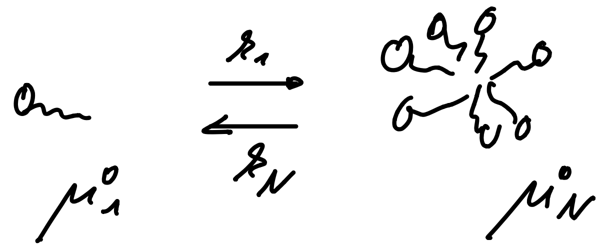
Wiederholung

5. Nov. 2019



$$x_1 = \frac{c_1}{c_1 + c_N}$$

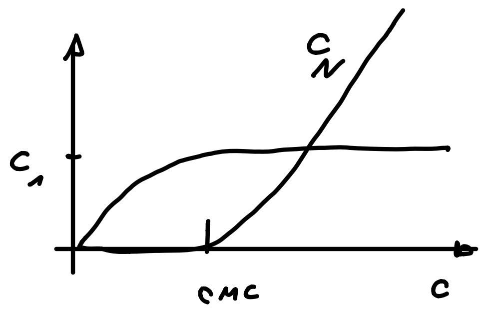
x : mol fraction

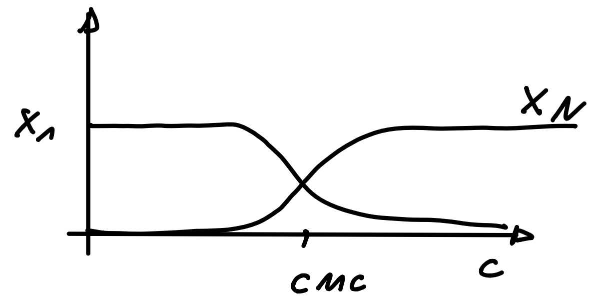
c : molar conc.

$$k_1 \cdot x_1^N = k_N \cdot \frac{x_N}{N}$$

$$k_1 / k_N = K = \exp \frac{-N \cdot (\mu_N - \mu_0)}{kT}$$

$$x_N = N \left[x_1 \cdot \exp\left(\mu_1^0 - \mu_N \right) / kT \right]^N$$





$$CMC = x_1^{crit} = \exp^{-(\mu_1^0 - \mu_N^0)/kT} = e^{-\alpha}$$

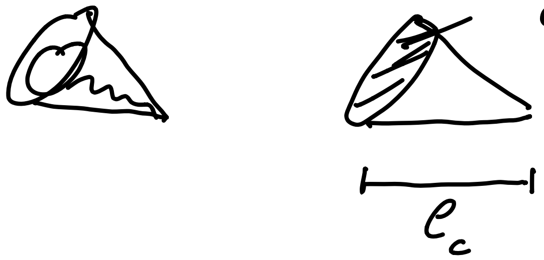
$$cmc_{micelle} \approx 10^{-2} - 10^{-5}\,M \qquad cmc_{bilayer} \approx 10^{-6} - 10^{-10}\,M$$

Note : if $\mu_N^0 = \mu_1^0 \Rightarrow x_N \ll 1$

if next neighbour interactions $\mu_N^0 \approx \mu_\infty^0 + \frac{\alpha\, kT}{N^{1/3}}$

$\alpha \cdot kT$: monomer-monomer bond energy

Molecular packing



a_H : head group area

l_c : chain length

v : volume

$$P = \frac{v}{a_H \cdot l_c}$$: shape factor (packing parameter)

$P < 1/3$ spherical

$1/3 < P < 1/2$ non-spherical

$1/2 < P < 1$ bilayer

$P > 1$ inverted

$$l_c \le l_{max} \approx (0.154 + 0,126 \cdot n)\ \text{nm}$$

$$\Delta \mu_{alkane} = 2.44 + 0,88\, n_c \qquad \text{kcal/Mol}$$

Tanford model

- hydrophobic interaction $\mu_N = \gamma \cdot a_H$

  γ: surface tension

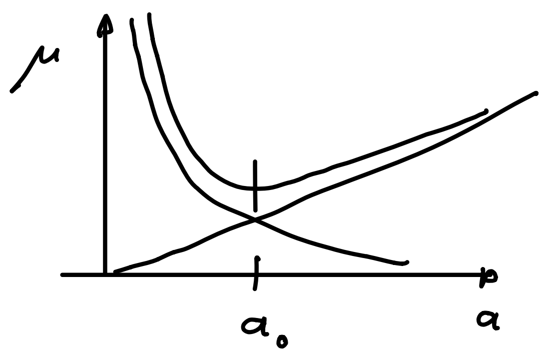
  [$\gamma_{hydrocarbon/water} = 50\, mJ \cdot m^{-2}$]

- head group repulsion $\mu_N = K_A / a_H$

  K_A: area compressibility

$$\Rightarrow \mu_{Ges} = \gamma \cdot a + \frac{K}{a}$$

$$\mu_{Ges}(min) = 2\gamma \cdot a_0 \qquad \text{with } a_0 = \sqrt{\frac{K}{\gamma}}$$

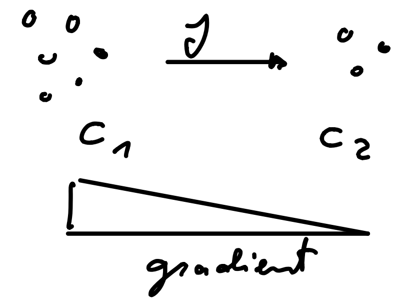


$$\mu_N = \gamma \cdot a + \frac{a_0^2 \gamma}{a}$$

$$= \gamma \cdot a + \frac{\gamma}{a}(a - a_0)^2$$

Passive diffusion across membrane

Diffusion



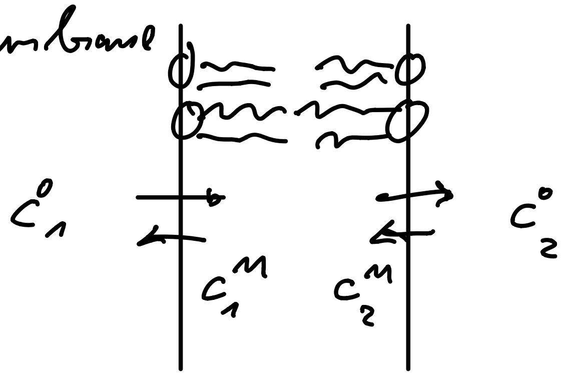
$$\vec{j} = D \cdot \nabla c(x) = \frac{dn}{dt} \cdot A$$

$\vec{j}$: particle flux density $[m^{-2} \cdot s^{-1}]$

D : diffusion const. $[m^2 s^{-1}]$

c : concentration $[m^{-3}]$

Membrane



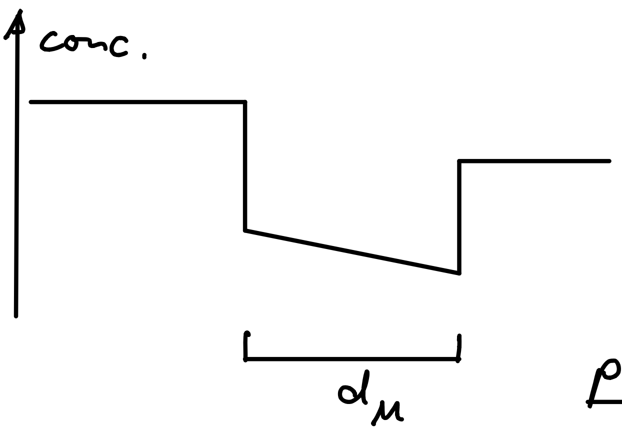
$$\frac{c_1^M}{c_1^o} = K = e^{-\Delta\mu}$$

K : partition coefficient

e.g. $K_{urea} = 2 \cdot 10^{-4}$

$K_{Na^+} \approx 10^{-30}$

due to Born energy



P: Permeability:

particle flux

$$\frac{dn}{dt} = P \cdot A \, (c_1^o - c_2^o)$$

$$= \frac{D}{d_M} \cdot A \cdot (c_1^M - c_2^M)$$

$$= \frac{D}{d_M} \cdot A \cdot K \cdot (c_1^o - c_2^o)$$

$$\boxed{P = \frac{K \cdot D}{d_M}}$$