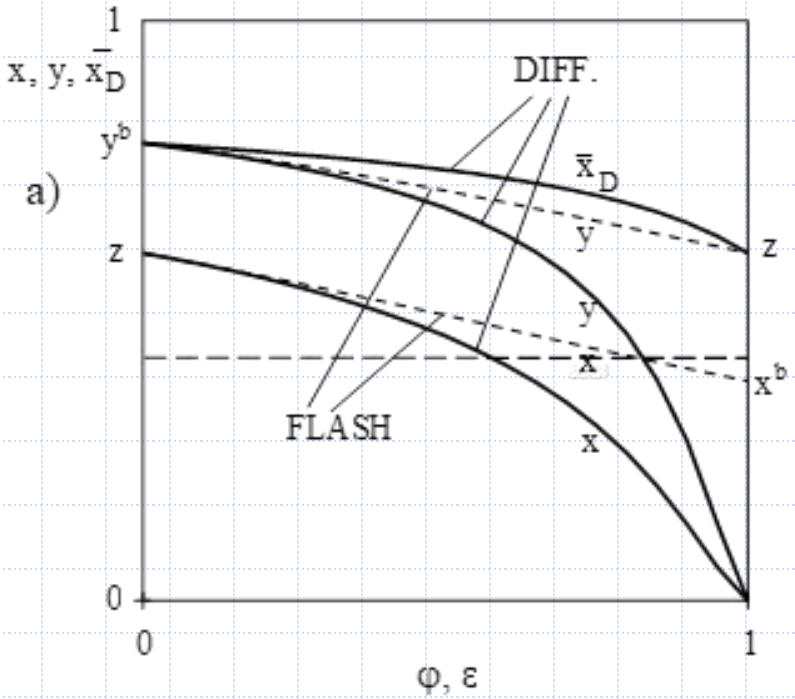


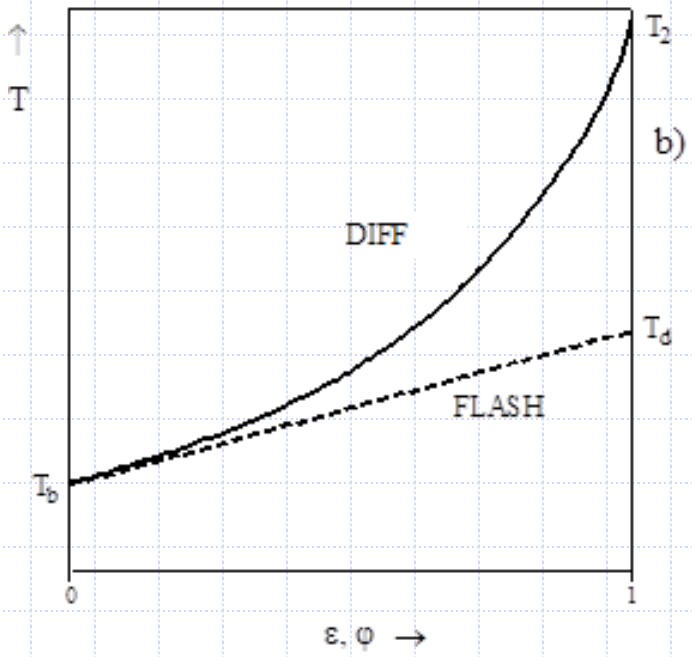
Products Separation

Differential vaporization for the system n-Hexane / n-heptane



Flash vs. differential vaporization





Exercise: flash methanol water at 1 atm

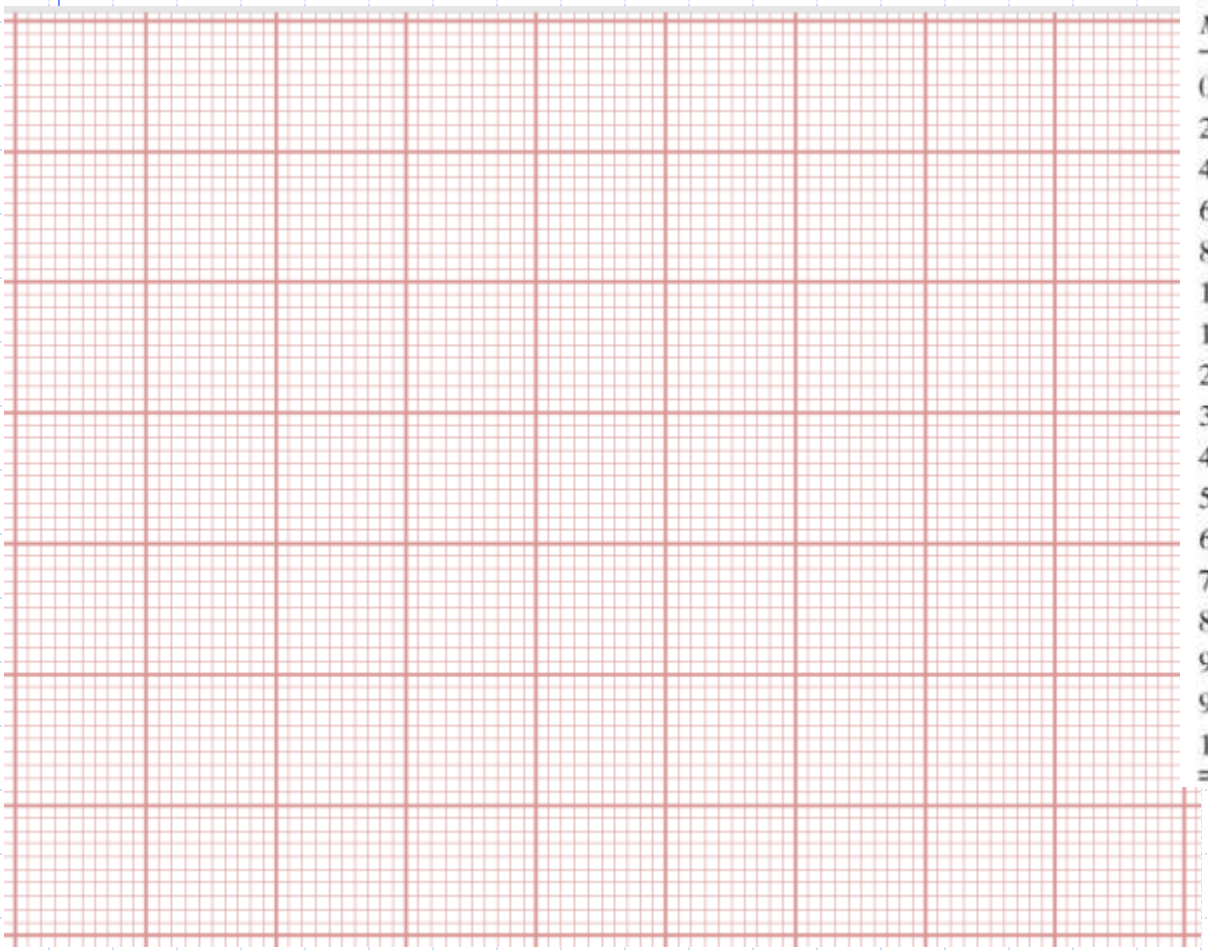
- A flash distillation chamber operating at 1 atm is separating a methanol-water mixture. The equilibrium data at 1 atm is reported in table.
  - **a.** Feed is 60 mol% methanol, and 40% of the feed is vaporized. What are the vapor and liquid mole fractions and flow rates? Feed rate is 100 kmol/h.
  - **b.** Repeat part a for a feed rate of 1500 kmol/h.
  - **c.** If the feed is 30 mol% methanol and we desire a liquid product that is 20 mol% methanol, what V/F must be used?
  - **d.** We are operating the flash drum so that the liquid mole fraction is 45 mol% methanol. L = 150 kmol/h, and V/F = 0.2. What must the flow rate and composition of the feed be?

Exercise: flash methanol water at 1 atm

- A flash distillation chamber operating at 1 atm is separating a methanol-water mixture. The equilibrium data at 1 atm is reported in table.
  - **e.** Find the dimensions of a vertical flash drum for Problem c. Data: ρ_w = 1.00 g/cm3, $\rho_{m,L}$ = 0.7914 g/cm3, MW_w = 18.01, MW_m = 32.04. Assume vapors are ideal gas.
  - **f.** If z = 0.4, p = 1 atm, and T_{drum} = 77°C, find V/F, x_m, and y_m.
  - **g.** If F = 50 mol/h, z = 0.8, p = 1 atm, and y_m = 0.892 mole fraction methanol, find V, L, and x_m
- Verify Flash results with Aspen+
  - For cases: a, b, c, d, f, g
  - Use Sensitivity analysis and Design specification

Exercise: flash methanol water at 1 atm

- Equilibrium data at 1 atm in mole%



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