

Application to reverse osmosis

$$J_r = \frac{\Theta K_s}{l} \left(\frac{C_{r,osm} - C_{r,ret}}{l} \right) = \frac{\Theta K_s}{l} \left\{ C_{r,s} - C_{r,p} \exp \left[\frac{-\tilde{F}_r (p_h - p_r)}{RT} \right] \right\}$$

$$\frac{\Theta K_s}{l} \gg \frac{\Theta K_s}{l} \quad (\text{selective membrane})$$

$$0 = J_r = \frac{\Theta K_s}{l} \left\{ C_{r,s} - C_{r,p} \exp \left[\frac{-\tilde{F}_r \cdot \Delta \Pi}{RT} \right] \right\} \Rightarrow C_{r,s} = C_{r,p} \exp \left[\frac{-\tilde{F}_r \cdot \Delta \Pi}{RT} \right]$$

$$J_r = \frac{\Theta K_s C_{r,s}}{l} \left\{ 1 - \exp \left[\frac{-\tilde{F}_r (\Delta p - \Delta \Pi)}{RT} \right] \right\} \approx \frac{\Theta K_s C_{r,s}}{l} \frac{\tilde{F}_r (\Delta p - \Delta \Pi)}{RT}$$

$$J_r = \frac{\Theta K_s (\Delta p - \Delta \Pi)}{l} \quad A: \text{Permeability of water}$$

$$J_r = \frac{\Theta K_s}{l} \left\{ C_{r,s} - C_{r,p} \exp \left[\frac{-\tilde{F}_r \cdot \Delta p}{RT} \right] \right\} \approx \frac{\Theta K_s}{l} (C_{r,s} - C_{r,p})$$

$$J_r = B_r (\Delta c_r) \quad B: \text{Permeability of solute}$$

Application to reverse osmosis

Equilibrium at the downstream interface:

$$H_{r,osm} = H_{r,p}$$

$$\mu_r^* + RT \ln(\gamma_{r,osm} \tilde{x}_{r,osm}) = \mu_r^* + RT \ln(\gamma_{r,p} \tilde{x}_{r,p}) + \tilde{F}_r (p_r - p_{r,osm})$$

$$\ln(\gamma_{r,p} \tilde{x}_{r,p}) = \ln(\gamma_{r,osm} \tilde{x}_{r,osm}) + \frac{\tilde{F}_r}{RT} (\tilde{F}_r (p_r - p_{r,osm}))$$

$$\gamma_{r,p} \tilde{x}_{r,p} = (\gamma_{r,osm} \tilde{x}_{r,osm}) \exp \left[\frac{\tilde{F}_r (p_r - p_{r,osm})}{RT} \right]$$

$$K_r = \frac{\gamma_{r,p}}{\gamma_{r,osm}} \frac{p_r}{p_{r,osm}}$$

$$C_{r,osm} = K_r C_{r,p} \exp \left[\frac{-\tilde{F}_r (p_h - p_r)}{RT} \right]$$

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Application to reverse osmosis

Equilibrium at the upstream interface:

$$H_{r,s} = H_{r,osm}$$

$$\mu_r^* + RT \ln(\gamma_{r,s} \tilde{x}_{r,s}) + \tilde{F}_r (p_h - p_{r,osm}) = \mu_r^* + RT \ln(\gamma_{r,osm} \tilde{x}_{r,osm}) + \tilde{F}_r (p_h - p_{r,osm})$$

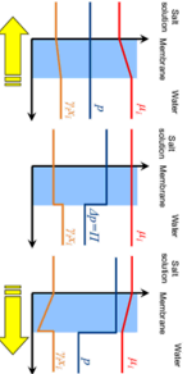
$$\tilde{x}_{r,s} = \frac{\gamma_{r,osm}}{\gamma_{r,s}} \tilde{x}_{r,osm}$$

$$c_r = \tilde{x}_r M \tilde{\rho} \Rightarrow c_{r,osm} = \frac{\gamma_{r,s}}{\gamma_{r,osm}} \frac{\tilde{\rho}_s}{\tilde{\rho}_{osm}} c_s = K_r c_s$$

$$K_r = \frac{\gamma_{r,s}}{\gamma_{r,osm}} \frac{\tilde{\rho}_s}{\tilde{\rho}_{osm}} \quad \text{The sorption coefficient}$$

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Application to reverse osmosis



Osmosis

Equilibrium

Reverse osmosis

Friction coefficient in a pipe

The friction coefficient f_r is defined as:

$$F = A_r \tilde{\tau}_r \cdot f_r$$

- F : the frictional force

- A_r : wetted area

- E_r : the kinetic energy per volume

In a pipe, we have:

$$F = (\pi \cdot DL) \left(\frac{1}{2} \rho v^2 \right) \cdot f_r = (-\Delta p) \left(\frac{\pi}{4} D^2 \right) \Rightarrow (-\Delta p) = 2 f_r \rho v^2 \frac{L}{D}$$

With f_r the Fanning's coefficient of friction (different from the Blasius' coefficient of friction f_D) $f_r = 4 f_D$

$$f_r = \frac{16}{Re} \quad \text{Poiseuille regime}$$

Re: Laminar regime

$$\frac{1}{f_r} = -4.0 \log_{10} \left(\frac{K' D}{3.7} + \frac{1.26}{Re \sqrt{f_r}} \right)$$

Colbrook, turbulent regime

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Pore-flow model

- Permeate flux calculation
- Porous membrane
- Particles or macromolecules are retained by a sieve effect
- Two situations

Screen filtration

Depth filtration



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Application to gas permeation

Equilibrium at the upstream interface:

$$H_{g,s} = H_{g,osm}$$

$$\mu_g^* + RT \ln(\gamma_{g,s} \tilde{x}_{g,s}) + \tilde{F}_g (p_h - p_{g,osm}) = \mu_g^* + RT \ln(\gamma_{g,osm} \tilde{x}_{g,osm}) + \tilde{F}_g (p_h - p_{g,osm})$$

$$\tilde{x}_{g,s} = \frac{\gamma_{g,osm}}{\gamma_{g,s}} \frac{p_{g,osm}}{p_{g,s}} \exp \left[\frac{-\tilde{F}_g (p_h - p_{g,osm})}{RT} \right] \approx \frac{\gamma_{g,osm}}{\gamma_{g,s}} \frac{p_{g,osm}}{p_{g,s}} = \frac{\gamma_{g,osm}}{\gamma_{g,s}} \frac{p_{g,osm}}{p_{g,s}}$$

$$c_g = \tilde{x}_g M \tilde{\rho} \Rightarrow c_{g,osm} = M \tilde{\rho}_s \frac{\gamma_{g,osm}}{\gamma_{g,s}} \frac{p_{g,osm}}{p_{g,s}} = K_g p_{g,s}$$

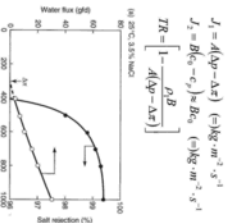
$$K_g = \frac{\gamma_{g,osm}}{\gamma_{g,s}} \frac{M \tilde{\rho}_s}{p_{g,s}} \quad \text{The sorption coefficient}$$

Equilibrium at the downstream interface: $c_{g,ret} = K_g p_{g,p}$

$$J_g = \frac{\Theta (C_{g,osm} - C_{g,ret})}{l} = \frac{\Theta K_g (p_{g,s} - p_{g,p})}{l} = \frac{P_g (p_{g,s} - p_{g,p})}{l}$$

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Application to reverse osmosis



Characterization: Water flux = 20-120 g/h (NaCl = 3.5%)
Castero et al. (1989)

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The Darcy's law

- Use of the Ergun's equation where the turbulent term is negligible

$$\frac{(-\Delta p)}{\rho u_0} \cdot \frac{d_p}{L} \cdot \frac{e^3}{1-e} = \text{Re} = \frac{150 (1-e)}{\rho u_0} \cdot \frac{d_p}{L}$$

$$u_0 = \frac{\mu L}{\rho u_0} \cdot \frac{d_p^2}{e^3} \cdot \frac{1}{1-e}$$

$$u_0 = \frac{K}{\mu} \cdot \frac{(-\Delta p)}{L} \Rightarrow u_0 = \frac{K}{\mu} \cdot \frac{d_p^2}{L} \cdot \frac{1}{1-e}$$

The darcy's law

$$K = \frac{d_p^2}{150} \cdot \frac{e^3}{(1-e)^2}$$

The intrinsic permeability

$$L_0 = \frac{K}{J} \cdot \frac{1}{(\Delta p - \Delta P)}$$

The solvent permeability

Friction coefficient in a porous medium

$$\frac{\pi \cdot d_p^2}{4} \cdot \frac{e^3}{(1-e)^2} = \frac{6}{d_p}$$

$$(-\Delta p) = 2 f / \rho u_0^2 \cdot \frac{L}{D_h} = 2 f / \rho \left(\frac{u_0}{e} \right)^2 \cdot \frac{4 \cdot (1-e)}{4 \cdot e} \cdot \frac{L}{D_h}$$

$$\frac{(-\Delta p)}{\rho u_0} \cdot \frac{d_p}{L} \cdot \frac{e^3}{1-e} = 3 \cdot f_f = \frac{1.75}{\text{Re}} \text{ r\`egime laminaire}$$

Blake and Plummer
Kozany and Carman

$$\frac{(-\Delta p)}{\rho u_0} \cdot \frac{d_p}{L} \cdot \frac{e^3}{1-e} = 1.75 \cdot \frac{150}{\text{Re}}$$

Ergun's relation

$$\text{Re} = \frac{\rho u_0 d_p}{\mu} \cdot \frac{e}{(1-e)}$$

Friction coefficient in a porous medium

$$F = k \cdot \dot{\epsilon}_1 \cdot f \Rightarrow (-\Delta p) = 2 f / \rho u_0^2 \cdot \frac{L}{D_h}$$

In a porous medium, we find: $(-\Delta p) = 2 f / \rho u_0^2 \cdot \frac{L}{D_h}$

- real velocity

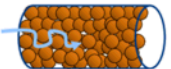
$$u_0 = \frac{Q}{S_0} = \frac{Q}{e \cdot S}$$

- mean velocity

$$u_0 = \frac{Q}{S} = e \cdot u_m$$

- D_h hydraulic diameter

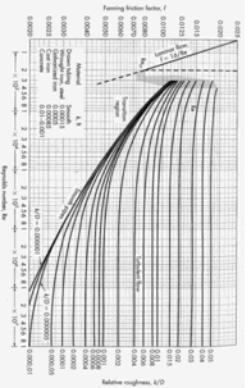
$$D_h = 4 \cdot \frac{\text{volume of vacuum}}{\text{wetted area}}$$



wetted area = area of a particle + volume of particle / radius of a particle
volume of particle = volume of bed

$$D_h = 4 \cdot \frac{eV}{a_p(1-e)} = 4 \cdot \frac{e}{a_p(1-e)}$$

The Moody's Diagram



The mass transfer coefficient.

Correlations

Sieder et Tate: influence of τ on μ

$$\text{Sh} = 0.023 \cdot \text{Re}^{0.8} \cdot \text{Sc}^{0.33} \cdot \left(\frac{\mu}{\mu_s} \right)^{0.14}$$

$$\text{Sh} = 1.36 \cdot \left(\text{Re} \cdot \frac{D_h}{L} \right)^{0.5} \cdot \left(\text{Sc}^{0.33} \cdot \left(\frac{\mu}{\mu_s} \right)^{0.14} \right)^{0.5}$$

Cheng et al: influence of τ on ν

$$\text{Sh} = 0.662 \cdot \sqrt{\text{Pe}}$$

Gekas et Hellstrom: roughness

$$\text{Sh} = \left(\frac{L}{D_h} \right)^{0.5} \cdot \text{Re}^{0.5} \cdot \text{Sc}^{0.33} \cdot \left(\frac{\mu}{\mu_s} \right)^{0.14}$$

$$f_f = \text{Re}^{-0.25}$$

$$\frac{1}{f_f} = 4.0 \log_{10} \left(\frac{3.7}{\text{Re}} + \frac{1.35}{\text{Re}^{0.75}} \right)$$

The mass transfer coefficient Dimensional analysis

$$k = k(D, \mu, D_h, \rho, \nu) \Rightarrow k = \alpha \cdot D^\gamma \cdot \mu^\beta \cdot D_h^\gamma \cdot \rho^\delta \cdot \nu^\epsilon$$

$$k(D) \cdot L^{-1} \cdot T^{-1}$$

$$D(D) \cdot L^2 \cdot T^{-1}$$

$$\mu(D) \cdot M \cdot L^{-1} \cdot T^{-1}$$

$$D_h(D) \cdot L$$

$$\rho(D) \cdot M \cdot L^{-3}$$

$$\nu(D) \cdot L^2 \cdot T^{-1}$$

$$k = \alpha \cdot D^{-\gamma+1} \cdot \mu^\beta \cdot D_h^{\gamma+1} \cdot \rho^\delta \cdot \nu^{\epsilon-2}$$

$$k = \alpha \left(\frac{\mu}{D} \right)^{\gamma+1} \left(\frac{D_h}{D} \right)^{\gamma+1} \Rightarrow \frac{HD}{D} = \alpha \left(\frac{\mu}{D} \right)^{\gamma+1} \left(\frac{D_h}{D} \right)^{\gamma+1}$$

$$\frac{HD}{D} = \text{Sh}$$

$$\frac{\mu}{D} = \text{Sc}$$

$$\frac{D\mu}{D} = \frac{\mu}{D} \cdot \frac{D\mu}{\mu} = \text{Sc} \cdot \text{Re} = \text{Pe}$$

Modeling of the concentration of polarisation

$$(E) \cdot (S) + (P) = (A)$$

$$J_f - J_f + \frac{D}{L} \cdot \frac{dc}{dx} = 0$$

$$\frac{dc}{dx} = \frac{J_f}{D} \cdot dx$$

$$c - c_0 = \frac{J_f}{D} \cdot x$$

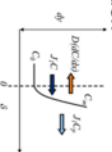
$$\ln(c - c_0) = \frac{J_f}{D} \cdot x$$

$$\ln(c_0 - c_0) = \frac{J_f}{D} \cdot x$$

$$\ln(c_0 - c_0) = \frac{J_f}{D} \cdot x$$

$$k = \frac{D}{\delta}$$

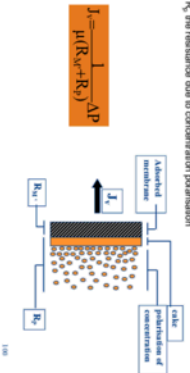
The mass Transfer Coefficient



5.2 Boundary layer film model

The resistance-in-series model

- Use of different mass resistance coefficients
- R_m the adsorbed membrane resistance
- R_p the resistance due to concentration polarisation



$$J_v = \frac{1}{\mu(R_{f,0} + R_p)} \Delta P$$

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The gel layer model

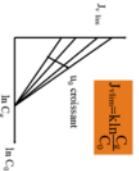
- Concentration polarisation can be very severe in ultrafiltration
- The solute concentration at the membrane surface reaches a maximum concentration, the gel concentration C_g

- C_g depends on the size, shape, chemical structure and degree of solvation
- C_g is independent of bulk concentration

$$J_{lim} = f(C_g) \text{ is a straight line}$$

λ is the slope

$$C_g \text{ is obtained at } J_{lim} = 0$$



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Correlations with suction effect

Colas et Hallerstein

$$R^* = \frac{J}{1 - \exp(-J/\lambda)}$$

De et Bhattacharya

$$S_0 = S_0 \left(\frac{S_0}{S_0^*} \right)^n \quad n = \text{refinement du solide, concentration}$$

$$S_0 = 1.35 \left(\frac{R_0 S_0}{L} \right)^{0.5} \left[1 + 0.324 + 0.02 R^* - 8.05 \cdot 10^{-3} R^* \right] \text{ canal rectangulaire}$$

$$S_0 = 1.65 \left(\frac{R_0 S_0}{L} \right)^{0.5} \left[1 + 0.374 + 0.03 R^* - 1.05 \cdot 10^{-3} R^* \right] \text{ canal tubulaire}$$

$$\lambda = \frac{P_0}{R_0 S_0}$$

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The mass transfer coefficient A new dimensional analysis

$$k = k(D, \mu, D_p, \rho, u, \eta)$$

$$k \propto D^{-1} \cdot r^{-1}$$

$$\partial \propto D^{1/2} \cdot r^{-1}$$

$$\mu \propto M \cdot D^{-1} \cdot r^{-1}$$

$$D_p \propto D \cdot L$$

$$k \propto M \cdot L^{-1}$$

$$u \propto D \cdot L^{-1}$$

$$\eta \propto D \cdot L^{-1}$$

$$J \propto D \cdot L^{-1}$$

$$\begin{cases} k = \alpha \cdot D^{-\beta} \cdot \mu^{\gamma} \cdot D_p^{\delta} \cdot \rho^{\epsilon} \cdot u^{\eta} \cdot \eta^{\zeta} \\ L_1: \beta = 2\beta - \gamma + \delta - 3\epsilon + \phi^+ + \eta \\ L_2: -1 = -\beta - \gamma - \phi^+ - \eta \\ M: 0 = \gamma + \epsilon \end{cases} \Rightarrow \begin{cases} \beta = \epsilon - \phi^+ + \eta \\ \gamma = -\epsilon \\ \delta = -1 + \phi^+ + \eta \end{cases}$$

$$k = \alpha \cdot D^{-\epsilon + \phi^+ + \eta} \cdot \mu^{\gamma} \cdot D_p^{-1 + \phi^+ + \eta} \cdot \rho^{\epsilon} \cdot u^{-\epsilon} \cdot \eta^{\zeta} \cdot \left(\frac{J D}{\partial} \right)^{\phi^+}$$

$$k D = \alpha \left(\frac{\mu}{\partial \eta} \right)^{\gamma} \left(\frac{D_p}{D} \right)^{-1 + \phi^+ + \eta} \left(\frac{J D}{\partial} \right)^{\phi^+} \left(\frac{D}{D_p} \right)^{\phi^+}$$

$$S_0 = \alpha_1 R_0^{\epsilon} S_0^{\epsilon} \eta^{\zeta} P_0^{\epsilon} \eta^{\zeta}$$

The Pressure osmotic model

$$J_v = \frac{\Delta P - \Delta \Pi - L_p (\Delta P - \Delta \Pi)}{\mu R_0}$$

- A high solute concentration at the membrane surface
- The osmotic pressure can not be neglected anymore

→ The real $\Delta P <$ The operating ΔP

With $\Delta \Pi = \Pi(C_m) - \Pi(C_p) - \Pi(C_m)$ because TR=1

- Dilute low molecular weight solutions
- $\Pi = a \cdot C$
- Macromolecular solution
- $\Pi = a \cdot C$ with $n > 1$

a and n depend both on molecular weight and type of polymer

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