Problem 1: Membrane gas separation (30p)

A mixed gas feed stream contains 50% of gas A and 50% of gas B. These two gases should be separated in a membrane separator. Gas A is the gas that permits the fastest, while gas B is the most valuable gas we want as clean as possible. This can be, for example, biogas, in other words: A = CO_2 and B = CH_4).

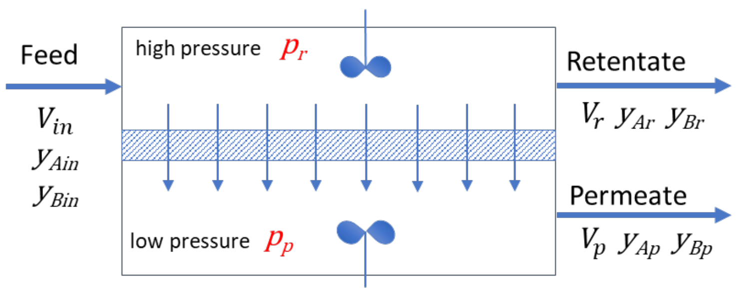
The following information is provided about the system:

Feed stream	$V_{in} = 2$ m^3(STP) / min	
Feed pressure	$p_r = 10$ bar	
Permeate pressure	$p_p = 1$ bar	1 bar = 76 cm Hg
Volumetric stage cut	$\theta = 0{,}53$	
Membrane thickness	$L = 10^{-6}$ m	
Permeability of A	$P_A = 400$ Barrer	1 Barrer = 10^{-10} cm^3(STP).cm/(s.cm^2.cm Hg)
Selectivity P_A/P_B	$\alpha = 30$	

The process can be described by the following equations assuming ideal mixing model:

- «transfer rate equation»
- «operating line» $$y_{Ap} = \frac{y_{Ain} - y_{Ar}(1-\theta)}{\theta}$$
- «volumetric flux equation»

a) Draw a sketch of the process with descriptions of all streams. Explain the ideal mixing model, where do the equations come from and what do they describe. **4p**



Ideal mixing model assumes that the fluid is completely mixed which means that there is no concentration gradient along the membrane from the entrance of the feed stream to the outlet. In addition, ideal gas behavior is assumed and no resistance for mass transfer in the gas phases. The only mass transfer resistance is the membrane.

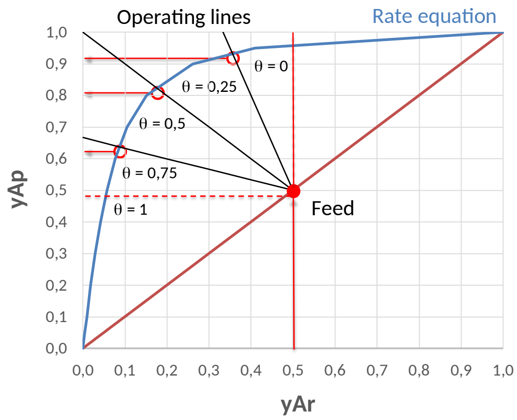
The provided equations:

- The operating line is a re-formulated balance equation combined with the definition of stage cut.
- The rate equation is a combination of the kinetic relations describing the fluxes of component A and B through the membrane respectively. The rate equation relates the molar fractions in retentate and permeate based on the membrane parameters and the driving force.
- The flux equation describes the rate of mass transfer through the membrane.

b) Calculate the minimum concentration of component A in the retentate stream that we can obtain. How clean would gas B be in this case? **5p**

The minimum concentration of A in retentate will be achieved in the limiting case of stage cut

$\theta = 1$ when $y_{Ap} = y_{Ain} = 0{,}5$



Using the transfer rate equation:

$$y_{Ar} = \frac{\left[\frac{p_p}{p_r}\left(1 - y_{Ap}\right)\left(\alpha - 1\right) + 1\right] y_{Ap}}{\alpha - \left(\alpha - 1\right) y_{Ap}}$$

Substituting the given information into the equation:

$y_{Ar} = ¿¿$

For gas B then:

$$y_{Br} = 1 - y_{Ar} = 1 - 0.079 = 0.921$$

c) Suppose that the concentration of A in the retentate that we are able to achieve for the system is 25% higher than the one you calculated under b). What is then the composition of the permeate stream? How much of component B (give the answer in%) do we lose with the permeate stream? **10p**

The real molar fraction of A in the retentate will be:

$$y_{Ar}=1.25\,y_{Ar}\,calculated \in part\,b¿$$

$$y_{Ar}=0.099$$

From the volumetric stage cut definition:

$$\theta=\frac{\dot{V}_p}{\dot{V}_{¿}}$$

by separating variable *Vp*:

$$\dot{V}_p=(0.53)\left(2\frac{m^3(STP)}{min}\right)=1.06\frac{m^3(STP)}{min}$$

Assuming ideal gases:

$$\dot{V}_{¿}=\dot{V}_r+\dot{V}_p$$

Therefore:

$$\dot{V}_r=\dot{V}_{¿}-\dot{V}_p=2.00\frac{m^3(STP)}{min}-1.06\frac{m^3(STP)}{min}=0.94\frac{m^3(STP)}{min}$$

Using the operating line for calculation of the real molar composition of A in the permeate stream:

$$y_{Ap}=\frac{y_{Ain}-y_{Ar}(1-\theta)}{\theta}=\frac{0.5-0.0988(1-0.53)}{0.53}=0.856$$

Gas B in permeate and assuming ideal gases:

$$\dot{V}_{Bp}=\dot{V}_p\,y_{Bp}=\dot{V}_p(1-y_{Ap})=1.06\frac{m^3(STP)}{min}*(1-0.856)=0.153\frac{m^3(STP)}{min}$$

The volumetric flow of gas B in the inlet is:

$$\dot{V}_{Bin}=\dot{V}_{¿}*y_{Bin}=2\frac{m^3(STP)}{min}*0.5=1.0\frac{m^3(STP)}{min}$$

The % of B lost is given by:

$$\% \, of \, B \, lost = \frac{\dot{V}_{Bp}}{\dot{V}_{Bin}} * 100 = \frac{0.153 \frac{m^3(STP)}{min}}{1.0 \frac{m^3(STP)}{min}} * 100 = 15.3 \% \, of \, B \, lost$$

d) How large membrane area is needed in order to perform this separation? **5p**

Using the volumetric flux equation:

$$J_{AV} = \frac{\dot{V}_{Ap}}{A} = \left(\frac{P_A}{L}\right)(p_r y_{Ar} - p_p y_{Ap})$$

where the volumetric flow of component A in the permeate stream could be calculated as:

$$\dot{V}_{Ap} = \dot{V}_p y_{Ap} = \theta \dot{V}_{¿} y_{Ap} = (0.53)\left(2 \frac{m^3(STP)}{min}\right)(0.856) = 0.907 \frac{m^3(STP)}{min}$$

and manipulating the equation and substituting the corresponding values in proper units (!):

$$A = \frac{\dot{V}_{Ap}}{\left(\frac{P_A}{L}\right)(p_r y_{Ar} - p_p y_{Ap})} = \frac{0.907 \frac{m^3(STP)}{min} * \left(\frac{1 \, min}{60 \, s}\right)\left(\frac{10^6 \, cm^3}{1 \, m^3}\right)}{¿¿}$$

The necessary membrane area is

$A = 374 \, m^2$

Problem 2: Adsorption (12p)

Water vapor should be removed from N_2 gas in a packed column at 28 °C using a molecular sieve. The height of the column is 0.3 m and the bulk density of the particles is 712.8 kg/m^3. The initial concentration of water in the particles in the column is 0.01 kg H_2O/kg particles and the mass velocity of the N_2 gas is 4052 kg/(m^2.h). Water concentration in the gas at inlet is $c_0 = 926 \times 10^{-6}$ kg H_2O/kg N_2. The break through data for the mass transfer zone is given in the table below. A value for $c/c_0 = 0.02$ is assumed to be the "break point".

time *t* [h]	0	9.0	9.2	9.6	10.0	10.4	10.8	11.3	11.5	12.0	12.5	12.8
Concentration *c* [kg H_2O/kgN_2 x 10^{-6}]	<0.6	0.6	2.6	21	91	235	418	630	717	855	906	926

a) Draw a typical break-through curve c/c_0 as a function of time. Describe the axes and explain the different points and areas in the figure. **4p**

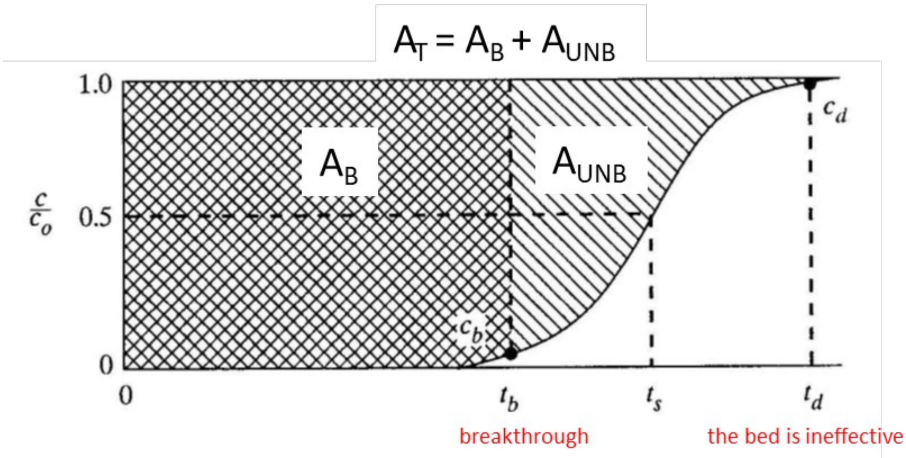


FIGURE 12.3-2. *Determination of capacity of column from breakthrough curve.*

- A_B is the used adsorption capacity of the column.
- A_{UNB} is the unused adsorption section of the column.
- t_b is the breakthrough or break point from which onwards the outlet concentration will exceed the required specified value
- t_d is the time when the adsorption bed is not adsorbing anything more and the outlet stream compositions are the same as the inlet stream compositions.

b) Explain which physical processes influence the shape of the curve? **4p**

The shape of the concentration profile will be affected by several simultaneous physical processes:

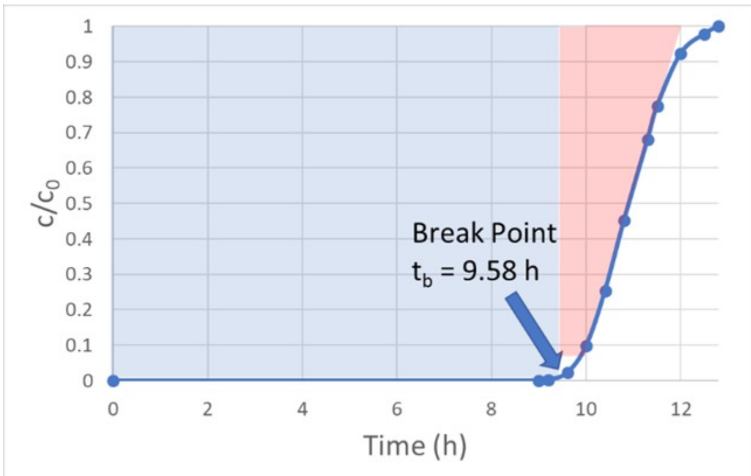
- adsorption equilibria = adsorption isotherm

- flow regime
- mass transfer a
- diffusion from the bulk to the surface
- diffusion in the pores
- possibly also surface diffusion

c) Determine the time needed to reach the "break point" t_b, and the height of the unused column H_{UB} assuming the following relationship for the ratio between the height of the used column H_B and the total height of the column H_T: **6p**

$$\frac{H_B}{H_T}=\frac{t_b}{t_{tot}}$$

time t [h]	Concentration c [kg H2O/kgN2 x 10-6]	c/c0
0	0	0
9	0.6	0.0006
9.2	**2.6**	**0.0028**
9.6	**21**	**0.0227**
10	91	0.0983
10.4	235	0.2538
10.8	418	0.4514
11.3	630	0.6803
11.5	717	0.7743
12	855	0.9233
12.5	906	0.9784
12.8	926	1



The breakthrough point time is between 9.2 and 9.6 hours

By interpolation: $t_b = 9.58\,h$

The area under the profile up to the break point is $A_B = t_b \cdot 1$

The time interval between the breakthrough point t_b and the time when the column is fully saturated t_d is $t_d - t_b = 12.8 - 9.58 = 3.22\,h$

This is the time interval when the profile is S-shaped. The S-shape is symmetrical so that the area bellow the curve between t_b and t_d (triangular shape in pink) can be estimated as ½ of the rectangular area given by $(t_d - t_b) \cdot 1$.

$$A_{UNB} = \frac{(t_d - t_b) \cdot 1}{2}$$

$$A_T = A_B + A_{UNB} = t_b \cdot 1 + \frac{(t_d - t_b) \cdot 1}{2}$$

or we can approximate the total area by a rectangular shape given by

$$A_T = t_{tot} \cdot 1$$

So that t_{tot} will be

$$t_{tot} = t_s = t_b + \frac{t_d - t_b}{2} = 9.58 + \frac{3.22}{2} = 11.19\,h$$

Then from the given relation:

$$H_B = \frac{t_b}{t_{tot}} H_T = \frac{9.58\,h}{11.19\,h} * 0.30\,m = 0.257\,m$$

The total height of the column is the used plus the unused bed:

$$H_T = H_B + H_{UNB}$$

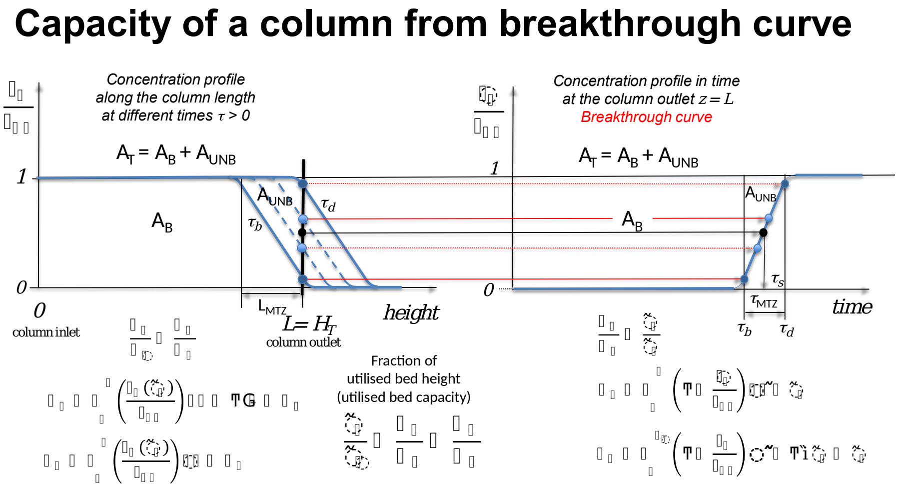
$$H_{UNB} = H_T - H_B$$

$$H_{UNB} = 0.30\,m - 0.257\,m = 0.043\,m$$

OR directly from the area ratio

$$\frac{A_{UNB}}{A_T} H_T = H_{UNB} = \frac{1.61}{11.19} \cdot 0.3 = 0.043$$

d) Explain how the ratio used under c is deduced from the break-through curve? **4p**



How the ratio between the utilized bed height and the total bed height is related to the ratio between the area corresponding to utilized bed and the total area could be seen from the concentration profiles along the column at breakthrough time τ_b and at full saturation of the column $\tau_{d.}$

The figure above illustrates how these "spacial" concentration profiles (on the left-hand side) are linked to the concentration time profile at the outlet of the column (on the right-hand side) where the later are the type of data we usually have available. The areas under the outlet concentration time profile up to the time t_b and the time t_d will the correspond to the utilized bed area and total bed are respectively.