

Packed column design

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Agenda

- ◆ Packed columns
- ◆ Packings
- ◆ Pressure drops and wetting rate
- ◆ Design and rating of randomly packed column
- ◆ Design and rating of structured packed column
- ◆ HETP
- ◆ Mass transfer in a packed column
- ◆ HTU and NTU

Mass transfer in distillation column

- ◆ **Mass transfer** in a column is strictly connected to the **contact surface** between liquid and vapor.
- ◆ Three types of L-V dispersion are possible:
 - Vapor bubbles or foam dispersion in liquid (continuum phase): **tray columns**
 - Liquid drops dispersion in vapor phase (continuum phase): **spray columns**
 - Dispersed liquid as a film immersed in vapor phase: **packed column** in which packing has the only effect of supporting the liquid phase – in this case **both phases are continuum**
- ◆ In stage columns the contact between the gas and the liquid phases **occurs on the tray**.
- ◆ The exchange area depends on the **hydrodynamics**

Packed columns

◆ In **continuous contact units**:

- packings are used rather than trays
- the gas and liquid phases flow counter currently
- the liquid forms a film on the packing
- the exchange area can be very high if a proper design of the packing is adopted (structured packings)

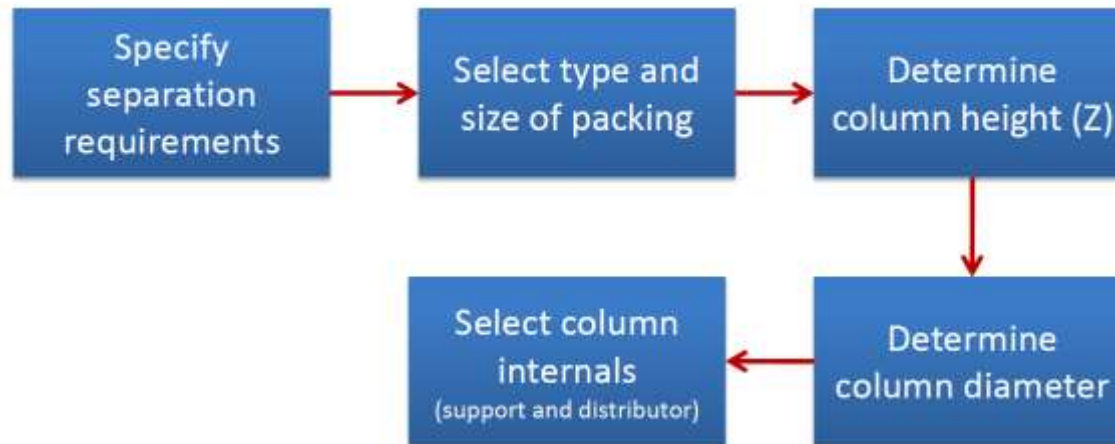
◆ Packed column are normally used for absorption while tray column for distillation

- Packed column may be used for distillation (vacuum distillation for pharma)
- Absorption can take place in tray columns

Advantages of Packed Columns

- ◆ For **corrosive liquids**, a packed column will usually be cheaper than the equivalent plate column.
- ◆ The liquid **hold-up is lower** in a packed column than a plate column.
 - This can be important when the inventory of **toxic or flammable liquids** needs to be kept as small as possible for safety reasons.
- ◆ Packed columns are more suitable for **handling foaming systems**.
- ◆ The **pressure drop can be lower** for packing than plates; and packing should be considered for **vacuum columns**.
- ◆ Packing should always be considered for **small diameter columns**, say less than 0.6 m, where plates would be difficult to install, and expensive.

Packed columns: design Procedure

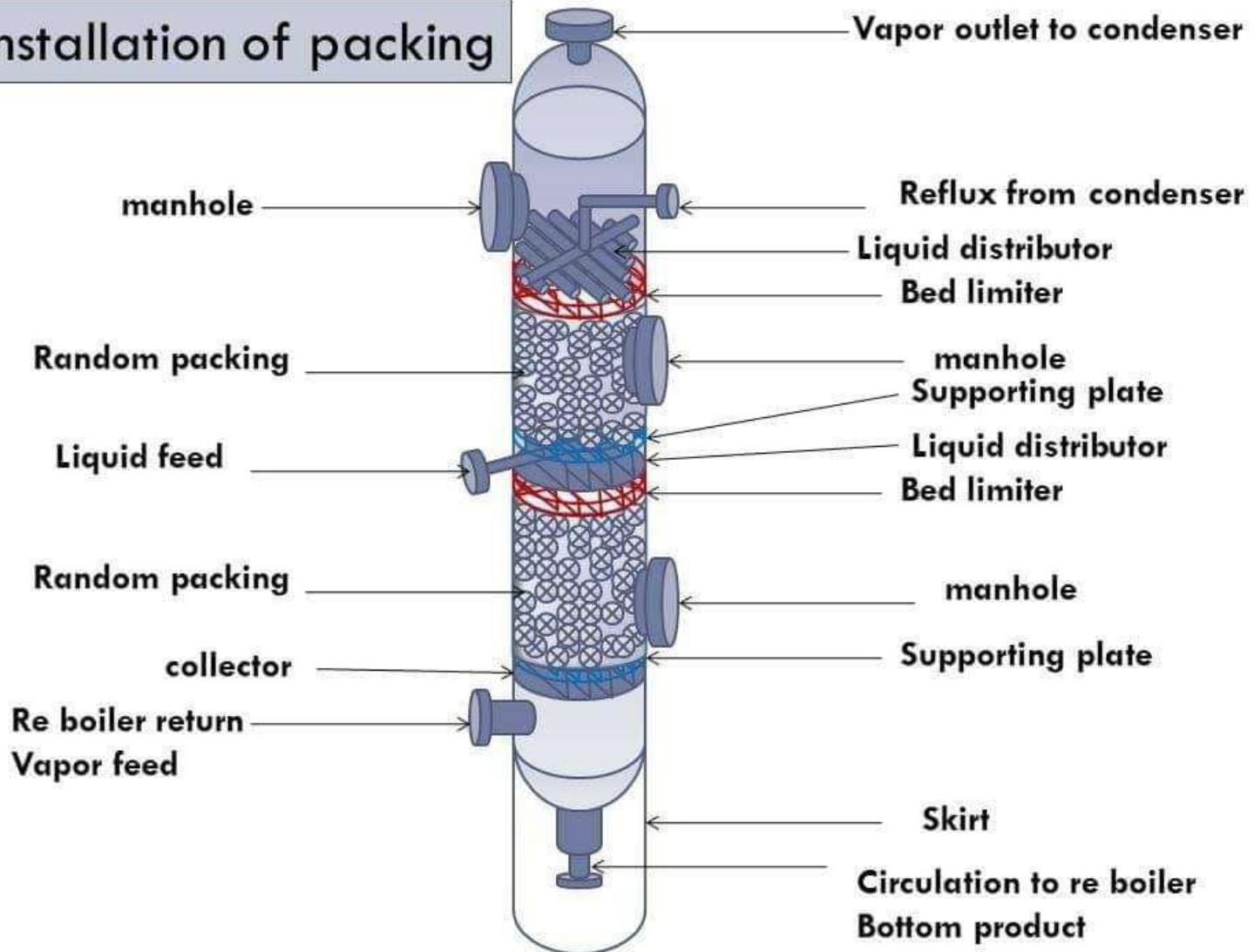


◆ Packing materials

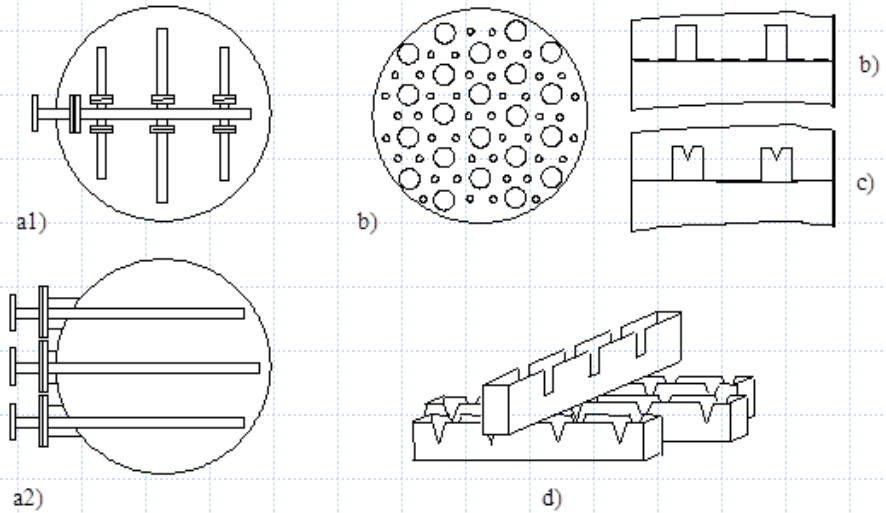
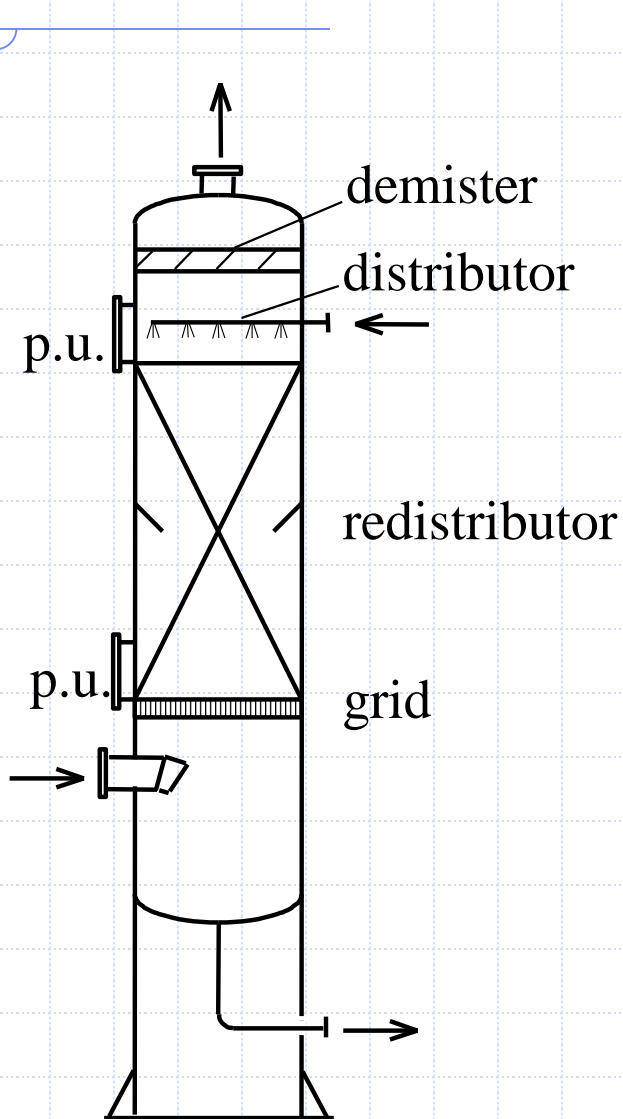
- **Ceramic:** superior wettability, corrosion resistance at elevated temperature, bad strength
- **Metal:** superior strength & good wettability
- **Plastic:** inexpensive, good strength but may have poor wettability at low liquid rate

Packed columns

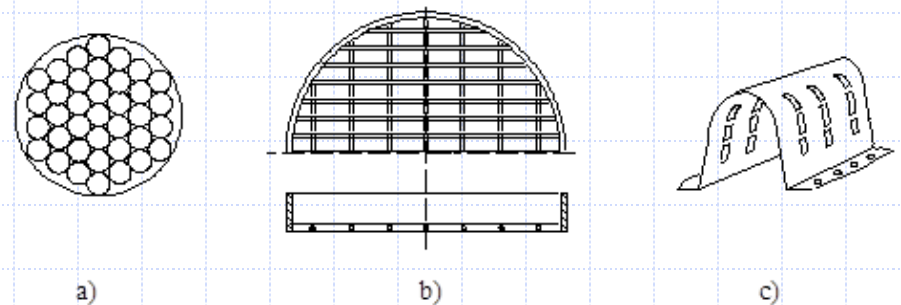
Installation of packing



Packed columns: mechanical details



Liquid distributors: a) drilled pipes; b) holes; c) weir.



Packing support: a) rings; b) grid; c) structured grid.

Packings

◆ Types of packings

- Random
- Structured

◆ Main packing characteristics :

- **High surface over volume ratio** in order to maximize the liquid vapor interface.
 - ◆ Consider that effective interface is less than the geometrical interface due to short circuits in the liquid film
- **Low pressure drops** to allow high flow rates without congestion
 - ◆ This requires high vacuum degrees in packings
- **Resistance to corrosion**
- **Good mechanical properties**
- **Low costs**

◆ Performances depends upon:

- Type of packing
- Dimension
- Material

Random packings



(a)



(b)



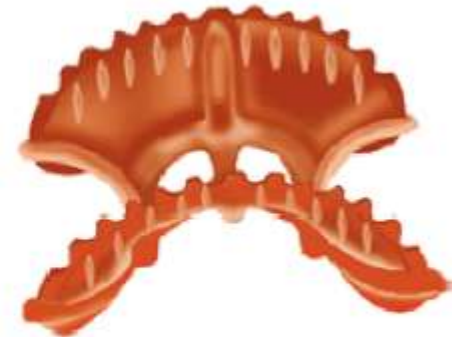
(c)



(d)



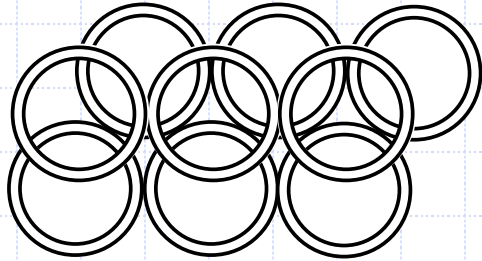
(e)



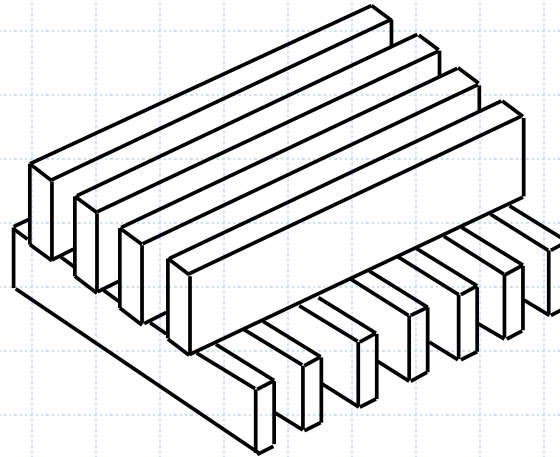
(f)

- Type of Random Packing: (a) Rascig rings, (b) Pall rings, (c) Berl saddles, (d) Intalox saddles, (e) Hy-pak, (f) Super Intalox.

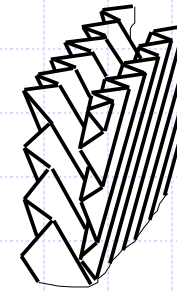
Structured packings



a)

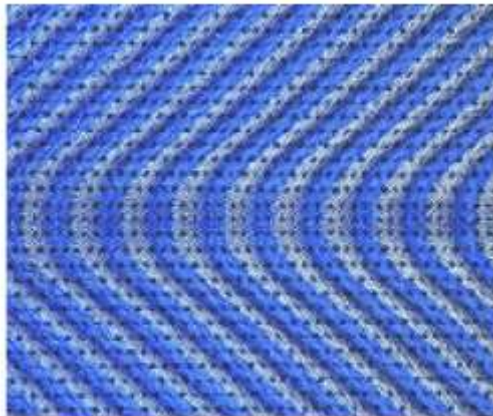


b)



c)

a) Raschig rings; b) wood or plastic grids; c) BX® Sulzer Material



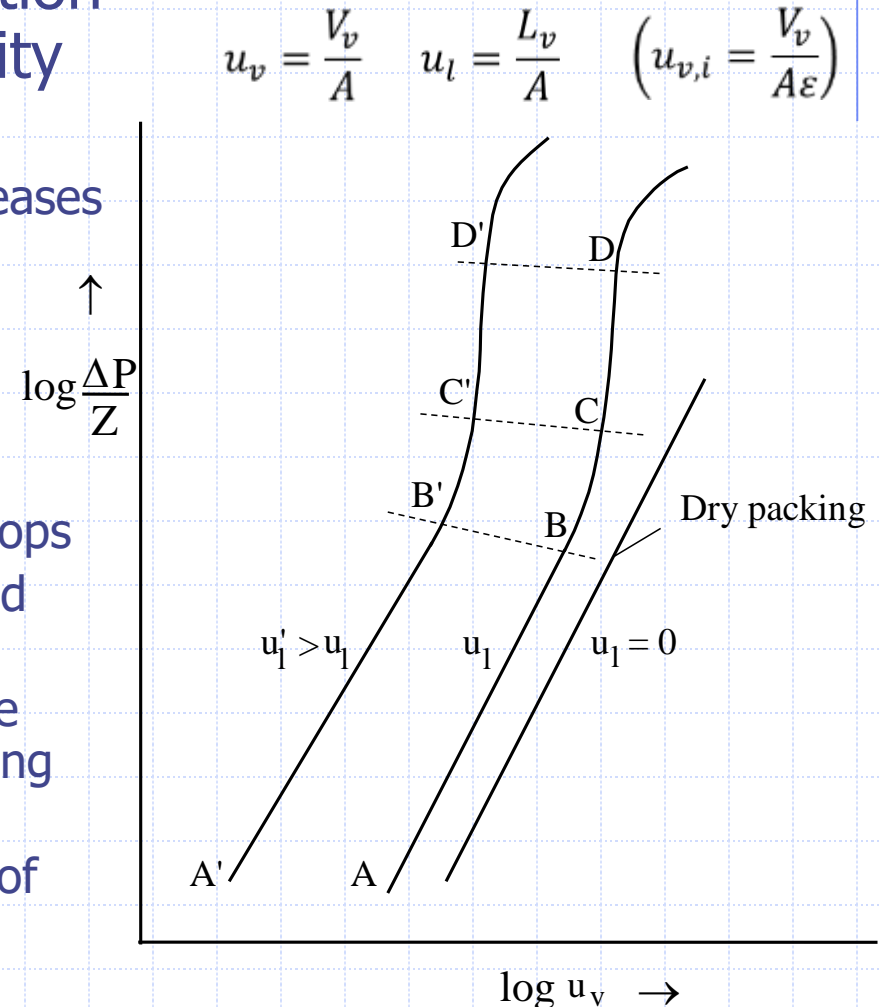
Hydrodynamics of a packed columns

- ◆ For a correct operation it should be
 - **Liquid flows as a film** over the packing
 - **Vapor** (or gas) **flows in the empty space** of packing
 - **Liquid film should wet** the highest amount of packing surface
- ◆ Operating limits
 - Upper operating limit is **FLOODING**. Like trays column this is characterized by a clogging of the column with increase of pressure drops. Vapor flow holds up the liquid in the column which at the end goes out from the top.
 - Lower limit is **LOADING**. Below loading there is not enough contact between liquid and vapor. This depends mainly on the liquid flowrate.

Pressure drops

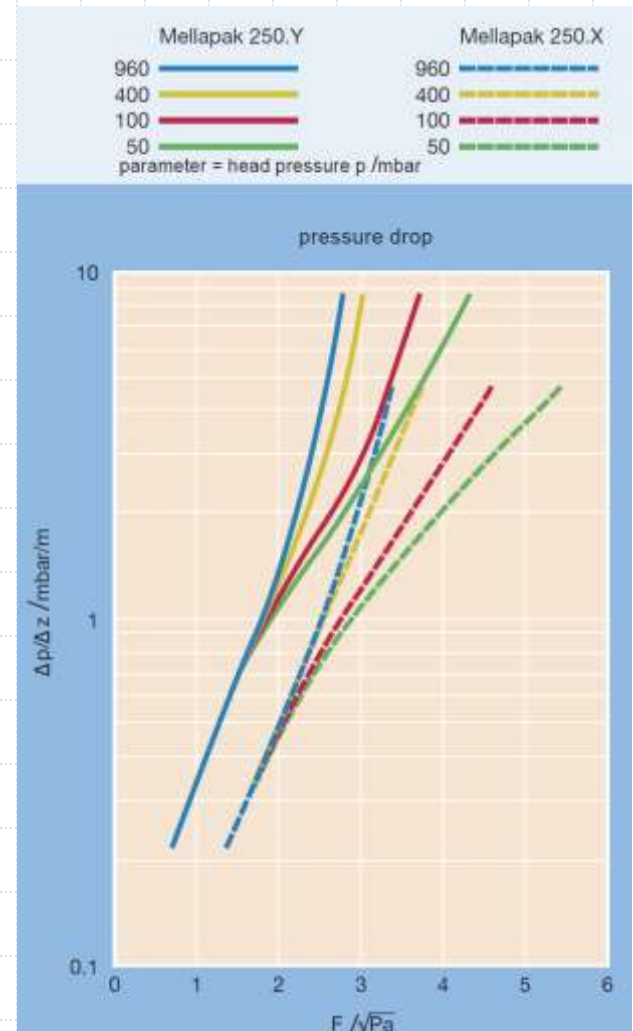
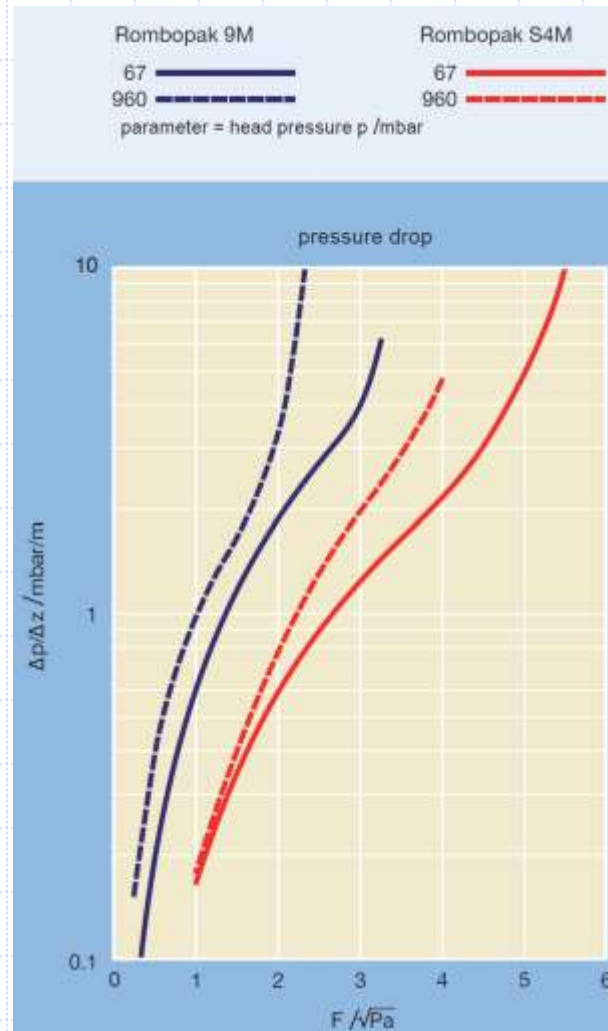
◆ Plot shows pressure drops per unit column height as a function of the liquid and vapor velocity (for a random packing)

- Initially vapor pressure drops increases with vapor velocity u_v squared
- When u_v increases, vapor starts interacting with the liquid.
- Liquid film starts growing due to friction, and reduces the space for vapor, thus increasing pressure drops
- This is LOADING (segments BC and B'C').
- If u_v increases further channels are closed and the column start clogging (flooding, points C, C')
- Above D and D' the column is full of liquid (bubbling column)



Pressure drops in commercial structured packings

◆ From Sulzer



$$F \text{ factor} = w_G \cdot \sqrt{\rho_G}$$

Wetting rate

- ◆ Column should operate **between loading and flooding**
- ◆ Once the diameter is chosen, wetting rate must be verified
 - Packing wetting increases with the liquid flow rate.
 - For random packings it is assumed that the packing is sufficiently wet if the Wetting rate (WR) is higher than the minimum wetting rate (MWR) defined as

$$WR = \frac{L_v/A}{a}$$

$$MWR = \frac{L_v/A_{\max}}{a}$$

$$L_v/A = a WR, \quad L_v/A_{\max} = a MWR$$

WR is expressed in m²/h, L_v/A is m³/m²h and a is m²/m³.

How to verify the wetting rate

◆ Random packings recommended minimum values

- $MWR = 0.08 \text{ m}^3\text{h}^{-1}\text{m}^{-1}$ for $d_p < 75 \text{ mm}$;
- $MWR = 0.12 \text{ m}^3\text{h}^{-1}\text{m}^{-1}$ for $d_p > 75 \text{ mm}$ ($d_p = \text{nominal packing dimension}$).

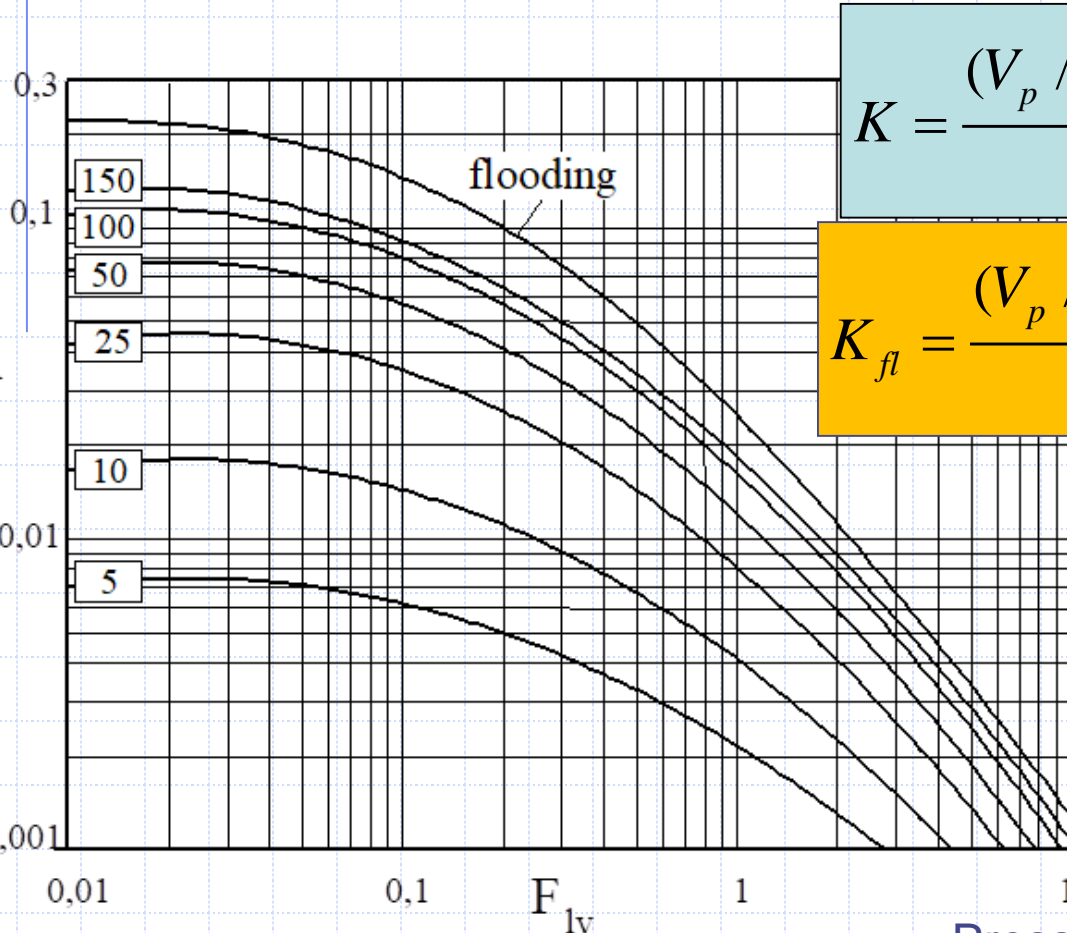
◆ Structured packings

- The minimum liquid velocity is directly given

Material	$u_{l,\min}, (\text{m}^3\text{h}^{-1})\text{m}^{-2}$
Ceramic row (not glazed)	0.5
Oxidised metal (C steel, brass)	0.75
Stainless steel with scratched surface	1
Glazed ceramic	2
Glass	2.5
Polished metal (steel, titania, ...)	3
PVC-CPVC	3.5
Polypropylene	4
fluoropolymers (as TEFLON)	5

Design and rating of randomly packed columns

◆ Flooding limit is evaluated by empirical **Eckert method**



$$K = \frac{(V_p / A)^2 C_f (\mu_l / \mu_{H_2O})^{0,2} (\rho_{H_2O} / \rho_l)}{g \rho_v \rho_l}$$

$$K_{fl} = \frac{(V_p / A)_{fl}^2 C_f (\mu_l / \mu_{H_2O})^{0,2} (\rho_{H_2O} / \rho_l)}{g \rho_v \rho_l}$$

V_p = mass flow rate (kg/sec)

$\mu_{H_2O}(20^\circ\text{C}) = 1\text{cP} = 0.001 \text{ Pa} \cdot \text{s}$

$\rho_{H_2O}(20^\circ\text{C}) = 1000 \text{ kg m}^3$

$g = 9.81 \text{ m s}^{-2}$

Pressure drops in $\text{N/cm}^2/\text{cm}$

$F_{LV} = L/G (\rho_v / \rho_L)^{-0,5}$ with L and G in kmol/h

Random packing table

◆ C_f is the packing parameter.

- It is determined from experimental data
- It is function of packing form, dimension and material
- Indicated as F in Wankat's book

Type	Nominal size mm	Elements, N. per m ³	Mass, kg per m ³	a m ² m ⁻³	ϵ	C_f m ⁻¹
Raschig rings	13	378000	880	370	0,64	2000
(ceramics)	25	47700	670	190	0,74	510
	38	13500	740	120	0,68	310
	50	5800	660	92	0,74	215
	75	8800	590	62	0,75	120
Pall rings	16				0,92	230
(metal)	25	49600	480	205	0,94	157
	38	13000	415	130	0,95	92
	50	6040	385	115	0,96	66
	90	1170	270	92	0,97	53
Pall rings	16	213700	116	341	0,87	310
(plastics)	25	50150	88	207	0,90	170
	38			128	0,91	130
	50	6360	72	100	0,92	82
	90			85	0,92	52
Berl saddles	13	590000	865	465	0,62	790
(ceramics)	25	77000	720	250	0,68	360
	38	22800	640	150	0,71	215
	50	8800	625	105	0,72	150
Intalox saddles	13	730000	720	625	0,78	660
(ceramics)	25	84000	705	255	0,77	320
	38	25000	670	195	0,80	170
	50	9400	670	118	0,79	130
	75	1870	590	92	0,80	70
Intalox saddles	25	168400	350		0,97	135
(metal)	38	50100	230		0,97	82
	50	14700	181		0,98	52
	70	4630	149		0,98	43
Intalox saddles	25	55800	76	206	0,91	105
(plastics)	50	7760	64	108	0,93	69
	75	1520	60	88	0,94	50

Flooding velocity calculation for randomly packed columns

- ◆ Flux parameter is given by

$$F_{lv} = \frac{L_v}{V_v} \sqrt{\frac{\rho_l}{\rho_v}} = \frac{L'}{V'} \sqrt{\frac{\rho_l}{\rho_v}} = \frac{L}{V} \sqrt{\frac{\rho_v}{\rho_l}}$$

- L_v and V_v are indicated as L' and V' (in Wankat book)

- ◆ K_{fl} is determined from Eckert's diagram

- ◆ **Massive flooding velocity G'_{fl}** is given by:

$$G'_{fl} = (V_p/A)_{fl} = \sqrt{\frac{K_{fl} g \rho_v \rho_l}{c_f (\mu_l / \mu_{H_2O})^{0.2} (\rho_{H_2O} / \rho_l)}} \text{ in lb/(ft}^2 \text{ sec)}$$

Randomly packed columns: diameter design

◆ Select the packing (type, dimension, material). Then

- Calculate massive flooding velocity
- Calculate massive vapor velocity based on a suitable K_5

$$G' = V_p/A = K_5 (V_p/A)_{fl}$$

- Calculate area and then the diameter:

$$A = \frac{V_p}{(V_p/A)} \quad D = \sqrt{\frac{4A}{\pi}}$$

- Select a value for D (commercially available) from which area is back calculated
- With the new value recalculate K_5 and verify it is below 80%;
- Calculate pressure drops per unit column height, knowing both F_{lv} and K.

Randomly packed columns: diameter rating

◆ Packing (type, dimension, material) and column diameter is known.

- Massive flooding velocity is calculated as before
- K_5 is calculated and verified it is below 80%

$$K_5 = \frac{V_p/A}{(V_p/A)_{fl}} = \sqrt{\frac{K}{K_{fl}}}$$

- Corresponding K value is calculated

$$K = \frac{(V_p/A)^2 C_f (\mu_l/\mu_{H_2O})^{0,2} (\rho_{H_2O}/\rho_l)}{g \rho_v \rho_l}$$

- Pressure drops per unit column height is calculated knowing both F_{lv} and K.

Parameters for dumped packings (F is 1/ft)

$$F = C_F$$

From

Eckert,

Ludwig,

Coker and
Geankoplis

Packing Type		Nominal				Packing Size, in					
		1/4	3/8	1/2	5/8	3/4	1	1 1/4	1 1/2	2	3
Raschig rings (metal, 1/32" wall)	F	700	390	300	170	155	115	—	—	—	—
	α				1.20						
	β				0.28						
Raschig rings (metal 1/16" wall)	F	—	—	410	290	220	137	110	83	57	32
	α					0.80	0.42	—	0.29	0.23	—
	β					0.30	0.21	—	0.20	0.14	—
Raschig rings (ceramic)	F	1600	1000	580	380	255	155	125	95	65	37
	α		4.70	3.10	2.35	1.34	0.97	0.57	0.39	0.24	0.18
	β		0.41	0.41	0.26	0.26	0.25	0.23	0.23	0.17	0.15
Pall rings (plastic)	F	—	—	—	97	—	52	—	32	25	—
	α						0.22			0.10	—
	β						0.14		—	0.12	—
Pall rings (metal)	F	—	—	—	70	—	48	—	28	20	—
	α				0.43		0.15		0.08	0.06	—
	β				0.17		0.16		0.15	0.12	—
Berl saddles (ceramic)	F	900	—	240	—	170	110	—	65	45	—
	α			1.2		0.62	0.39	—	0.21	0.16	—
	β			0.21		0.17	0.17	—	0.13	0.12	—
Intalox saddles (ceramic)	F	725	330	200	—	145	98	—	52	40	22
	α			1.04		0.52	0.52		0.13	0.14	—
	β			0.37		0.25	0.16		0.15	0.10	—
Intalox saddles (plastic)	F	—	—	—	—	—	33	—	—	21	16
Intalox saddles (metal)	F						41			18	
Flexirings (plastic)	F				78	—	45	—	28	22	—
Ballast ring (plastic)	F					97	—	52	32	25	—
Cascade miniring (plastic)	F				—	30	25	18	—	15	—
Hy-Pak (plastic)	F						25			12	

Source: Eckert (1970), Ludwig (1987), Coker (1991), Geankoplis (2003)

Packed column diameter calculation

◆ A distillation column is separating **n-hexane from n-heptane** using 1-inch ceramic Intalox saddles.

- The allowable pressure drop in the column is 0.5 inches of water per foot.
- Average column pressure is 1 atm.
- Separation in the column is essentially complete, so the distillate is almost pure hexane and the bottoms is almost pure heptane.
- Feed is a 50-50 mixture and is a saturated liquid.
- In the top, $L/V = 0.8$.
- If $F = 1000$ lbmol/h and $D = 500$ lbmol/h, estimate the column diameter required at the top.

Packed column diameter calculation

◆ Solution

- The *top* is essentially pure n-hexane. Then,

$$\rho_v = \frac{p(\text{MW})}{RT} = \frac{(1 \text{ atm})(86.17 \frac{\text{lb}}{\text{lbmol}})}{(1.314 \frac{\text{atm ft}^3}{\text{K lbmol}})(342 \text{ K})} = 0.1917 \frac{\text{lb}}{\text{ft}^3}$$

$$\frac{L'}{G'} = \left(\frac{L}{V}\right)\left(\frac{\text{MW liquid}}{\text{MW vapor}}\right) = (0.8)\left(\frac{86.17}{86.17}\right) = 0.8$$

- Using graph: x value: $\frac{L'}{G'} \left(\frac{\rho_v}{\rho_L}\right)^{1/2} = (0.8) \left[\frac{0.1917 \text{ lb/ft}^3}{(0.659 \frac{\text{g}}{\text{cm}^3})(\frac{62.4 \text{ lb/ft}^3}{\text{g/cm}^3})} \right]^{1/2} = 0.055$

- y value ($\Delta P = 40 \text{ N/cm}^2/\text{cm}$) is: $\frac{G'^2 F \phi \mu^{0.2}}{\rho_G \rho_L g_c} = 0.055$

Packed column diameter calculation

◆ Solution

■ Then G' is:

$$G' = \left(\frac{0.055 \rho_G \rho_L g_c}{F \psi \mu^{0.2}} \right)^{1/2}$$

■ With $C_F = 98$:

$$G' = \left[\frac{(0.055)(0.1917)(0.659)(62.4)(32.2)}{98 \left(\frac{0.9783}{0.659} \right) (0.22)^{0.2}} \right]^{1/2} = 0.360 \frac{\text{lb}}{\text{s ft}^2}$$

■ Using equation:

$$\text{Area} = \frac{\left(V \frac{\text{lbmol}}{\text{s}} \right) (\text{MW})}{G'}$$

■ Calculate V from $V=L+D=(L/D+1) D$, with $L/D=L/V / (1-L/V) = .8/.2= 4$

■ And $V = (5) * D = (5*500/3600) = 0.6944 \text{ lbmol/sec}$

■ Area is given by $(0.6944)*(86.17) / (0.360) = 166 \text{ ft}^2$

■ Diameter $D = (4*\text{Area}/\pi)^{1/2} = (4/31.4 * 166)^{1/2} = 14.54 \text{ ft}$

Packed column diameter calculation

◆ *Alternative method using table by Eckert et al.:*

- *Estimate pressure drops use Equation (α and β from tables):*
- *Since $L'/G' = L/V$, have $L' = (L/V)G'$. Then Equation becomes:*

$$\Delta p = \alpha(10^{\beta(L/V)G'})\left(\frac{G'^2}{\rho_G}\right)$$

- From Table (see text), $\alpha = 0.52$ and $\beta = 0.16$. Then the equation is

$$0.50 = (0.52)(10^{(0.16)(0.8)G'})\left(\frac{G'^2}{0.1917}\right)$$

- This is an equation with one unknown, G' , so it can be solved for G' . Rearranging the equation,

$$G' = \left(\frac{0.1843}{10^{0.128G'}}\right)^{1/2}$$

- Using our previous answer, $G' = 0.360$, as the first guess and using direct substitution, we obtain $G' = 0.404$ as the answer in two trials. This equation is also easy to solve on a spreadsheet with Goal Seek.

Packed column diameter calculation

- Then:

$$\text{Area} = \frac{V(\text{MW})}{G'} = \frac{(0.6944)(86.17)}{0.404} = 148.1 \text{ ft}^2$$

$$\text{Diameter} = \left(\frac{4 \text{ Area}}{\pi} \right)^{1/2} = 13.73 \text{ ft}$$

- Note that there is a 6% difference between this answer and the one we obtained graphically.
- Since α and β in are specific for this packing and are not based on generalized curves, the lower value is probably more accurate and a 14-foot diameter would be used.
- If we wanted to be conservative (safe), a 14.5-foot diameter would be used.
- Additional safety factors (see Fair, 1985) might be employed if the pressure drop is critical.

Design and rating of structured packed columns

◆ The GPDC-KG (Generalized Pressure Drop Correlation) diagram proposed by Kister and Gill is used to estimate flooding velocity:

- Capacity parameter is defined as

$$Y = u_v \sqrt{\frac{\rho_v}{\rho_l - \rho_v}} C_f^{0,5} v_l^{0,05}$$

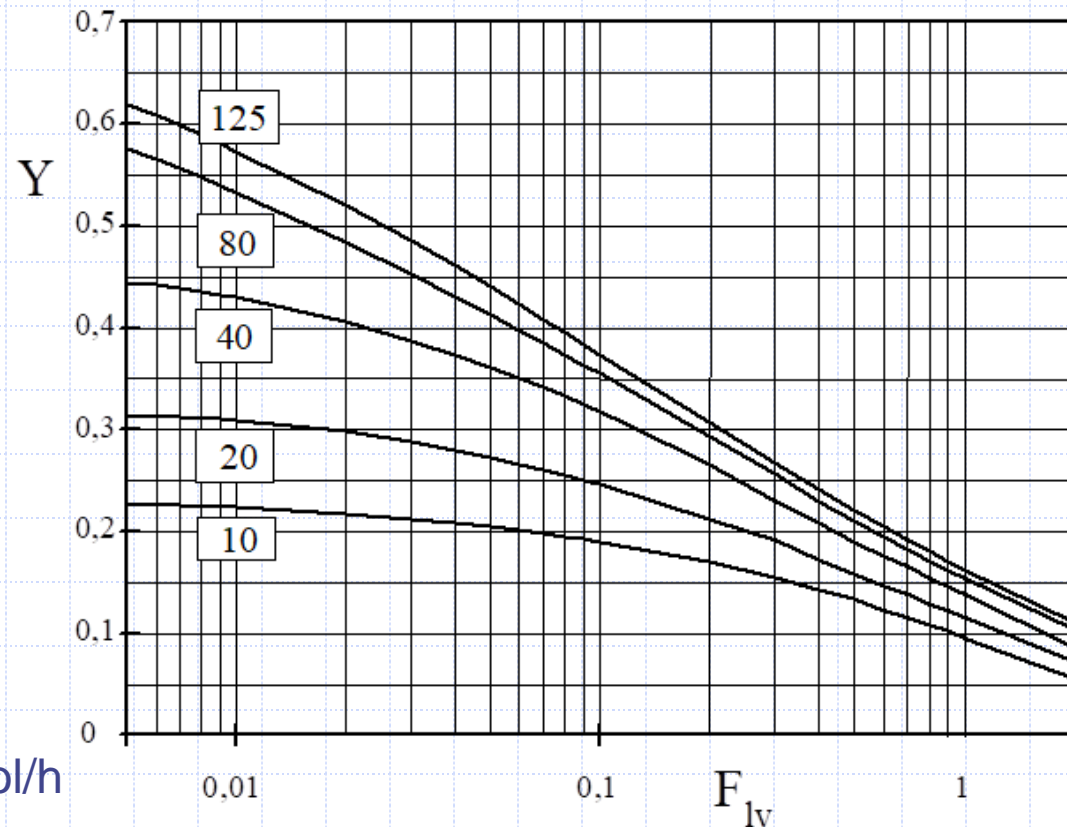
$$v_l = \frac{\mu_l}{\rho_l} = \text{kinematic viscosity}$$

- The ΔP at flooding is given by

$$\left(\frac{\Delta P}{L}\right)_{fl} = 4,17 C_f^{0,7}$$

Pressure drops in N/cm²/cm

$F_{IV} = L/G (\rho_v / \rho_l)^{0,5}$ with L and G in kmol/h



Structured packing table

◆ C_f is the packing parameter.

- It is determined from experimental data
- It is function of packing form, dimension and material

Packing	Type	C_f, m^{-1}	Packing	Type	C_f, m^{-1}
Koch-Sulzer	CY	230	Flexeramic Koch	#88	49
	BX	69	Gempak Glitsch	4A	105
Mellapak Sulzer (metal)	500Y	112		3A	69
	350Y	75		2A	52
	250Y	66		1,5A	39
	125Y	33		1A	30
Mellapak Sulzer (plastics)	250Y	72		0,5A	20
Flexipak Koch	#1	98	Montz B - 1	300	108
	#2	43		250	66
	#3	26	Intalox Norton (structured)	1T	66
	#4	20		2T	56
Flexeramic Koch	#28	131		3T	43
	#48	79	Jaeger MacPac		39

Structured packed columns: diameter **design**

◆ Select the packing (type, dimension, material). Then

- Calculate flooding curve with the graphical correlation
 - ◆ the capacity parameter Y_{fl} is determined

- Calculate vapor flooding velocity:
$$u_{v,fl} = \frac{Y_{fl}}{C_f^{0,5} v^{0,05}} \sqrt{\frac{\rho_l - \rho_v}{\rho_v}}$$

- Calculate vapor velocity based on a suitable K_5 value:
$$u_v = K_5 u_{v,fl}$$

- Calculate area and then the diameter:

$$A = \frac{V_v}{u_v} \quad D = \sqrt{\frac{4A}{\pi}}$$

- Select a value for D (commercially available) from which area is back calculated
- With this new value recalculate K_5 and verify it is below 80%;
- Calculate pressure drops per unit column height, knowing both F_{IV} and Y .

Structured packed columns: diameter rating

◆ Packing (type, dimension, material) and column diameter is known.

- Calculate flooding curve as above: the capacity parameter Y_{fl} is determined

- Calculate vapor flooding velocity:
$$u_{v,fl} = \frac{Y_{fl}}{C_f^{0,5} v^{0,05}} \sqrt{\frac{\rho_l - \rho_v}{\rho_v}}$$

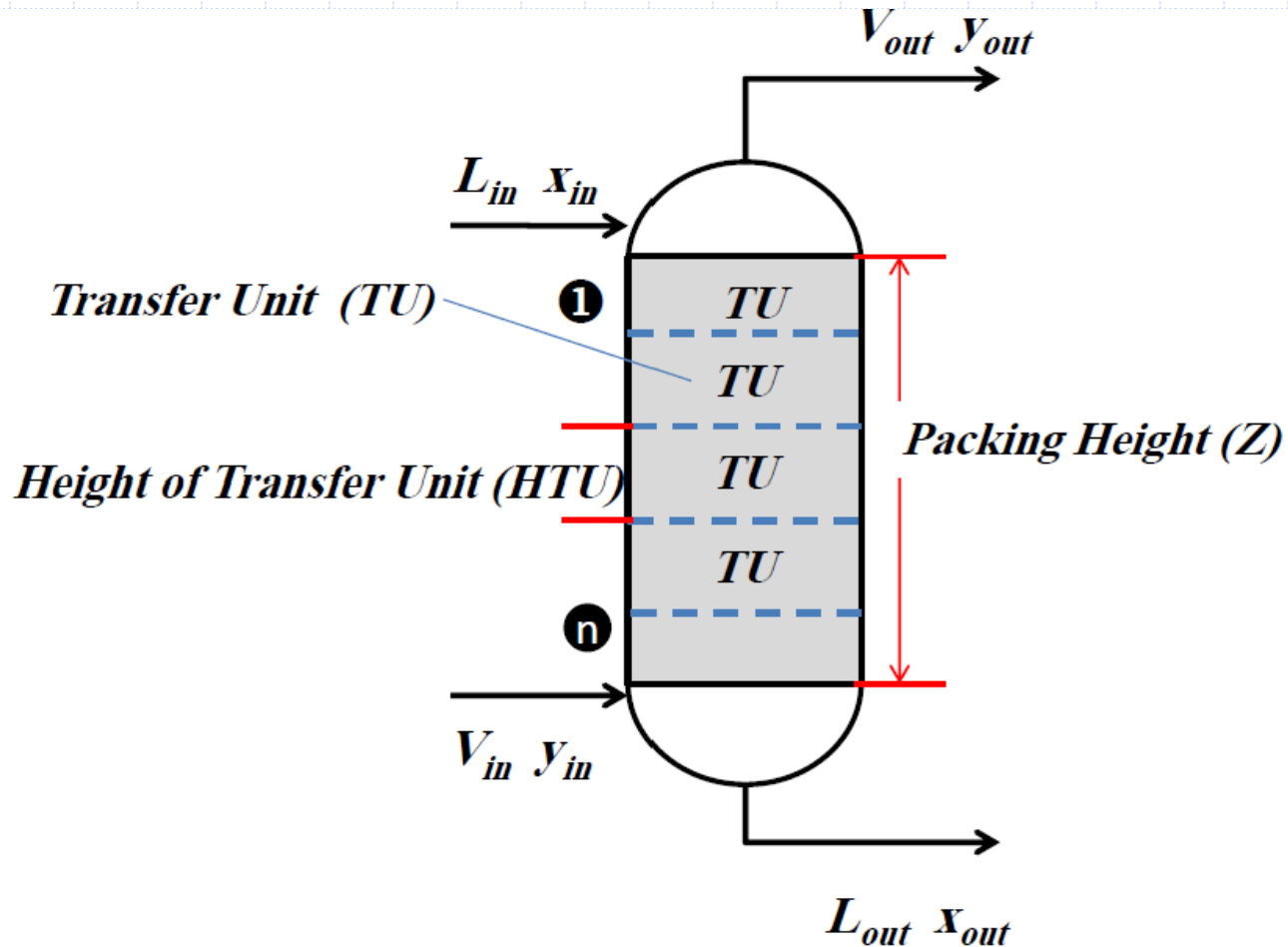
- Case 1: K_5 is calculated and verified that is lower than 80%

$$K_5 = \frac{u_v}{u_{v,fl}}$$

- Case 2: Maximum vapor flow rate is calculated: $V_{v,max} = u_{v,fl}A$
 - ◆ If the value of $V_{v,max}$ is lower than V_v the liquid flow rate for that packing must be recalculated
- Pressure drops per unit column height is calculated from both F_{lv} and Y .

Packing Height (Z)

- ◆ Packing Height (Z) = height of transfer unit (HTU) * number of transfer units (n)



Methods for Packing Height (Z)

2 methods

Equilibrium stage analysis
HETP method

Mass Transfer analysis
HTU method

More common

$$Z = \text{HETP} \times N$$

N = number of theoretical stages obtained from McCabe-Thiele method

HETP

- Height Equivalent to a Theoretical Plate
- Represents the height of packing that gives similar separation to as a theoretical stage.
- HETP values are provided for each type of packing

$$Z = \text{HTU} \times \text{NTU}$$

HTU = Height of a Transfer unit

NTU = Number of Transfer Units (obtained by numerical integration)

$$Z = \frac{V}{K_y a A_c} \int_{y_{Ain}}^{y_{Aout}} \frac{dy}{(y_A^* - y_A)} \quad Z = H_{OG} \times N_{OG}$$

$$Z = \frac{L}{K_x a A_c} \int_{x_{Ain}}^{x_{Aout}} \frac{dx_A}{(x_A - x_A^*)} \quad Z = H_{OL} \times N_{OL}$$

HETP: Height of the Equivalent Theoretical Plate

- ◆ It is common practice express the height of packing in terms of HETP

$$Z = (HETP) (NETP)$$

- Where NETP (Number of Equivalent Theoretical Plates) is the number of theoretical ideal stages obtainable with a McCabe-Thiele plot.
 - Unfortunately, no general model for predicting HETP is available.
 - HETP is not used for design, only for rating
- ◆ It is common using HETP for describing the efficiency of a portion of packing with respect to mass transfer: the lower HETP, the higher the efficiency

$$HETP = \frac{Z}{NETP}$$

The concept of HETP

◆ At **very low gas rates** liquid is not well distributed

- Low efficiency
- Lower than MWR.

◆ **Pre-loading regime** is characterized by

- Good mass transfer and constant efficiency

◆ **Loading zone**

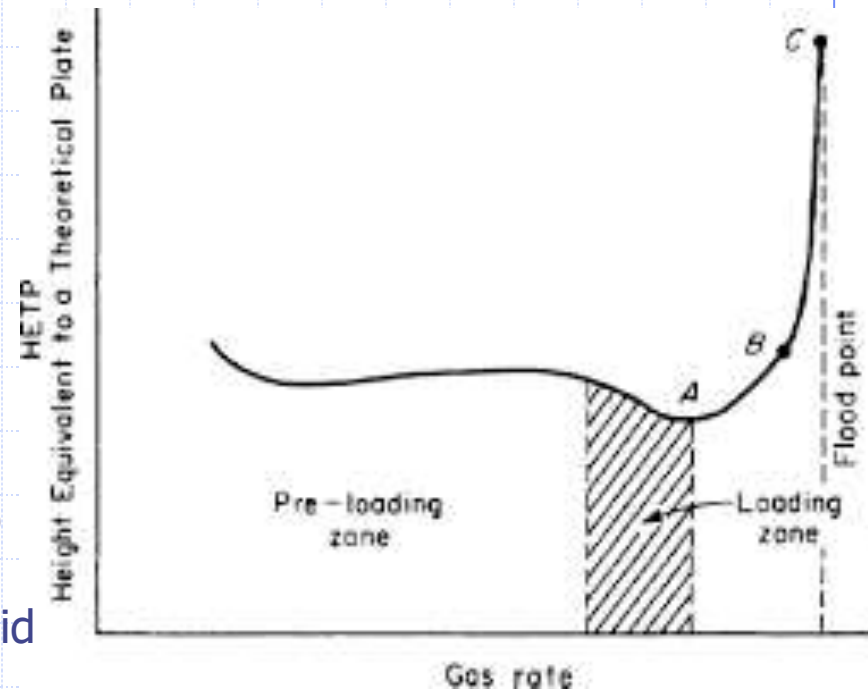
- efficiency increases with liquid hold up
- It goes through a maximum (A)
- And decreases rapidly (AC) due to liquid drag

◆ **Flooding regime** (above point C)

- Characterized by instability, liquid dragging and low efficiency

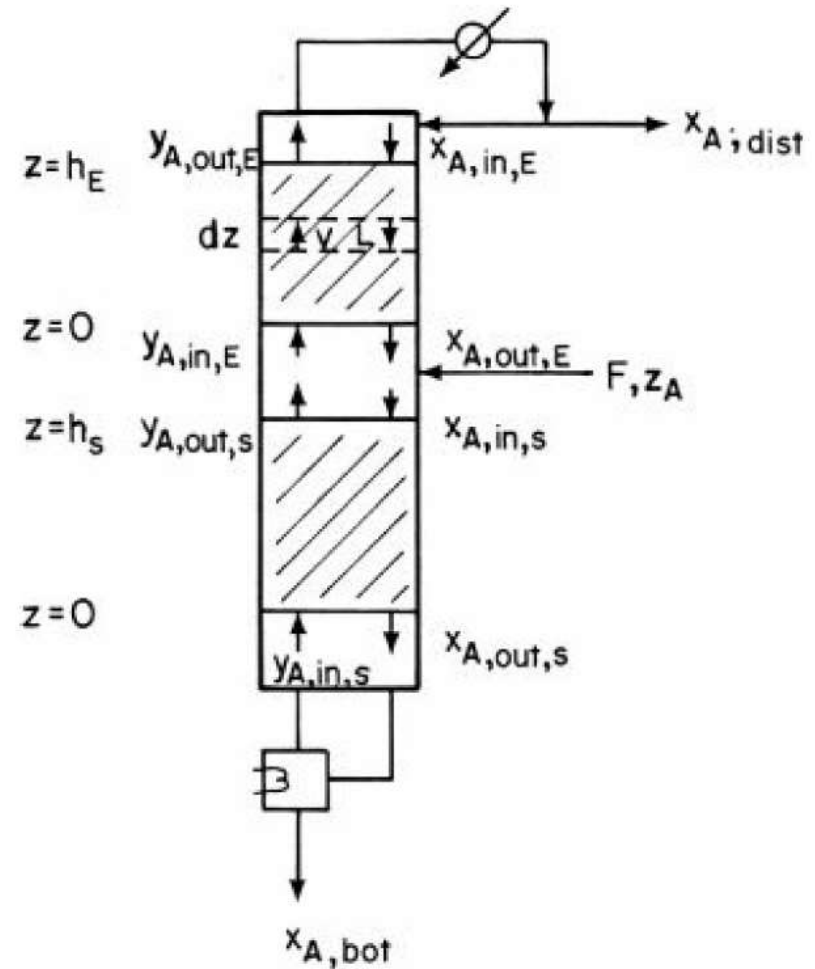
◆ Columns are design to operate in the region of **constant efficiency**

- Pressure drops increases uniformly with vapor flow rate



HTU-NTU Analysis of Packed Distillation Columns

- ◆ Packed distillation tower in Figure.
- ◆ Assumptions:
 - Binary distillation with (CMO).
 - A is the more volatile component and B the less volatile component.
- ◆ CMO means:
 - $L/V = \text{constant}$
 - energy balances satisfied
 - equimolal counter diffusion,
 - ◆ $N_A = -N_B$.
 - Perfect plug flow of the liquid and vapor.
 - ◆ Therefore, no eddy mixing to reduce the separation.



Mass Transfer fundamentals

- ◆ Molar flow of component A depends on concentration gradient (mol.m⁻².s⁻¹)

$$\vec{W}_A = \vec{J}_A + \vec{B}_A$$

\vec{J}_A = is molecular diffusive flux (relative to the motion of the bulk of the mixture),

\vec{B}_A = flux resulting from the motion of the bulk of the mixture

$$\vec{B}_A = y_A \sum \vec{W}_j \quad \vec{B}_A = C_A \vec{V} = C_A \sum y_j \vec{V}_j$$

V and V_j are mean molar velocity and particle j velocity respectively

Fick's and Fourier's laws

◆ Fick's law for binary mixtures:

- c = total concentration (mol/dm³)
- D_{AB} = diffusivity of A in B (dm²/s)

$$\vec{J}_A = -c D_{AB} \vec{\nabla} y_A$$

◆ Analogy with Fourier's law:

- k thermal conductivity

$$\vec{q} = -k \vec{\nabla} T$$

◆ For binary mixtures:

$$\vec{W}_A = -c D_{AB} \vec{\nabla} y_A + y_A (\vec{W}_A + \vec{W}_B)$$

◆ For multicomponent mixtures, the flux of component j may be generated not only by its concentration gradient but also by concentration gradients of other components

◆ The concept of effective binary diffusion is used

- diffusion of component j through the mixture D_{jm} :

$$\vec{W}_j = -c D_{jm} \vec{\nabla} y_j + y_j \sum_{k=1}^N \vec{W}_k$$

Diffusivity is function of T and P

Phase	Order of Magnitude		Temperature and Pressure Dependences ^a
	cm ² /s	m ² /s	
Gas			
Bulk	10 ⁻¹	10 ⁻⁵	$D_{AB}(T_2, P_2) = D_{AB}(T_1, P_1) \frac{P_1}{P_2} \left(\frac{T_2}{T_1}\right)^{1.75}$
Knudsen	10 ⁻²	10 ⁻⁶	$D_A(T_2) = D_A(T_1) \left(\frac{T_2}{T_1}\right)^{1/2}$
Liquid	10 ⁻⁵	10 ⁻⁹	$D_{AB}(T_2) = D_{AB}(T_1) \frac{\mu_1}{\mu_2} \left(\frac{T_2}{T_1}\right)$
Solid	10 ⁻⁹	10 ⁻¹³	$D_{AB}(T_2) = D_{AB}(T_1) \exp \left[\frac{E_D}{R} \left(\frac{T_2 - T_1}{T_1 T_2} \right) \right]$

^a μ_1, μ_2 , liquid viscosities at temperatures T_1 and T_2 , respectively; E_D , diffusion activation energy.

Different situations for diffusion - 1

◆ Equimolar counter-diffusion: $\vec{W}_A = -\vec{W}_B$

$$\vec{W}_A = \vec{J}_A + y_A (\vec{W}_A + (-\vec{W}_A)) = \vec{J}_A = -c D_{AB} \vec{\nabla} y_A = -D_{AB} \vec{\nabla} C_A$$

◆ Dilute concentrations: second term can be neglected (y_A is small):

$$\vec{W}_A \approx \vec{J}_A = -c D_{AB} \vec{\nabla} y_A = -D_{AB} \vec{\nabla} C_A$$

- In case of diffusion in aqueous solutions with negligible convective motion
- In case of Knudsen diffusion with very small pore dimensions

Different situations for diffusion - 1

- ◆ Knudsen diffusion: occurs when the scale length of a system is comparable to or smaller than the mean free path of the particles involved.

$$\vec{W}_A = \vec{J}_A = -D_K \vec{\nabla} C_A$$

- with D_K Knudsen's diffusivity

- ◆ Diffusion through stagnant gas: $W_B = 0$

$$\vec{W}_A = c D_{AB} \vec{\nabla} \ln(1 - y_A) = c D_{AB} \vec{\nabla} \ln y_B$$

- ◆ Forced convection: diffusion term if the flow direction is small compared to the bulk motion and therefore is neglected

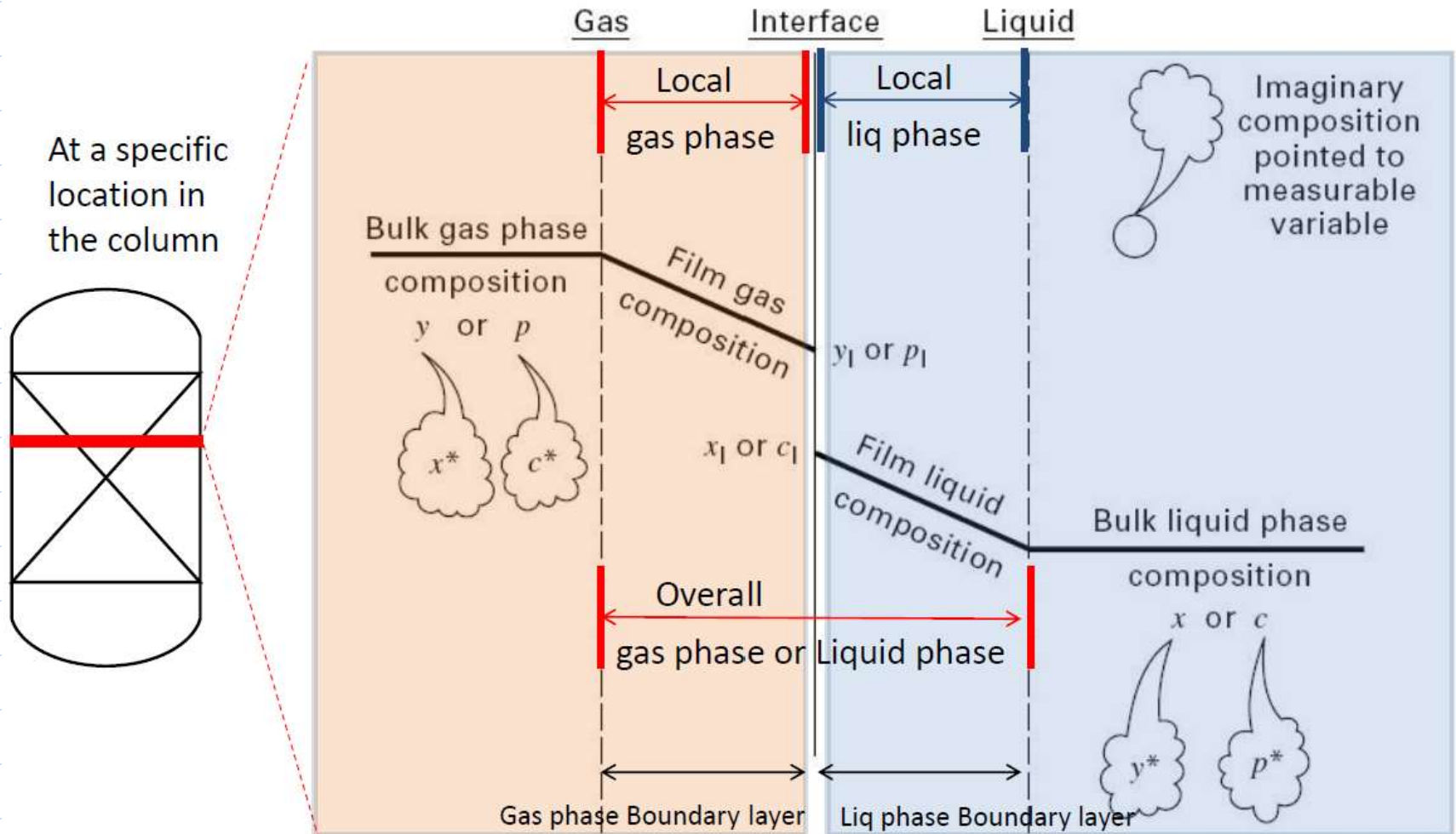
$$W_{Az} = B_{Az} = y_A W_{Az} = C_A V_z$$

- ◆ Diffusion and convective transport

- All effects are considered → complete equation

Two-Film Theory of Mass Transfer

◆ Interface properties in terms of bulk properties



HTU-NTU Analysis of Packed Distillation Columns

- ◆ For the differential height dz in the rectifying section, the mass transfer rate in terms of the individual coefficients is

$$N_A a A_C dz = k_y a (y_{AI} - y_A) A_C dz$$

- where N_A is the flux of A in kmol/m²-h or lbmol/ft²-h and A_C is the column cross-sectional area in m² or ft².
- This equation has units of kmol/h or lbmol/h.

- ◆ The mass transfer rate must also be equal to the changes in the amount of the more volatile component in the liquid and vapor phases

$$N_A a A_C dz = V dy_A = L dx_A$$

- Where L and V are constant molar flow rates.

- ◆ Combining equations:

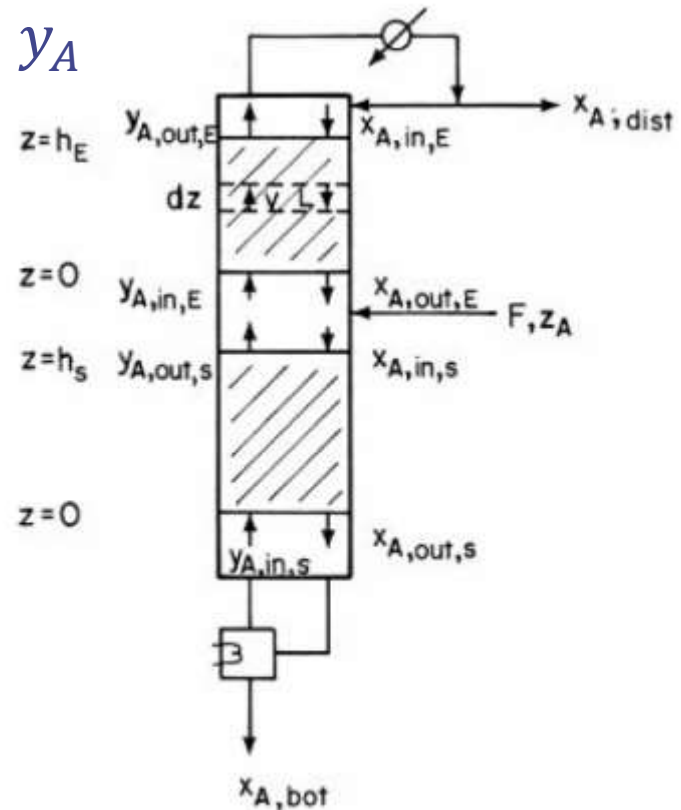
$$dz = \frac{V}{k_y a (y_{AI} - y_A) A_C} dy_A$$

HTU-NTU Analysis of Packed Distillation Columns

- ◆ Integrating this from $z = 0$ to $z = h$, where h is the total height of packing in a section, we obtain

$$h = \frac{V}{k_y a A_C} \int_{y_{A,in}}^{y_{A,out}} \frac{dy_A}{y_{AI} - y_A}$$

- We have assumed that the term $V/(k_y a A_C)$ is constant.
- The limits of integration for y_A in each section are shown in Figure.
- Equation (16-4) is often written as $h = H_G n_G$ where
- Height of a gas phase transfer unit H_G is the pre integral factor (HTU)
- Number of gas transfer units n_G is the integral (NTU)



HTU-NTU Analysis of Packed Distillation Columns

- ◆ Same analysis can be done for the liquid phase:

$$h = \frac{L}{k_x a A_C} \int_{x_{A,out}}^{x_{A,in}} \frac{dx_A}{x_A - x_{AI}}$$

- Defining H_L and n_L in a similar way.
- ◆ In order to do the integrations to calculate n_G and n_L we must relate the interfacial mole fractions y_{AI} and x_{AI} to the bulk mole fractions y_A and x_A .
- ◆ To do this we need to go back to equimolar transfer systems.
- ◆ The gas and liquid compositions at the interface are always assumed at equilibrium: $y_i = K x_i$

Mass transfer in packed columns

- ◆ Previous equations are normally written in the form:

$$h = Z = (HTU)_l(NTU)_l = (HTU)_v(NTU)_v$$

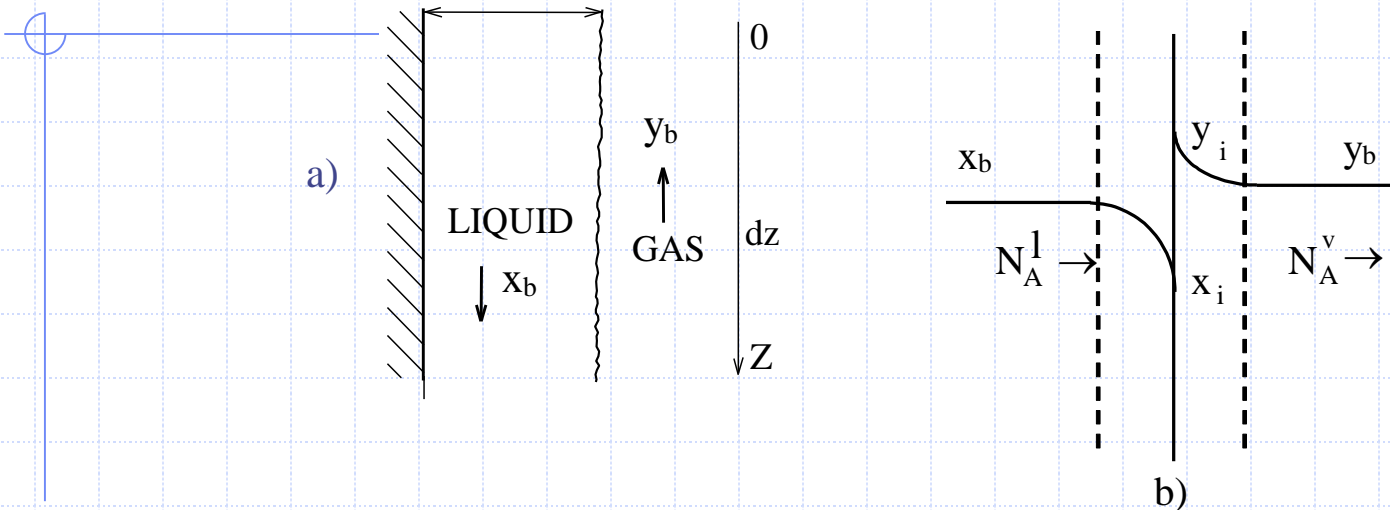
- ◆ Height of transfer units: $HTU_l = \frac{L}{k_x a A_C}$ $HTU_v = \frac{V}{k_y a A_C}$

- ◆ Number of transfer units:

$$NTU_l = \int_{x_{A,out}}^{x_{A,in}} \frac{dx_A}{x_A - x_{Ai}} \qquad NTU_v = \int_{y_{A,in}}^{y_{A,out}} \frac{dy_A}{y_{Ai} - y_A}$$

- ◆ For random packings a general relationship exists for calculating HTU: Bolles and Fair method

Mass transfer in packed columns



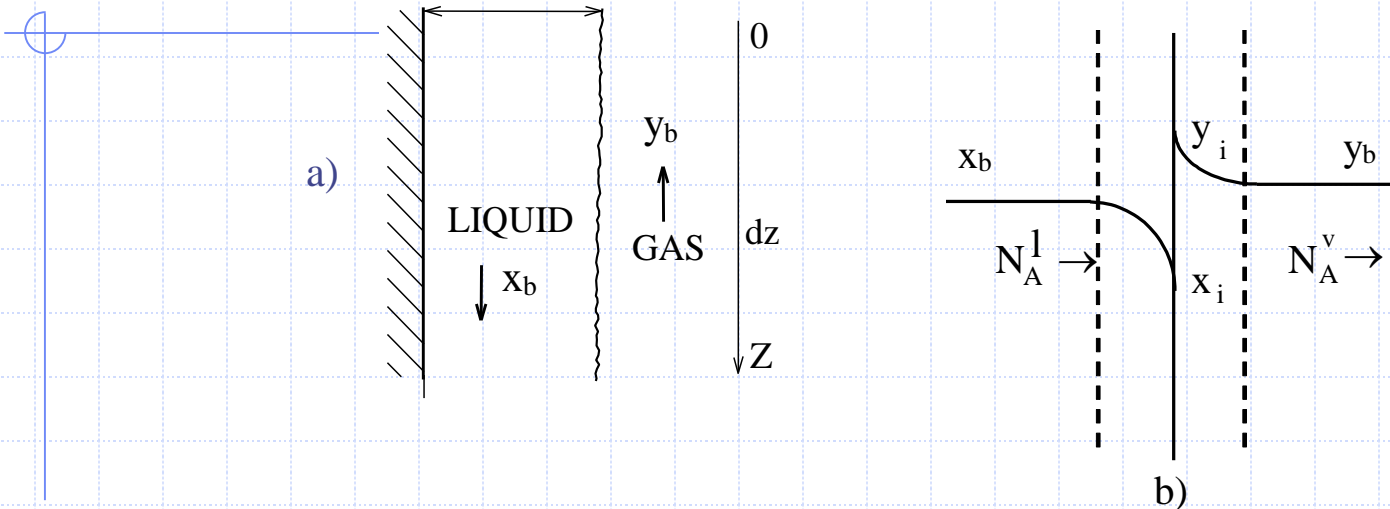
- ◆ Mass transfer equation for dilute or equimolar counter diffusion is:

$$N_{A,z,gas} = J_{A,z,gas} = k_{c,gas}(y_{A,0} - y_{A,\delta})$$

- Or, in terms of concentrations

$$N_{A,z,gas} = J_{A,z,gas} = k_{c,gas}(C_{A,gas,0} - C_{A,gas,\delta})$$

Mass transfer in packed columns



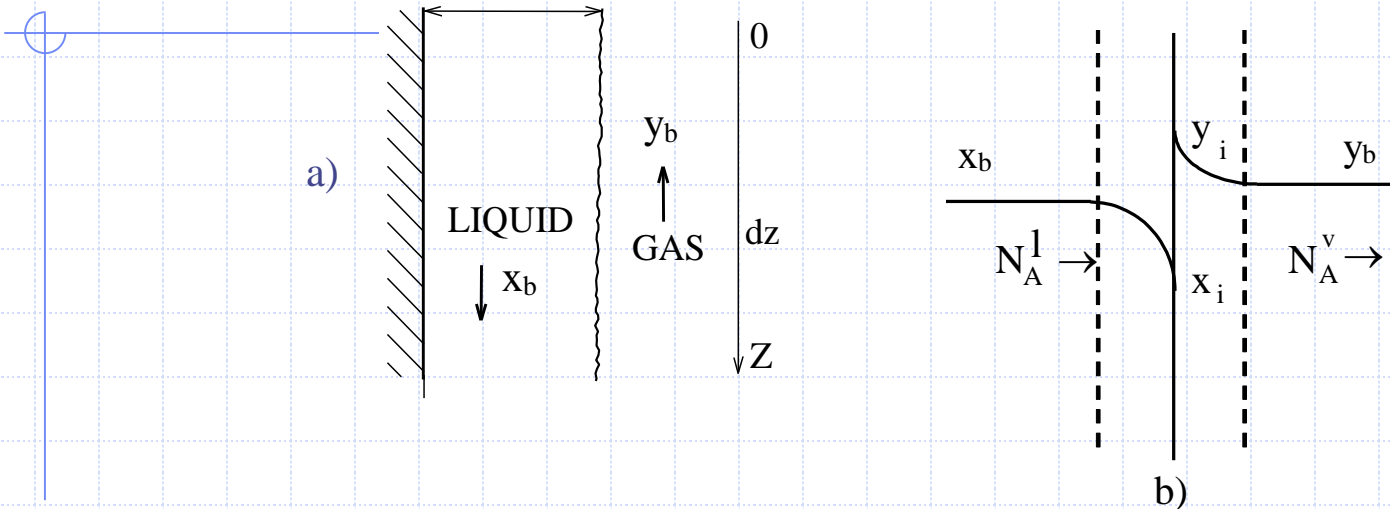
◆ For equilibrium staged and sorption separations, we are interested in mass transfer from one phase to another (see figure above)

- x_I and y_I are the interfacial mole fractions.
- For dilute absorbers and strippers and for distillation where there is equimolar counter transfer of the more volatile and less volatile components, the mass-transfer equations can be written for each stage in the following forms:

$$A_I N_{A,z,gas} = A_I k_y (y_{A,I} - y_A)$$

$$A_I N_{A,z,liq} = A_I k_x (x_A - x_{A,I})$$

Mass transfer in packed columns



- ◆ The two equations are set equal to each other:

$$\frac{(y_{A,I} - y_A)}{(x_{AI} - x_A)} = -\frac{k_x a}{k_y a} = -\frac{L H_G}{V H_L}$$

- ◆ where the last equality on the right comes from the definitions of H_G and H_L .

Mass transfer in packed columns

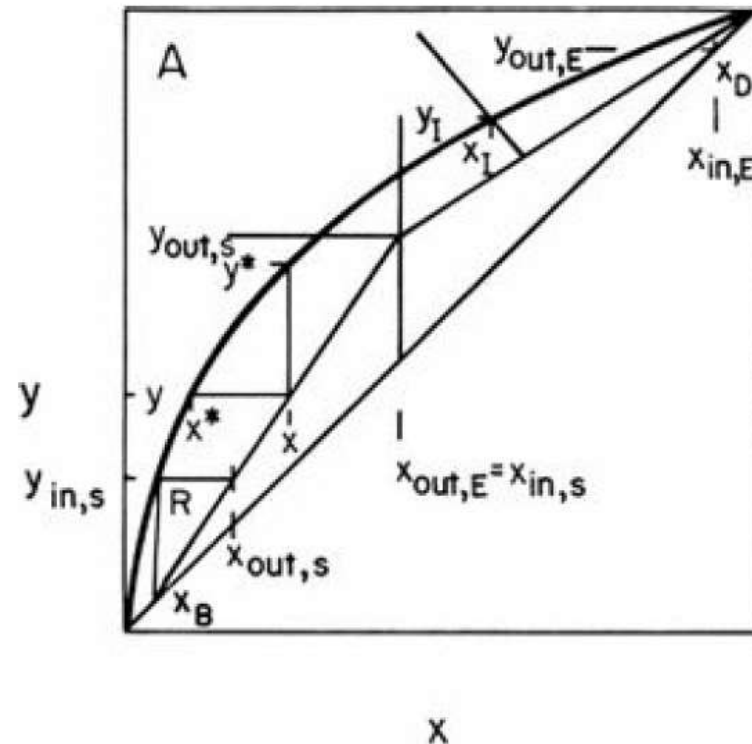
- ◆ The left-hand side of this equation is the slope of a line from the point representing the interfacial mole fracs ($y_{A,I}$, $x_{A,I}$) to the point representing the bulk mole fracs ($y_{A,r}$, $x_{A,r}$).
- ◆ Since there is no interfacial resistance, the interfacial mole fracs are in equilibrium and must be on the equilibrium curve.
- ◆ The bulk mole fracs are related by a mass balance through segment dz around the top or the bottom.
- ◆ This *operating line* in the rectifying section is

$$y_A = \frac{L}{V}x + \left(1 - \frac{L}{V}\right)x_{A,\text{dist}}$$

- ◆ And the *stripping line* is:

$$y_A = \frac{L'}{V'}x + \left(\frac{L'}{V'} - 1\right)x_{A,\text{bot}}$$

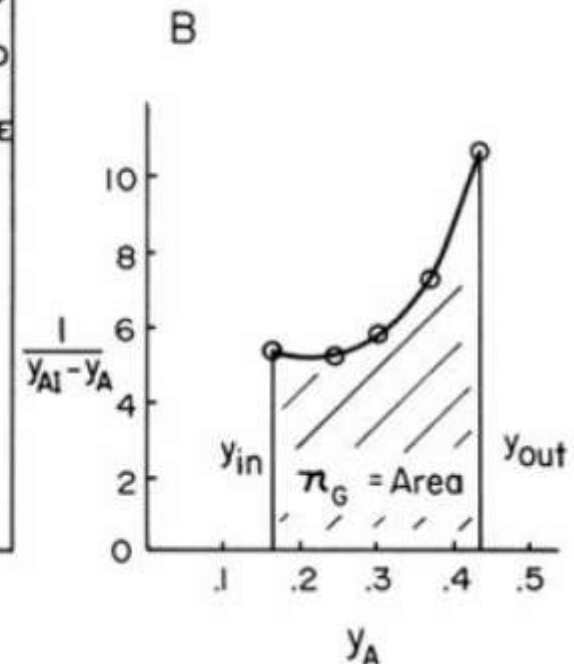
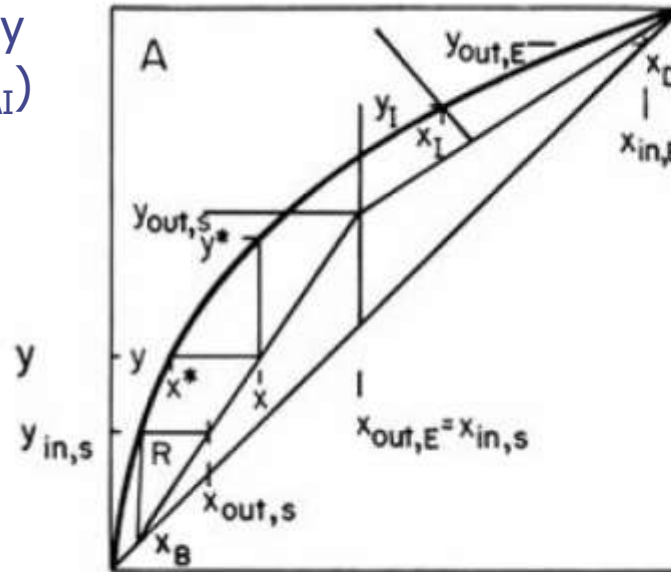
$$\frac{(y_{A,I} - y_A)}{(x_{A,I} - x_A)} = -\frac{k_x a}{k_y a} = -\frac{L H_G}{V H_L}$$



Mass transfer in packed columns

◆ We can now use a modified McCabe-Thiele diagram to determine x_{AI} and y_{AI} .

- From any point (y_A, x_A) on the operating line, draw a line slope $-k_{xa}/k_{ya}$. The intersection of this line with the equilibrium curve gives the interfacial mole fracs that correspond to y_A and x_A .
- Calculation is done for a series of points \rightarrow plot $1/(y_{AI} - y_A)$ vs y_{AC}
- The area under the curve is n_G .
- n_L is determined by plotting $1/(x_A - x_{AI})$ versus x_A .
- The areas can be determined from graphical or numerical integration.

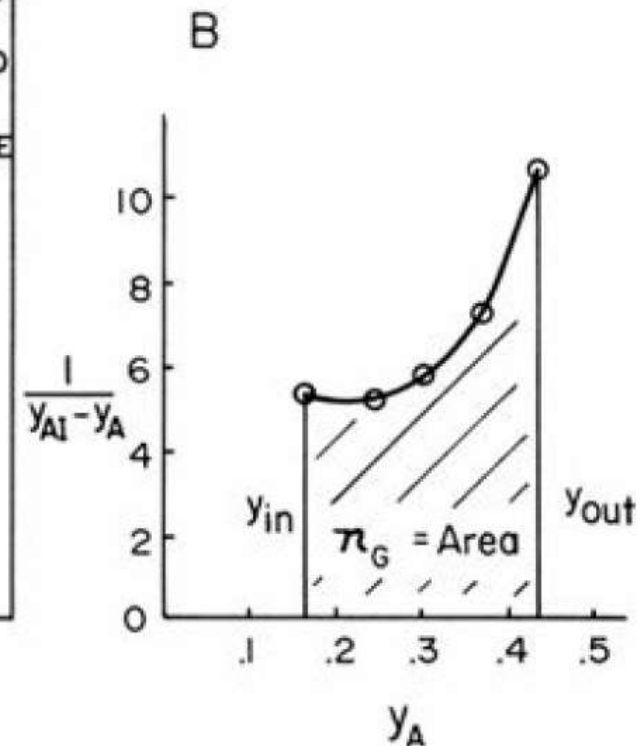
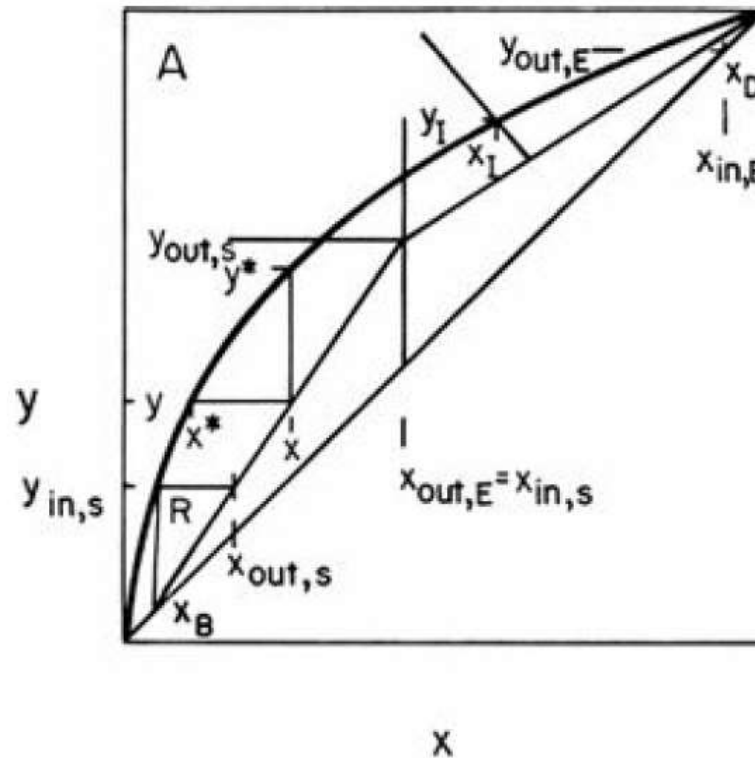


x

y_A

Mass transfer in packed columns

- ◆ In the determination of n_G for the stripping section, $y_{A,in,S}$ is the vapor mole frac leaving the reboiler.
- ◆ Mole frac $y_{A,out,S}$ is the mole frac leaving the stripping section.
 - This mole frac can be estimated at the intersection of the operating lines. Note that this estimate makes $y_{A,out,S} = y_{A,in,E}$.



How can packing height be calculated?

About NTU:

- ◆ just perform a numerical integration

About HTU:

- ◆ It depends on mass transfer and hydrodynamics
- ◆ Different methods, rough estimation anyway (average error: $\pm 50\%$)
- ◆ examples:
 - Bolles and Fair method (random packings)
 - Bravo method (structured packings)
 - proprietary methods

Bolles and Fair method

◆ HTU in liquid:

$$HTU_l = 0,305 \phi C_{fl} (0,33Z)^{0,15} S c_l^{0,5}$$

◆ HTU in vapor

$$HTU_v = 0,305 \frac{\beta S c_v^{0,5} (3,3D)^{C_1} (0,33Z)^{1/3}}{\left(737 \frac{L_p}{A} C_\sigma C_\rho C_\mu\right)^{C_2}}$$

- With empirical parameters: β , ϕ , C_{fl}

$$C_\sigma = \left(\frac{\sigma}{\sigma_{H_2O}}\right)^{-0,8} ; \quad C_\rho = \left(\frac{\rho_l}{\rho_{H_2O}}\right)^{-1,25} ; \quad C_\mu = \left(\frac{\mu_l}{\mu_{H_2O}}\right)^{0,16}$$

- $C_1 = 1,24$ for rings; $C_1 = 1,11$ for saddles; $C_2 = 0,6$ for rings; $C_2 = 0,5$ for saddles
- D is column diameter (= 0,6 when $D > 0,6$) and Z is the height of packings
- An iterative procedure is necessary

Bolles and Fair method

C_{fl}

V/V _{fl}	0	0,4	0,44	0,48	0,51	0,60	0,70	0,78	0,85
C _{fl}	1	1	1	0,98	0,96	0,87	0,74	0,61	0,45

ϕ

L _p /A, kg (m ² s) ⁻¹ =		0,3	0,5	1	2	5	10	20	50
	d _p , mm								
Raschig rings (ceramics)	13	0,0380	0,0360	0,0354	0,0423	0,0610	0,0905	0,1433	0,2857
	25	0,0420	0,0430	0,0456	0,0495	0,0590	0,0722	0,0981	0,1975
	38	0,0364	0,0394	0,0466	0,0574	0,0774	0,1014	0,1371	0,2516
	50	0,0472	0,0499	0,0551	0,0617	0,0741	0,0925	0,1207	0,1709
Raschig rings (metal)	13	0,0338	0,0328	0,0321	0,0377	0,0590	0,0876	0,1253	0,2585
	25	0,0380	0,0390	0,0410	0,0443	0,0541	0,0649	0,0882	0,1778
	38	0,0325	0,0354	0,0420	0,0518	0,0699	0,0909	0,1240	0,2263
	50	0,0472	0,0499	0,0551	0,0617	0,0741	0,0925	0,1207	0,1709
Berl saddles (ceramics)	13	0,0371	0,0387	0,0420	0,0479	0,0623	0,0761	0,0938	0,1266
	25	0,0197	0,0230	0,0298	0,0377	0,0538	0,0708	0,0932	0,1394
	38	0,0243	0,0262	0,0305	0,0374	0,0525	0,0669	0,0882	0,1237
Pall rings (metal)	13	0,0338	0,0328	0,0321	0,0377	0,0551	0,0817	0,1289	0,2575
	25	0,0380	0,0390	0,0410	0,0443	0,0541	0,0649	0,0882	0,2263
	38	0,0325	0,0354	0,0420	0,0518	0,0699	0,0909	0,1240	0,2263
	50	0,0525	0,0554	0,0613	0,0679	0,0827	0,1023	0,1335	0,1902

Bolles and Fair method

β

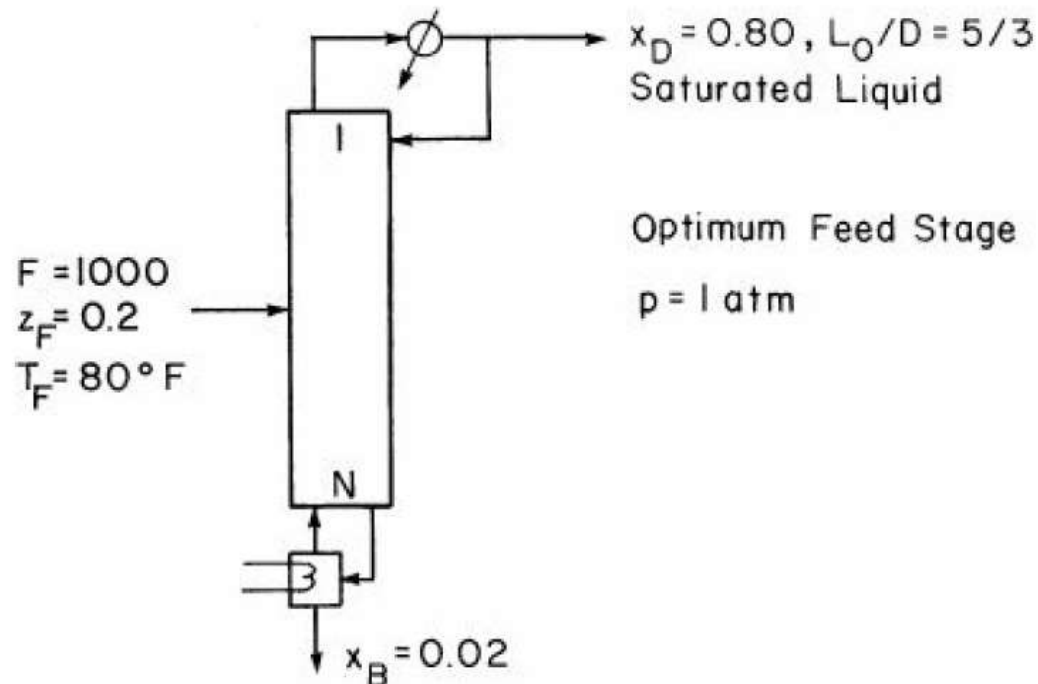
	V/V _{fl} =	0,2	0,3	0,4	0,5	0,6	0,7	0,8
	d _p , mm							
Raschig rings	13	109	137	154	161	161	153	134
(ceramics)	25	85	99	99	99	95	85	68
	38	124	140	144	144	144	144	144
	50	166	185	189	189	189	189	189
Raschig rings	13	41	51	57	60	60	57	50
(metal)	25	49	57	57	57	55	49	39
	38	72	81	83	83	83	83	83
	50	96	107	109	109	109	109	109
Berl saddles	13	29	37	42	46	48	50	51
(ceramics)	25	37	46	50	50	50	50	50
	38	53	60	63	64	64	64	64
Pall rings	13	51	64	72	75	75	71	62
(metal)	25	60	69	69	69	67	60	47
	38	87	98	101	101	101	101	101
	50	124	137	141	141	141	141	141

Example: distillation in a packed column

- ◆ We wish to repeat the example (distillation of ethanol and water) done with McCabe Thiele method except that a column packed with 2-inch metal Pall rings will be used.
- ◆ Previous example data: 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.

Example: distillation in a packed column

- ◆ Same data and specification as in the previous example.
- ◆ Further data:
 - Use a vapor flow rate that is nominally 75% of flooding.
 - in the enriching section $HG = 0.4054$ m and $HL = 0.253$ m
 - in the stripping section $HG = 0.2835$ m and $HL = 0.1067$ m

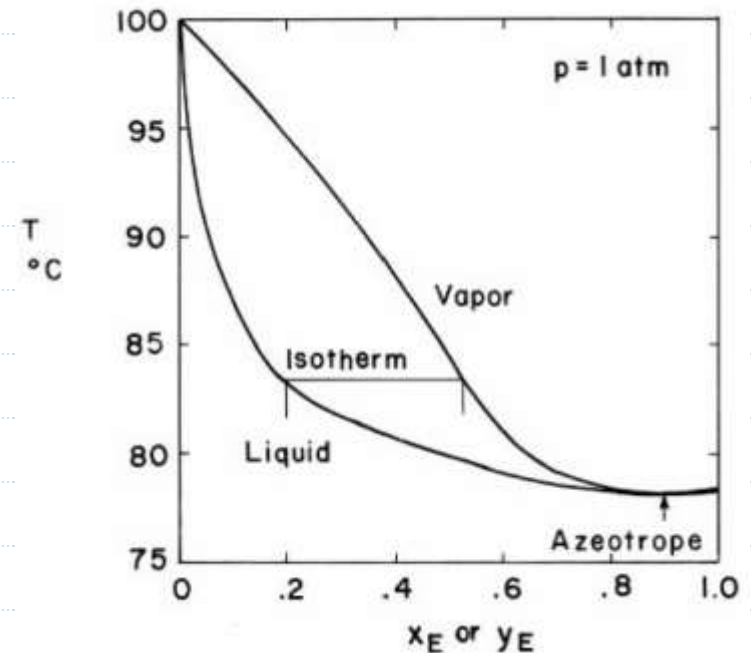
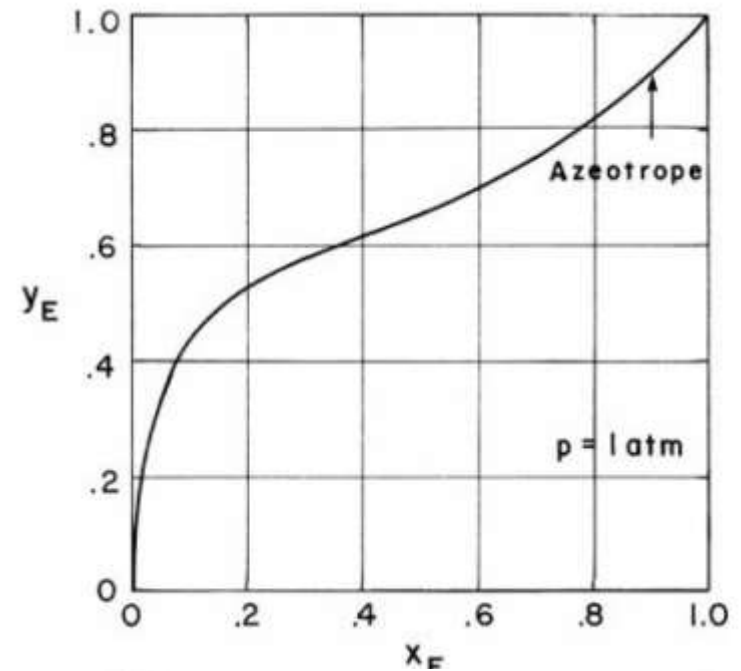


Example

◆ Equilibrium data

x_{EtOH}	x_w	y_{EtOH}	y_w	$T, ^\circ C$
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: distillation in a packed column

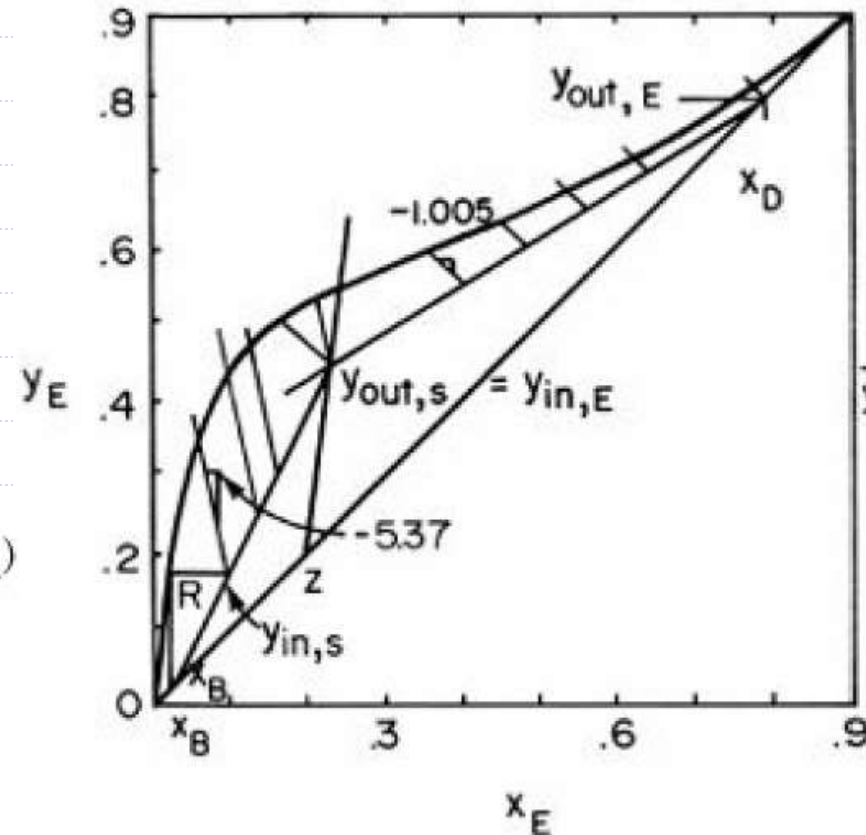
◆ Solution

- The equilibrium and operating lines are plotted in the following figure.
- In the *stripping* section, slope of the OL is ($L/V=2.04$ from mass balance)

$$\text{slope} = -\frac{L}{V} \frac{H_G}{H_L} = -2.04 \frac{0.2835}{0.1067} = -5.37$$

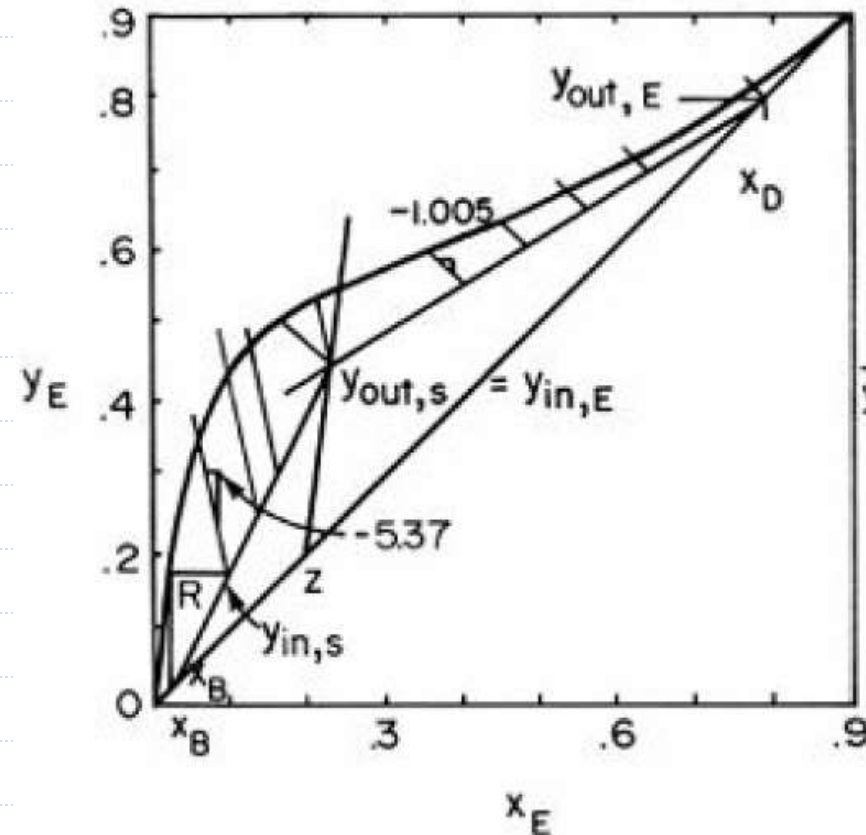
- Lines with a slope = -5.37 are drawn from arbitrary points on the stripping section operating line to the equilibrium curve.
- Values of y_A are on the operating line, while y_{AI} values are on the equilibrium line.
- Table with values:

y_{AI}	y_A	$y_{AI} - y_A$	$1/(y_{AI} - y_A)$
0.354	0.17	0.184	5.44
0.44	0.25	0.19	5.26
0.477	0.306	0.171	5.85
0.512	0.375	0.137	7.30
0.535	0.442	0.093	10.75



Example: distillation in a packed column

- A plot can easily be constructed with $(1/(y_{A1}-y_A))$ vs. y_A curve.
- The area under the curve from $y_{A,in,S} = 0.17$ to $y_{A,out,S} = 0.442$ can be estimated.
- $y_{A,in,S}$ is the vapor mole fraction leaving the partial reboiler.
- Determination of $y_{A,in,S}$ is shown in Figure.
- $y_{A,out,S}$ is the vapor mole fraction at the intersection of the operating lines.
- The area in Figure B can be estimated by Simpson's rule.
- $n_{G,S} = 1.79$
- $h_S = H_{G,S} * n_{G,S}$
- $h_S = 0.507$ m



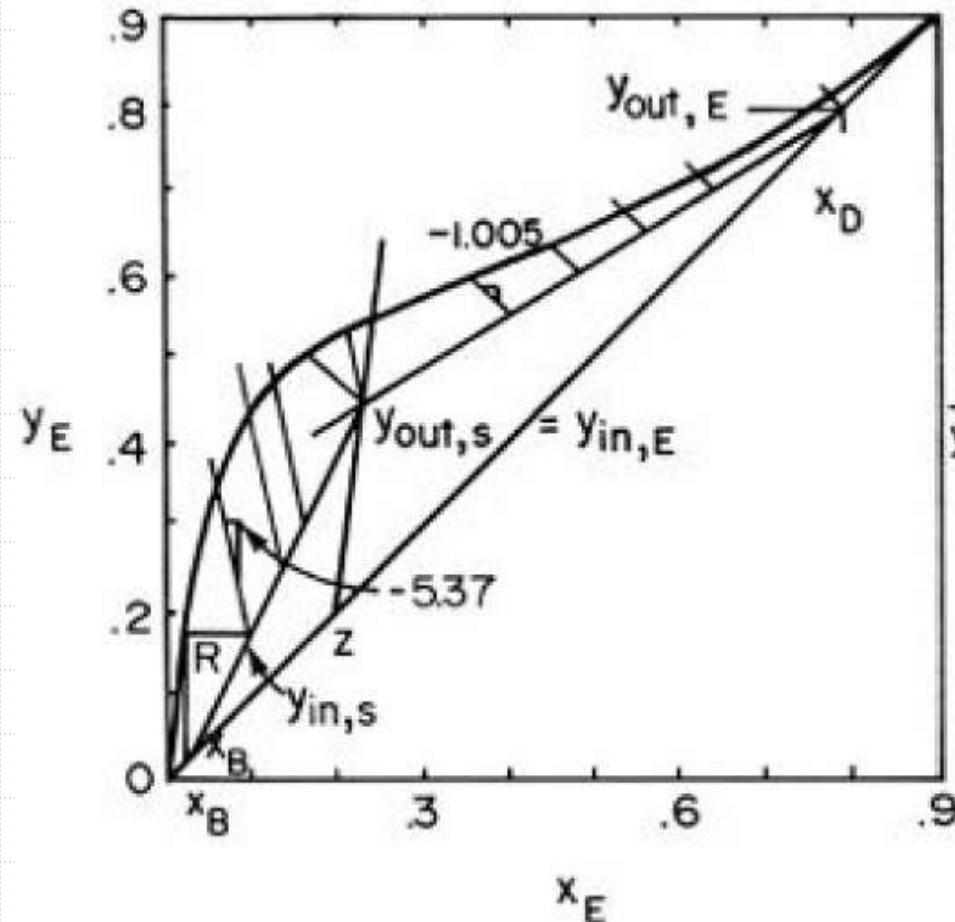
Example: distillation in a packed column

- In the *enriching* section, slope of the OL is ($L/V=2.04$ from mass balance)

- $slope = -\frac{L}{V} \frac{H_G}{H_L} = -5/8 \frac{0.4054}{0.253} = -1.005$

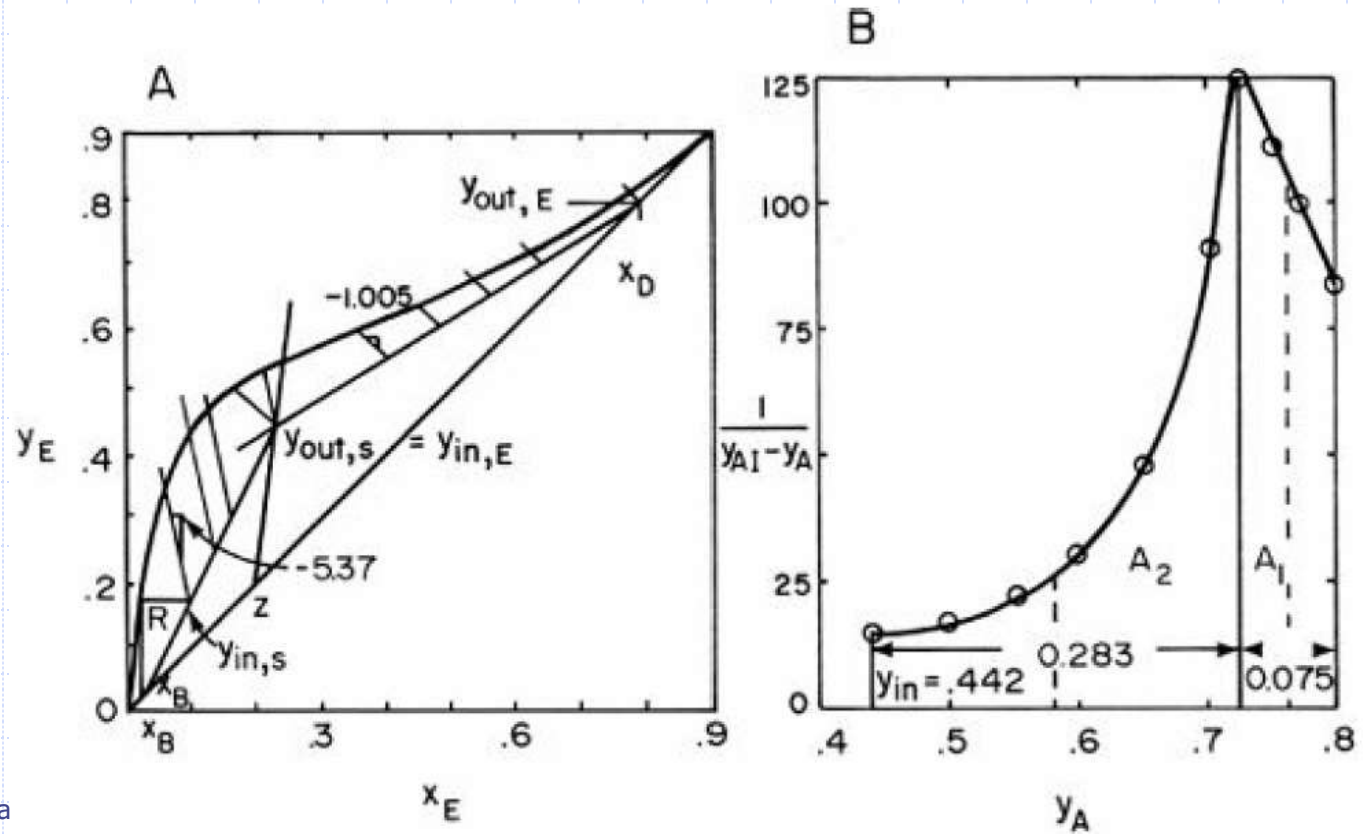
- Lines with a slope = -1.005 are drawn from arbitrary points on the enriching section operating line to the equilibrium curve.
- Values of y_A are on the operating line, while y_{AI} values are on the equilibrium line.
- Table with values:

y_{AI}	y_A	$y_{AI} - y_A$	$1/(y_{AI} - y_A)$
0.505	0.442	0.063	15.9
0.557	0.5	0.057	17.5
0.594	0.55	0.044	22.7
0.632	0.60	0.032	31.25
0.671	0.65	0.021	47.6
0.711	0.7	0.011	90.9
0.733	0.725	0.008	125
0.759	0.75	0.009	111.1
0.785	0.775	0.01	100
0.812	0.8	0.012	83.3



Example: distillation in a packed column

- The plot B shows the $(1/(y_{A1}-y_A))$ vs. y_A curve for enriching section.
- The area under the curve from $y_{A,in,E} = 0.442$ to $y_{A,out,E} = 0.8$.
- $y_{A,out,E}$ is the vapor mole fraction leaving the condenser.
- $y_{A,in,E} = y_{A,out,S}$ is the vapor mole fraction at the intersection of the OL.
- The area in Figure B can be estimated by Simpson's rule.
- $n_{G,E} = 19.6$
- $h_E = H_{G,E} * n_{G,E}$
- $h_E = 7.95$ m



Tray columnn vs. packed columns

	Tray column	Random packed columnn	Structured packed column
HETP	0.75 m	1-1.25 m	0.2 m
$\Delta P/Z$	200 mmH ₂ O/m	70 mmH ₂ O/m	5-10 mmH ₂ O/m
or $\Delta P/NETP$	150 mmH ₂ O/N _{id}	40 mmH ₂ O/N _{id}	3-5 mmH ₂ O/N _{id}
Wetting	No problem	Bad (10-20 m ³ m ⁻² h ⁻¹)	Good (0.2 m ³ m ⁻² h ⁻¹)
Capital costs	€€	€	€€€€€
Corrosion	No	Yes	Yes
Foaming	No	Yes	Yes
Suspended solids	Yes	No	No
Liquid hold-up	High	Low	Low

◆ Tray columns are preferred when

- The process generates high quantity of heat, that must be removed
- High vapor flow rates and low liquid flow rates are involved
- Side streams and multiple feeds are present

What is provided by popular Process Simulators?

◆ For Tray Columns:

- Many methods for the design and rating of tray diameter
- the possibility for the user to provide plate efficiency values

◆ For Packed Columns:

- many methods for the design and rating of column diameter
- no methods for calculating the column height (except in special programs such as RATEFRAC®)
- common use of the concept HETP=height equivalent of a theoretical plate → which is indeed an old and misleading approach

Example: packed column design with Radfrac

- ◆ We wish to distill 80.0 mol/s of a feed at 25°C and 15.0 atm.
- ◆ The feed is 0.100 mole fraction ethane, 0.300 mole fraction propane, 0.500 mole fraction n-butane, and 0.100 mole fraction n-pentane.
- ◆ The column operates at 15.0 atm, has a partial condenser, and produces a vapor distillate.
- ◆ A kettle type reboiler is used.
- ◆ Use equilibrium column calculation and design packed column internals with pall rings
- ◆ Specifications:
 - Max. n-C4 mole fraction in the vapor distillate of $y_{D,C4,max} = 0.00875$
 - Max. C3 mole fraction in the liquid bottoms of $x_{Bot,C3,max} = 0.005833$.

Example: packed column design with Radfrac

Setup



Internals

Status: Active

Column description: Input Complete

Buttons: Add New, Auto Section, Duplicate, Import Template, Export Template, View Internals Summary

Name	Start Stage	End Stage	Mode	Internal Type	Tray/Packing Type	Tray Details		Packing Details		
						Number of Passes	Number of Downcomers	Vendor	Material	Dimension
CS-1	2	15	Rating	Packed	PALL			MTL	METAL	0.625-IN OR
CS-2	16	34	Rating	Packed	PALL			MTL	METAL	0.625-IN OR

Options:

- Don't update pressure drop
- Update pressure drop from top stage
- Update pressure drop from bottom stage
- Include static vapor head in pressure drop calculations
- Calculate pressure drop across sump

Sump

- Diameter: 2.34009 meter
- Liquid residence time: 0.0156667 hr
- Liquid level: meter

Example: packed column design with Radfrac

◆ Hydraulic plots

