

Membrane processes

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Lecture 12

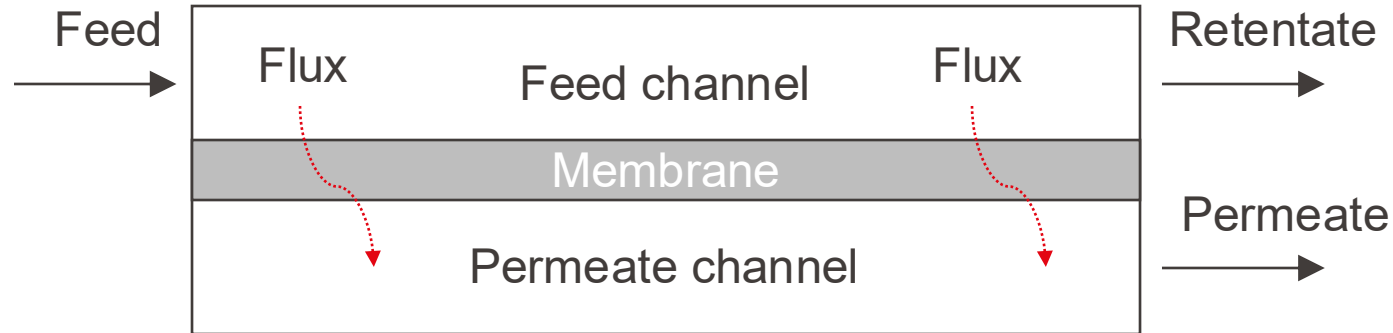
21.05.2025

Reference book: Membrane Technology and Applications, R. W. Baker, Wiley 2012 (3rd ed.)

THEORY

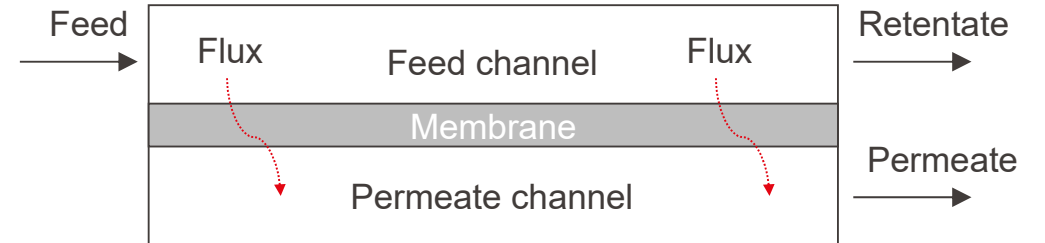
- What is a membrane stage?
- How to calculate transmembrane flux?
- How to model a membrane stage?
- How to design multi-stage processes?
- How to implement the model for membrane process?

Part 1



- ✓ **Driving force:** gradient of pressure, concentration or chemical potential that drives the trans-membrane flux from the feed to the permeate channel;
- ✓ **Membrane permeance:** measure of the flux of a component through the membrane for a given driving force;
- ✓ **Membrane selectivity:** ratio between the permeance of two components;
- ✓ **Product recovery:** ratio between the content of the product in the permeate stream and the content in the feed stream;
- ✓ **Product purity:** concentration of the product in the outlet permeate stream.

Overall balances on the membrane stage



- Total mass balance

$$Q_f = Q_r + Q_p$$

- Mass balance for component i

$$X_{i,f} Q_f = X_{i,r} Q_r + X_{i,p} Q_p$$

$$\sum X_{i,f} = \sum X_{i,r} = \sum X_{i,p} = 1$$

- Total mass balance on the feed channel

$$Q_f = Q_r + \int_0^A J \, dA$$

- Mass balance for component i on the feed channel

$$X_{i,f} Q_f = X_{i,r} Q_r + \int_0^A J_i \, dA$$

$$\sum J_i = J$$

How do we
calculate J ?

Dense membranes

Flux driven by the concentration gradient

Transport based on solution-diffusion

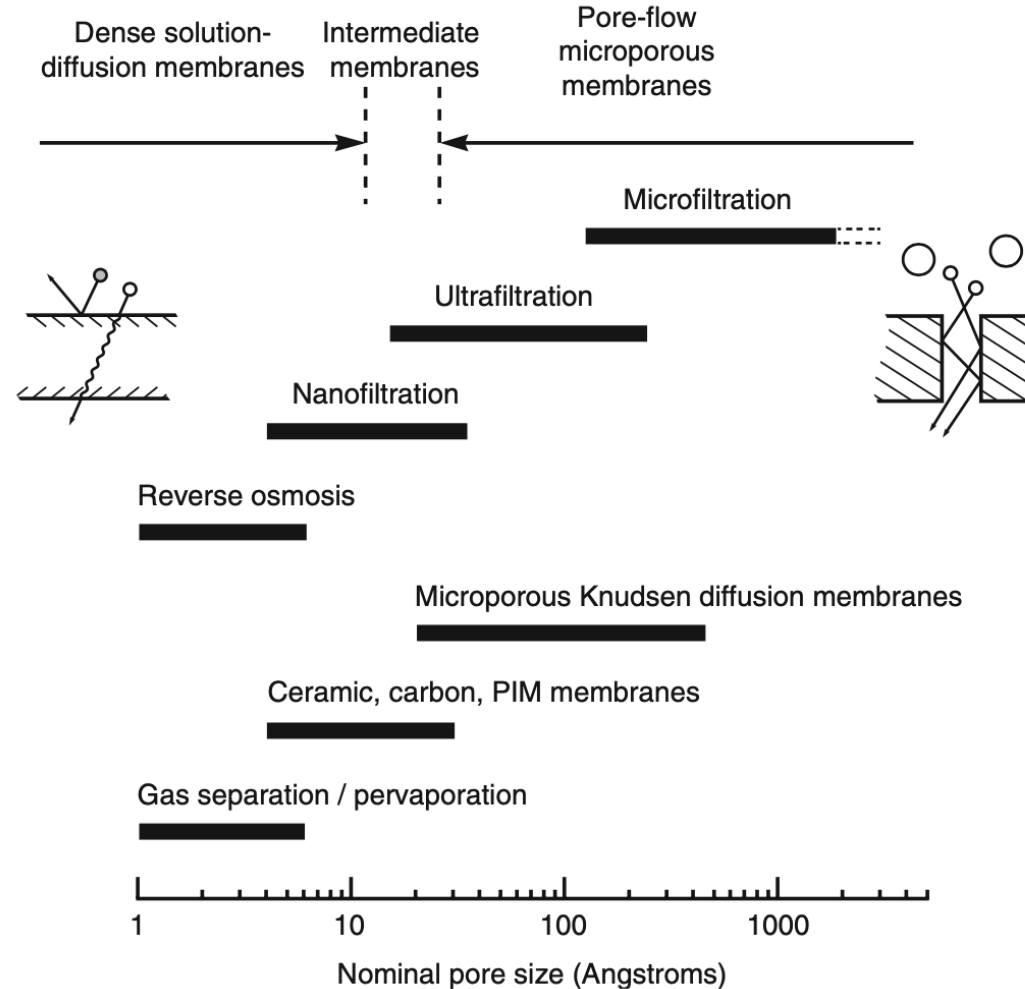
Selectivity based on solubility and diffusivity

Porous membranes

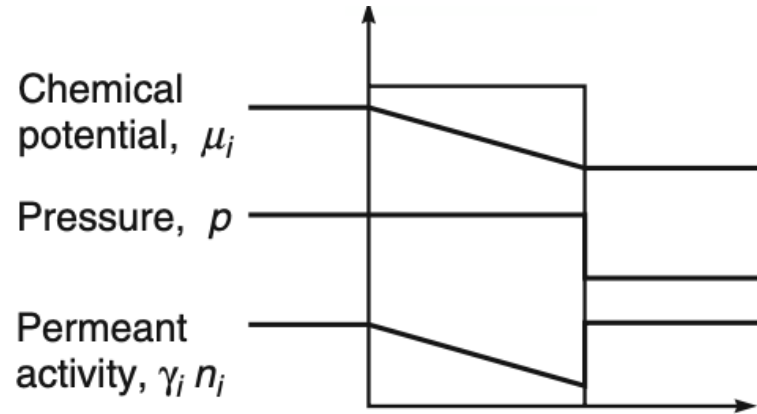
Flux driven by the total pressure gradient

Transport based on viscous flow and diffusion

Selectivity based on pore size



Flux from solution-diffusion model in gas separation



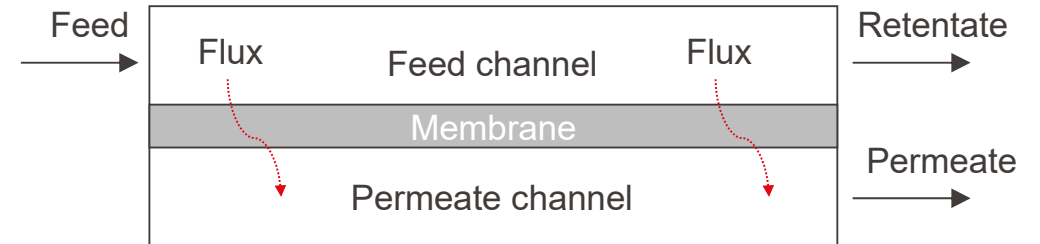
$$J_i = \frac{D_i K_{i,G}}{\delta} (p_{i,feed} - p_{i,perm}) = \frac{\bar{N}_i}{\delta} (p_{i,feed} - p_{i,perm})$$

Permeability coefficient given by the product of diffusivity D_i and sorption coefficient $K_{i,G}$

Well-mixed system

$$J_i = \frac{\bar{N}_i}{\delta} (p_{i,ret} - p_{i,perm})$$
$$= N_i (P_{ret} X_{i,ret} - P_{perm} X_{i,perm})$$

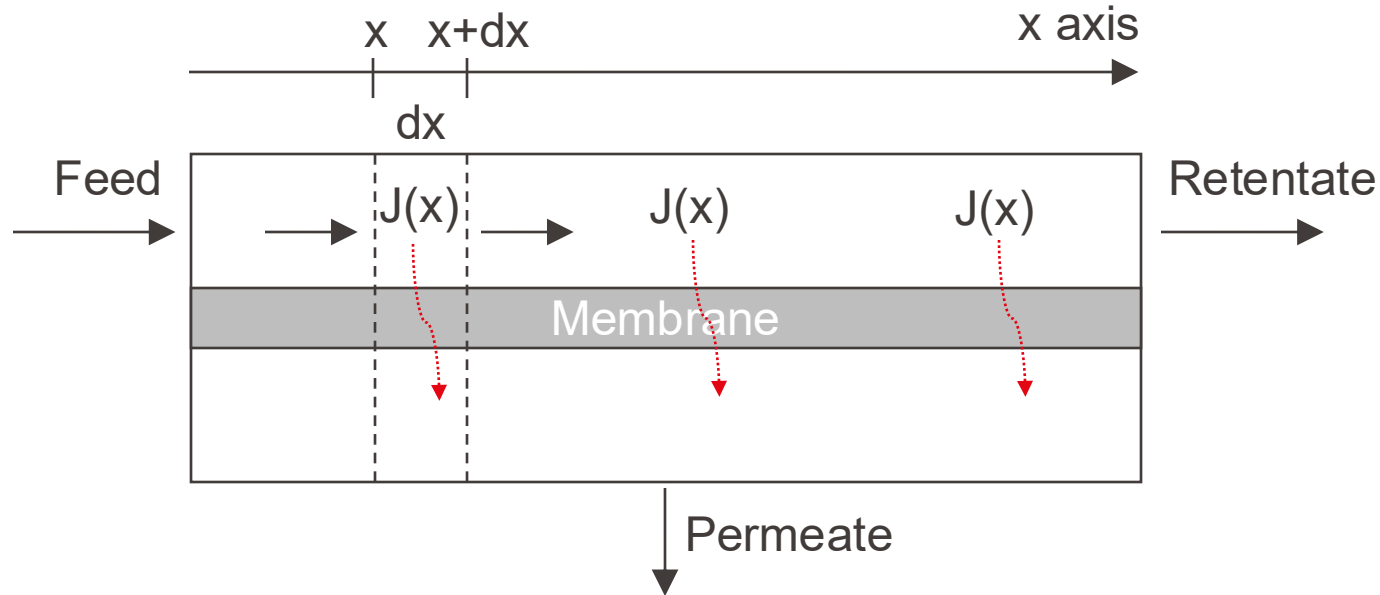
$$J = \sum_{components} J_i$$



Modelling a membrane module

1-dimensional model: discretization along the direction of the feed stream (x axis)

Cross-current flow arrangement



Assumptions

- No variation along the width
- Permeance independent of X
- Negligible pressure drops
- Isothermal process
- No mixing in permeate channel

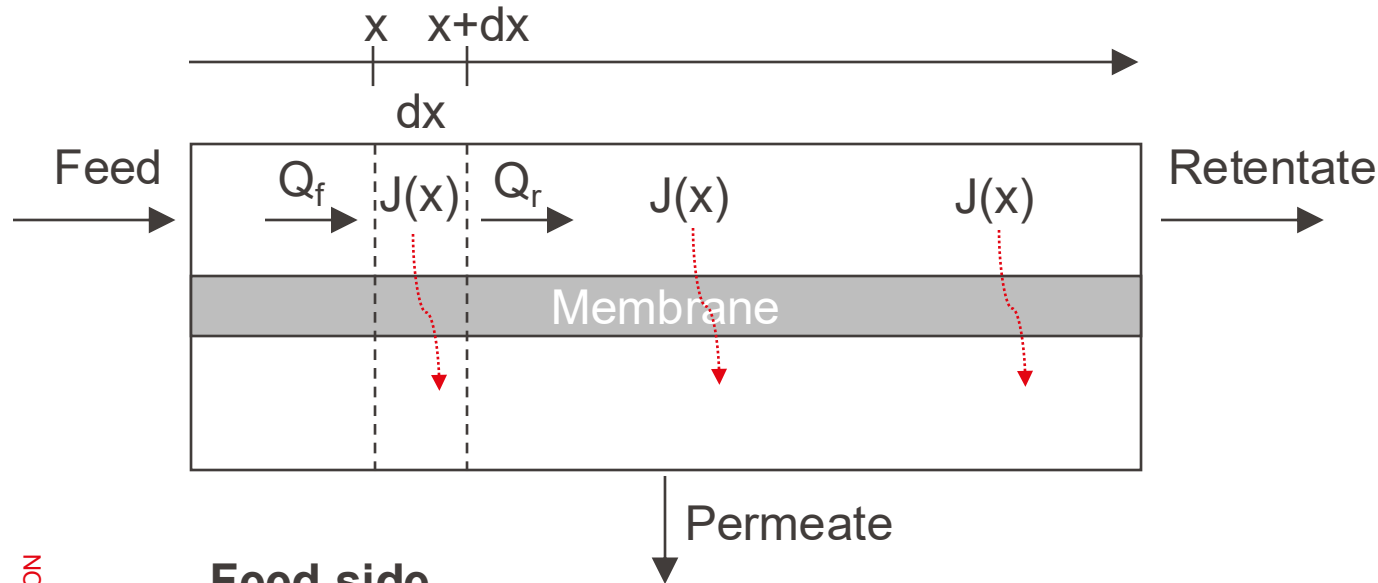
$$J_i(x) = \frac{\bar{N}_i \left(p_{i,feed}(x) - p_{i,perm}(x) \right)}{\delta} = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,perm}(x) \right)$$

$$J(x) = \sum_{components} J_i(x)$$

Modelling a membrane module

1-dimensional model: discretization along the direction of the feed stream (x-axis)

Cross-current flow arrangement



Feed side

$$Q_r(x) = Q_f(x) - J(x) dA$$

$$X_{i,r}(x) Q_r(x) = X_{i,f}(x) Q_f(x) - J_i(x) dA$$

$$Q_f(x + dx) = Q_r(x)$$

$$X_{i,f}(x + dx) = X_{i,r}(x)$$

$$J_i(x) = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,perm}(x) \right)$$

$$J(x) = \sum_{components} J_i(x)$$

Permeate side

$$Q_{p,out} = Q_{feed} - Q_{r,out}$$

$$X_{i,p,out} Q_{p,out} = X_{i,feed} Q_{feed} - X_{i,r,out} Q_{r,out}$$

$$1 \quad J_{CO_2}(x) = N_{CO_2} (P_{feed} X_{CO_2,feed}(x) - P_{perm} X_{CO_2,perm}(x))$$

$$X_{N_2,perm}(x) = 1 - X_{CO_2,perm}(x) \quad X_{N_2,feed}(x) = 1 - X_{CO_2,feed}(x)$$

$$2 \quad J_{N_2}(x) = N_{N_2} (P_{feed} (1 - X_{CO_2,feed}(x)) - P_{perm} (1 - X_{CO_2,perm}(x)))$$

$$3 \quad J_{TOT}(x) = J_{CO_2}(x) + J_{N_2}(x)$$

$$4 \quad J_{TOT}(x) = J_{CO_2}(x) / X_{CO_2,perm}(x)$$

α selectivity

β pressure ratio: P_{perm}/P_{feed}

$$X_{CO_2,perm}(x) = \frac{1 + (\alpha - 1) (\beta + X_{CO_2,feed}(x)) - \sqrt{[1 + (\alpha - 1) (\beta + X_{CO_2,feed}(x))]^2 - 4\alpha\beta(\alpha - 1) X_{CO_2,feed}(x)}}}{2\beta(\alpha - 1)}$$

Modelling a membrane module

Equation	N equation
$J_i(x) = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,perm}(x) \right)$	$N_{components} \times N_{elem}$
$J(x) = \sum_{components} J_i(x)$	N_{elem}
$J_i(x) = J(x) X_{i,perm}(x)$	$N_{components} \times N_{elem}$
$Q_r(x) = Q_f(x) - J(x) dA$	N_{elem}
$X_{i,r}(x) Q_r(x) = X_{i,f}(x) Q_f(x) - J_i(x) dA$	$N_{components} \times N_{elem}$
$Q_{p,out} = Q_{feed} - Q_{r,out}$	1
$X_{i,p,out} Q_{p,out} = X_{i,feed} Q_{feed} - X_{i,r,out} Q_{r,out}$	$N_{components}$
$Q_f(x + dx) = Q_r(x)$	$N_{elem} - 1$
$X_{i,f}(x + dx) = X_{i,r}(x)$	$N_{components} \times (N_{elem} - 1)$
$Q_f(0) = Q_{feed}$	1
$X_{i,f}(0) = X_{i,feed}$	$N_{components}$
	total: $4 N_{components} \times N_{elem} + 3 N_{elem} + N_{components} + 1$

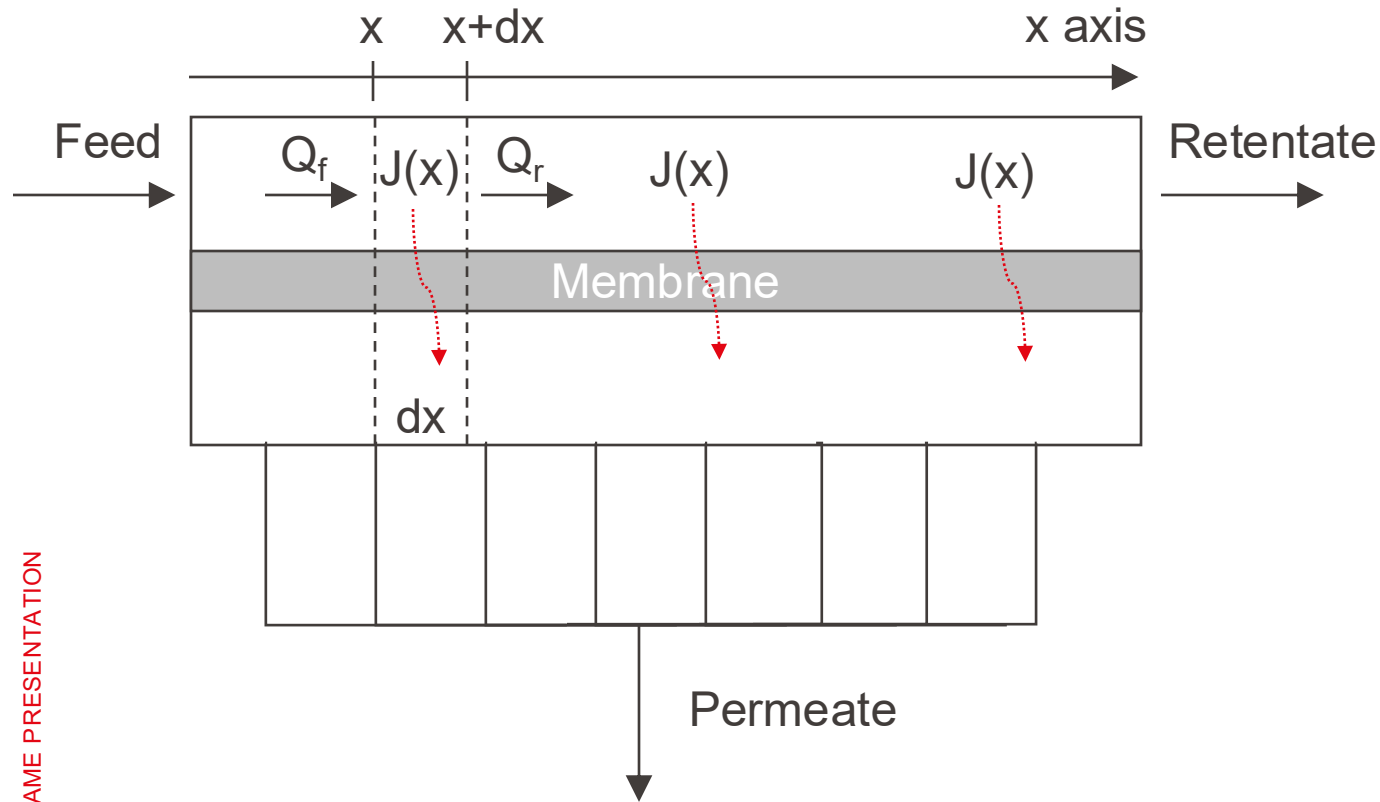
Variable	N variable
$J_i(x)$	$N_{components} \times N_{elem}$
$J(x)$	N_{elem}
$X_{i,perm}(x)$	$N_{components} \times N_{elem}$
$Q_r(x)$	N_{elem}
$X_{i,r}(x)$	$N_{components} \times N_{elem}$
$Q_{p,out}$	1
$X_{i,p,out}$	$N_{components}$
$Q_f(x)$	N_{elem}
$X_{i,f}(x)$	$N_{components} \times N_{elem}$
	total: $4 N_{components} \times N_{elem} + 3 N_{elem} + N_{components} + 1$

For given P_{feed} , P_{perm} and A

$$N_{equations} = N_{variables}$$

Part 2

Cross-current flow arrangement



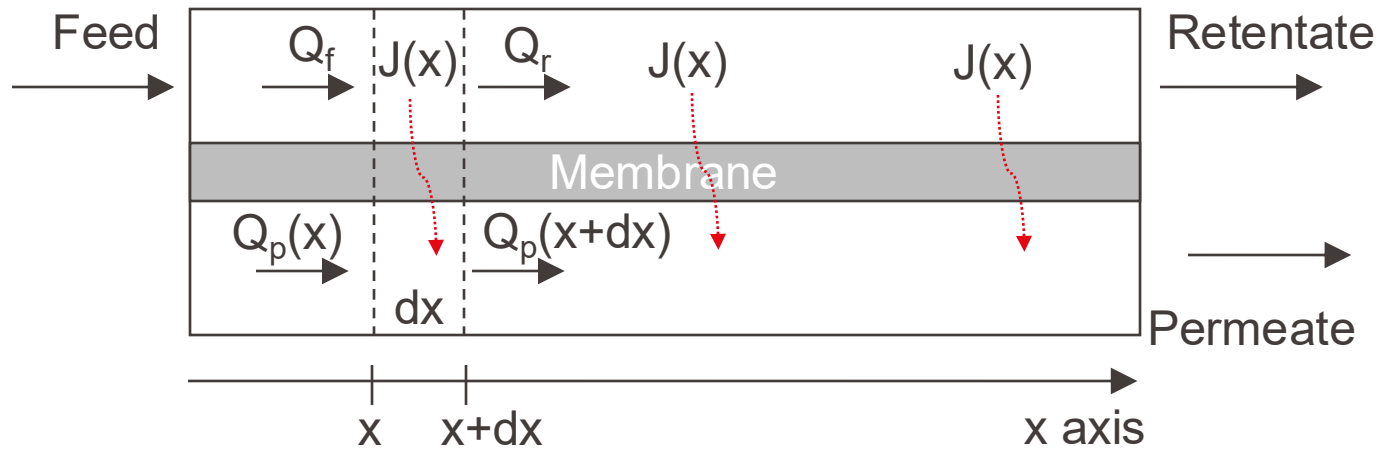
No mixing in the permeate channel

$$J_i(x) = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,perm}(x) \right)$$

$$Q_{p,out} = \sum_{x=0}^L J(x) dA$$

$$X_{i,p,out} = \frac{\sum_{x=0}^L J_i(x) dA}{Q_{p,out}}$$

Co-current flow arrangement



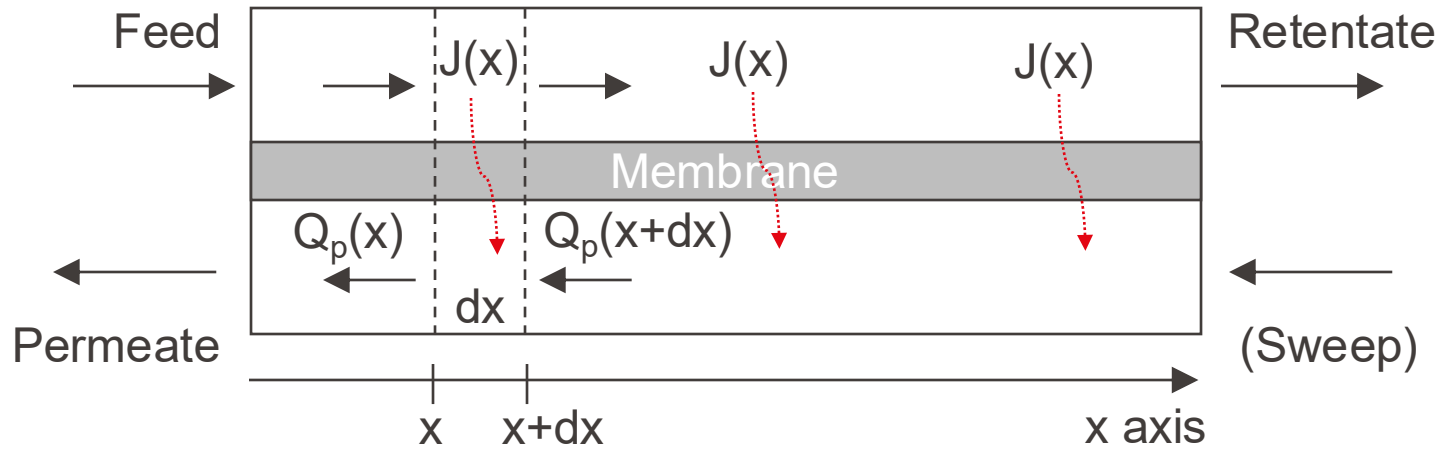
$$J_i(x) = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,p}(x) \right)$$

Permeate side

$$Q_p(x + dx) = Q_p(x) + J(x) dA$$

$$X_{i,p}(x + dx) Q_p(x + dx) = X_{i,p}(x) Q_p(x) + J_i(x) dA$$

Counter-current flow arrangement



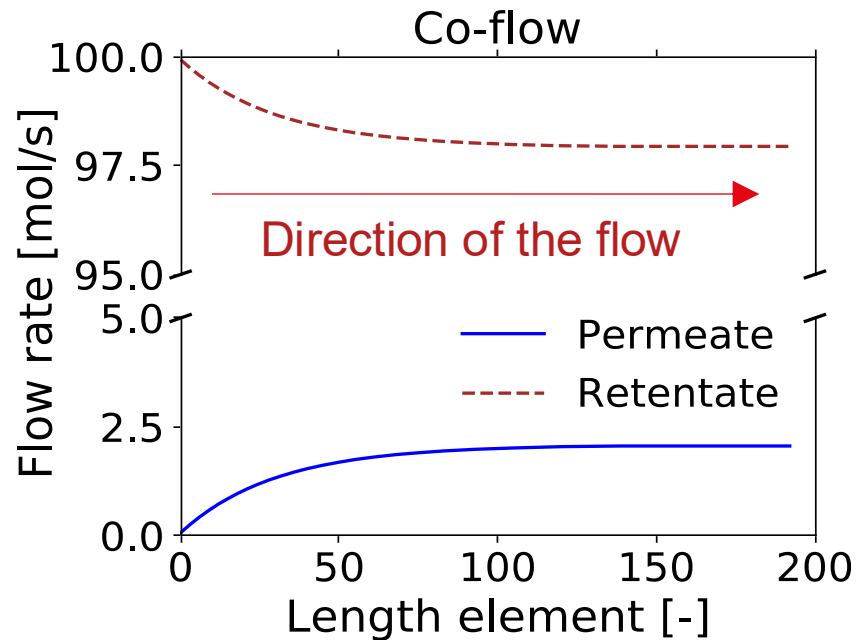
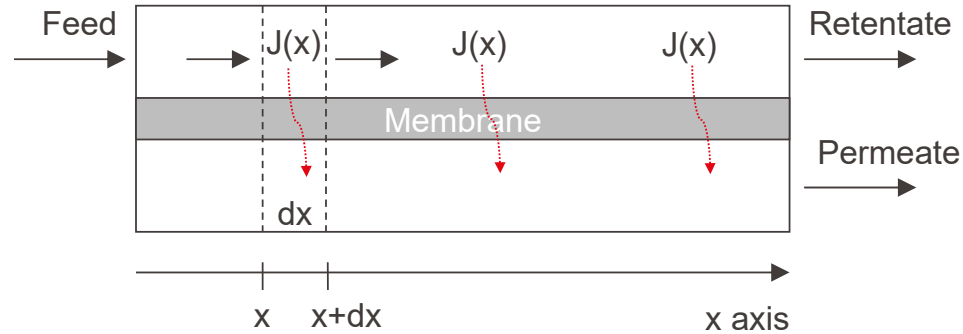
$$J_i(x) = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,p}(x) \right)$$

Permeate side

$$Q_p(x) = Q_p(x + dx) + J(x) dA$$

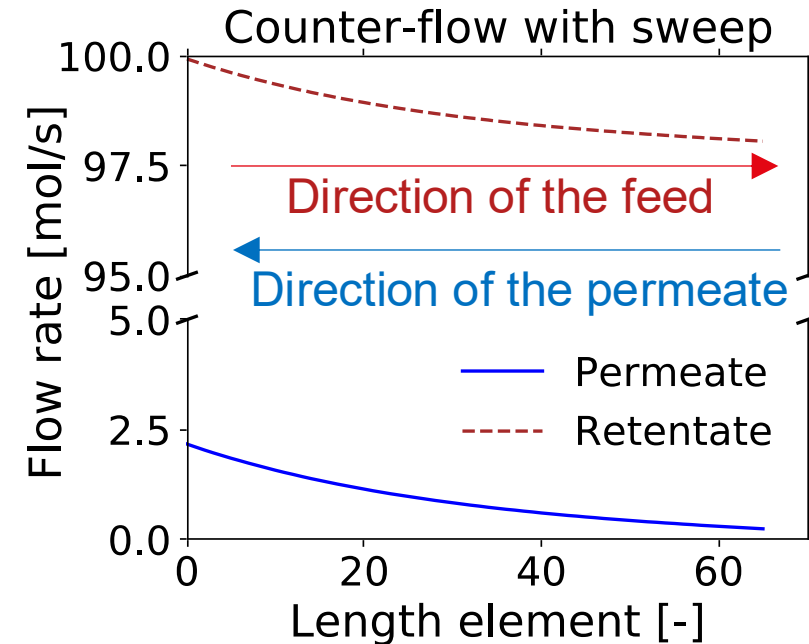
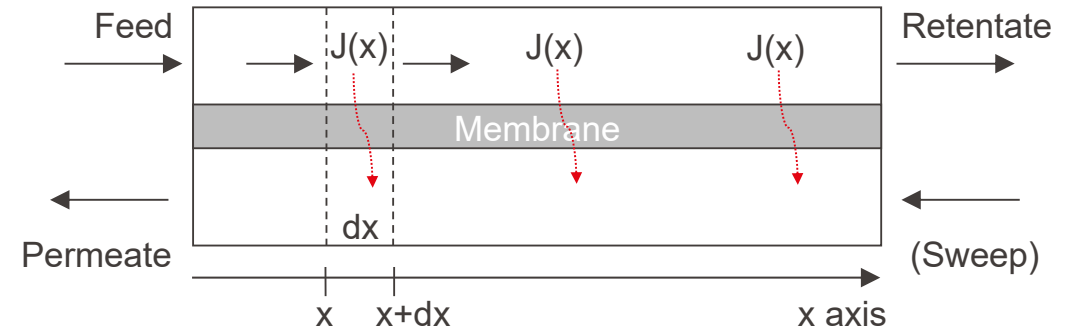
$$X_{i,p}(x) Q_p(x) = X_{i,p}(x + dx) Q_p(x + dx) + J_i(x) dA$$

Co-current flow arrangement



■ Reduced driving force along the length

Counter-current flow arrangement



Almost constant driving force along the length

To achieve purity and recovery > 90% with one module, one would need very high permeance and selectivity & very high driving force (high P_{feed} , low P_{perm})

$$J_i(x) = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,perm}(x) \right) > 0 \text{ if } \frac{P_{feed}}{P_{perm}} > \frac{X_{i,perm}}{X_{i,feed}} \quad \text{Max separation limited by pressure ratio}$$

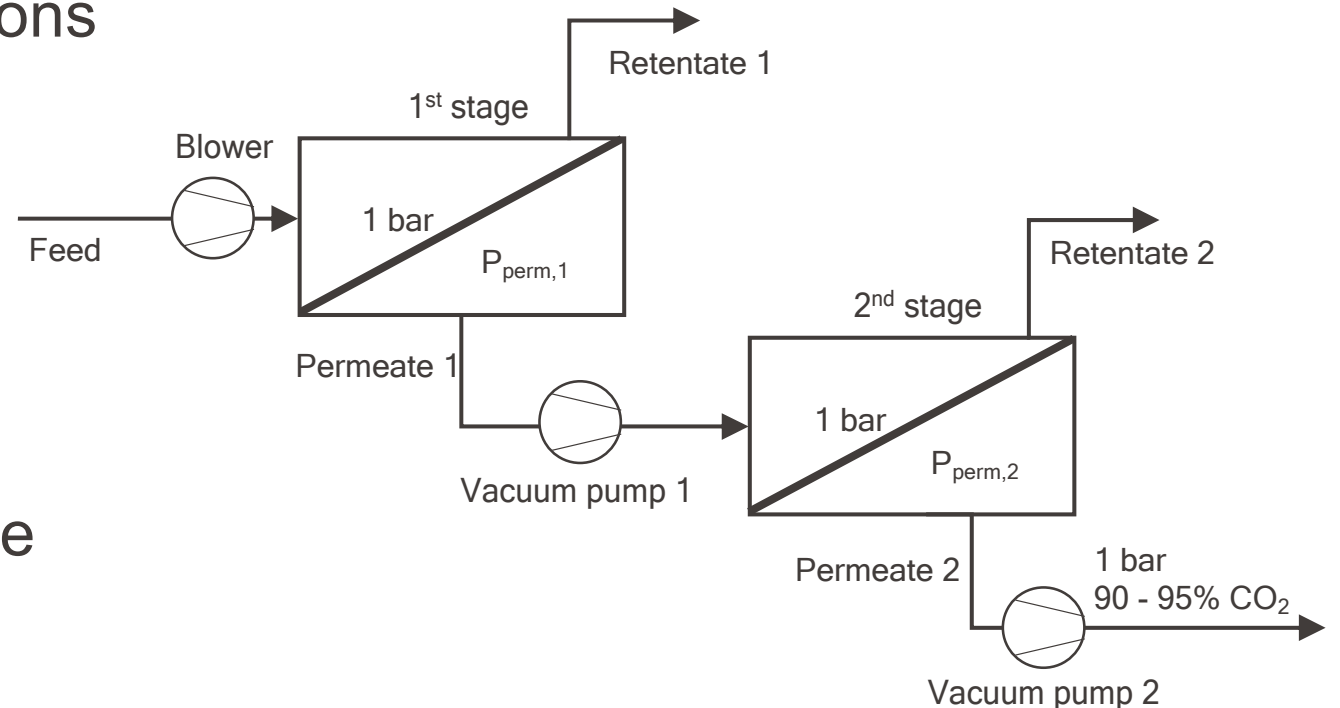
Alternative: multi-stage configurations

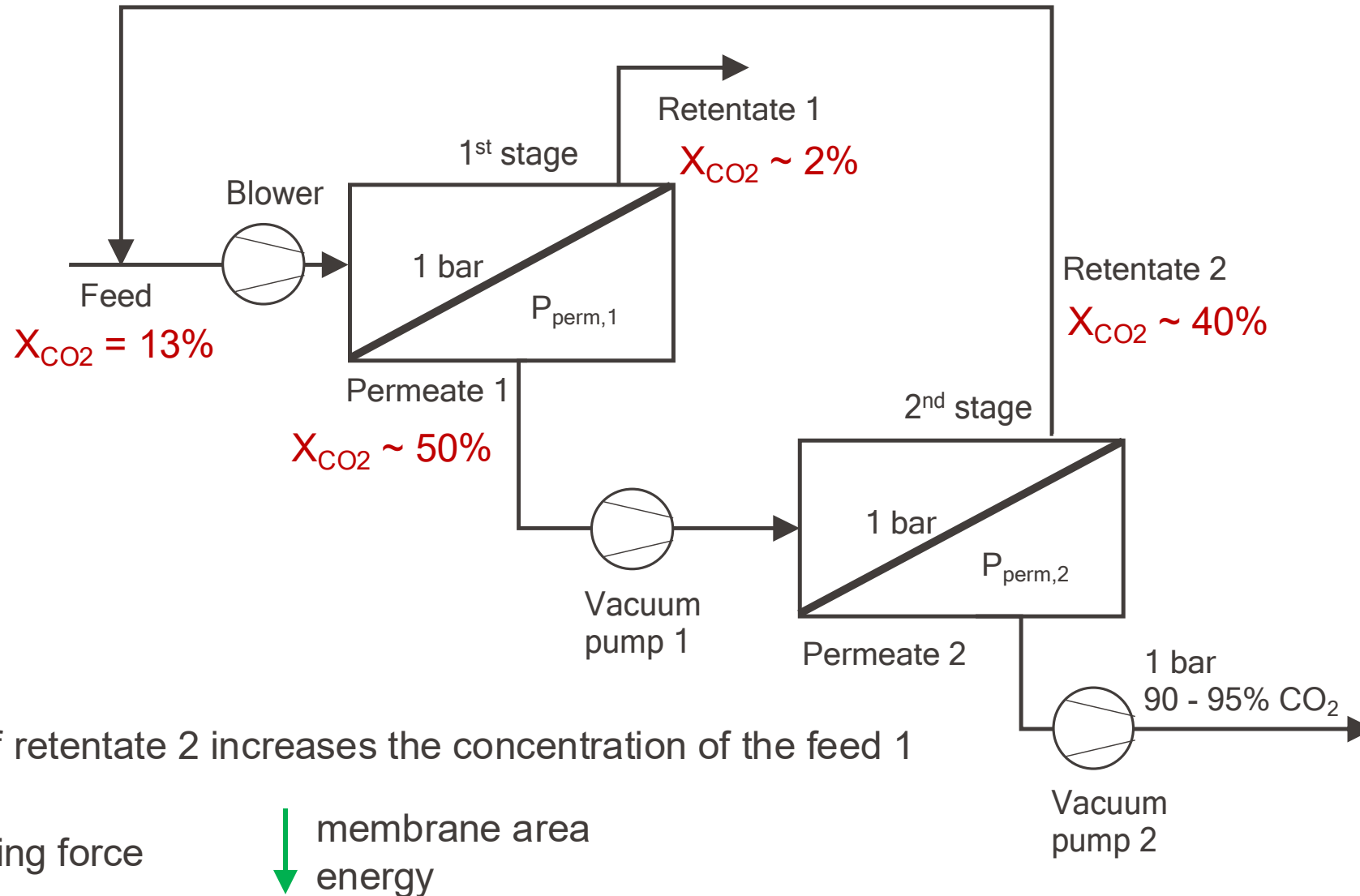
$$Q_{feed,2} = Q_{perm,1}$$

$$X_{CO_2,feed,2} = X_{CO_2,perm,1}$$



Higher driving force in the 2nd stage





Part 3

- How to model a membrane stage?
- How to design multi-stage processes?
- Results at variable membrane **permeance and selectivity**
- Results at variable **feed concentration and flow rate**
- Results at variable **feed and permeate pressure**
- Results at variable **membrane areas**



next lecture

Building the model for a single-stage process

Inputs:

- feed concentration
- feed flow rate
- feed pressure
- permeate pressure
- membrane area

Parameters:

- membrane permeance
- membrane selectivity
- physical properties
- geometrical properties

class single stage



method solver:

- flux definition
- total flux definition
- mass balance on the retentate
- mass balance on the permeate
- next element feed definition

Outputs:

- permeate concentration
- permeate flow rate
- retentate concentration
- retentate flow rate

$$J_i(x) = N_i \left(P_{feed} X_{i,feed}(x) - P_{perm} X_{i,perm}(x) \right)$$

$$J(x) = \sum_{components} J_i(x)$$

$$Q_r(x) = Q_f(x) - J(x) dA$$

$$Q_{P,out} = Q_{feed} - Q_{r,out}$$

$$Q_f(x+1) = Q_r(x)$$

Building the model for a double-stage process

Inputs:

- feed concentration
- feed flow rate
- feed pressure (1 and 2)
- permeate pressure (1 and 2)
- membrane area (1 and 2)

Parameters:

- membrane permeance
- membrane selectivity
- physical properties
- geometrical properties

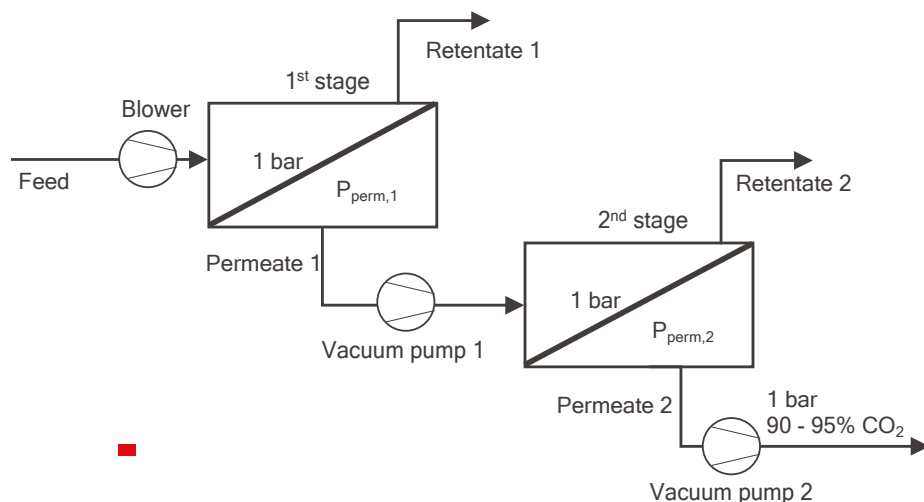
class double stage

Outputs:

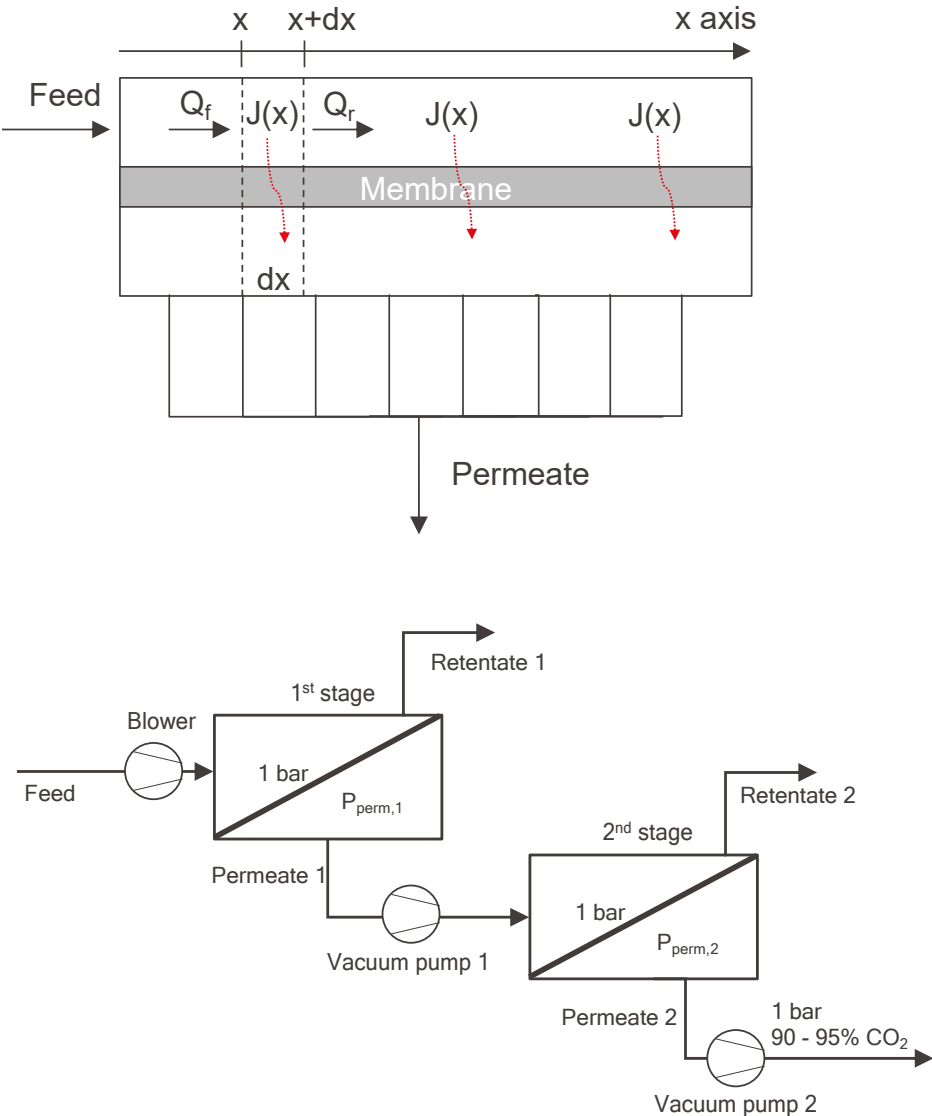
- permeate concentration (1 and 2)
- permeate flow rate (1 and 2)
- retentate concentration (1 and 2)
- retentate flow rate (1 and 2)

method solver:

- def stage 1 as ***class*** single stage (inputs stage 1, parameters stage 1)
- def feed stage 2 = permeate stage 1
- def stage 2 as ***class*** single stage (inputs stage 2, parameters stage 2)



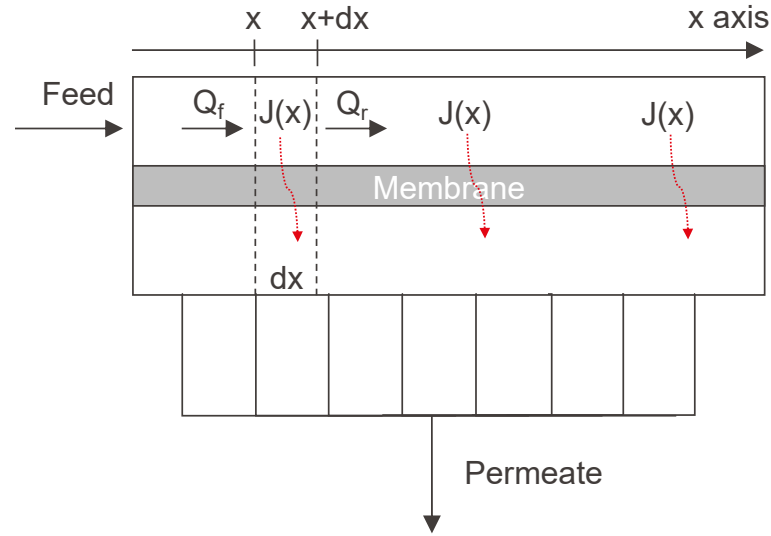
Simulations - inputs



P_{feed}	1 bar
P_{permeate}	0.1 bar
$X_{\text{feed,CO2}}$	0.1
Q_{feed}	2.5 mol/s
A_{membrane}	10 m ²
CO ₂ Permeance	10000 GPU
CO ₂ /N ₂ Selectivity	30

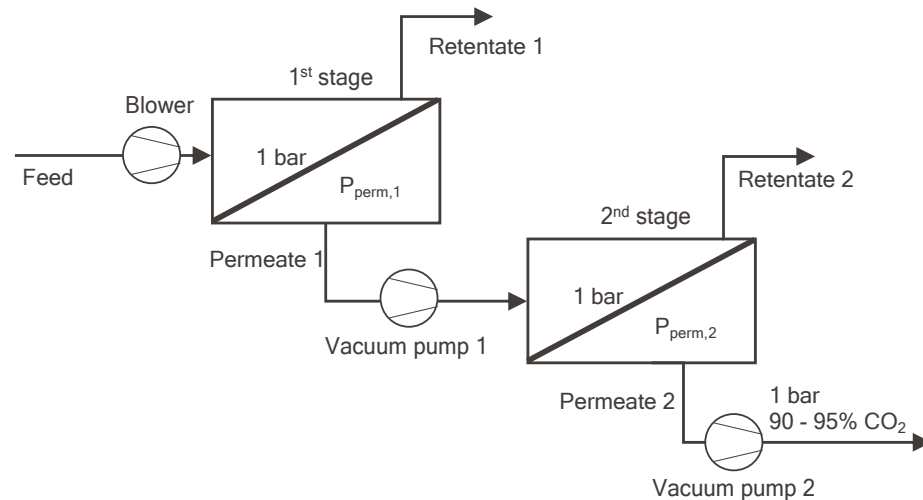
P_{feed}	1 bar
$P_{\text{permeate,1}}$	0.1 bar
$P_{\text{permeate,2}}$	0.2 bar
$X_{\text{feed,CO2}}$	0.1
Q_{feed}	2.5 mol/s
$A_{\text{membrane,1}}$	10 m ²
$A_{\text{membrane,2}}$	5 m ²
CO ₂ Permeance	10000 GPU
CO ₂ /N ₂ Selectivity	30

Simulations - outputs



$$Purity = X_{CO_2,p,out}$$

$$Recovery = \frac{Q_{P,out} X_{CO_2,p,out}}{Q_{feed,in} X_{CO_2,feed,in}}$$



$$Purity = X_{CO_2,p,out,stage2}$$

$$Recovery = \frac{Q_{P,out,stage2} X_{CO_2,p,out,stage2}}{Q_{feed,in} X_{CO_2,feed,in}}$$