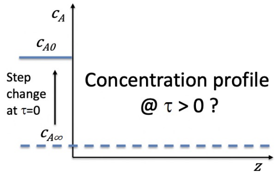
Øving 7

1

Unsteady diffusion into a semi-infinite slab



Consider the following problem:

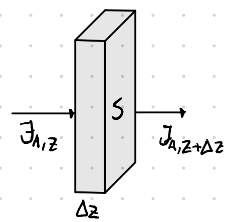
- a large volume of solution that starts at an interface z=0 and extends a relatively very long distance away from the interface $z \to \infty$
- first the concentration is constant all-over the system $c_A = c_{A\infty}$ for all z
- at initial time $\tau = 0$ the concentration at the interface suddenly (step change) increases to a higher constant value $c_A(0) = c_{A0}$ and the solute starts to diffuse into the system of lower concertation
- we observe the system for relatively short enough times for the concentration far away from the interface ($z \to \infty$) to remain un-affected by the diffusion of A equal to the initial concentration for all times ($c_A(\infty) = c_{A\infty}$)
- this corresponds to the conceptual idea of infinitely thick slab

1. Derive the differential equation describing the system and formulate the boundary and initial conditions

Massebalanse

$$\text{Inn} - \text{Ut} + \cancelto{0}{\text{Generert}} = \text{Akkumulert}$$

Vi ser på diffusjon. Anta tynt volumelement



$\Delta V = \Delta z \cdot S$

Får

$$J_{A,z} \cdot S - J_{A,z+\Delta z} \cdot S = \frac{\partial C_A}{\partial \tau} S \Delta z$$

$$\frac{\partial C_A}{\partial \tau}\Delta z = J_{A,z} - J_{A,z+\Delta z} = \cancel{J_{A,z}} - \cancel{J_{A,z}} - \Delta J_{A,z}$$

$$\frac{\partial C_A}{\partial \tau} = -\frac{J_{A,z}}{\Delta z}$$

Anta at Δz er veldig liten
$\Delta z \to \partial z$

$$\frac{\partial C_A}{\partial \tau} = -\frac{\partial J_{A,z}}{z}$$

Fick's lov

$$\frac{\partial C_A}{\partial \tau} = -\frac{\partial}{\partial z}\left(-D\frac{\partial C_A}{\partial z}\right)$$

$$\underline{\underline{\frac{\partial C_A}{\partial \tau} = D\frac{\partial^2 C_A}{\partial z^2}}}$$

Boundary og initial conditions

$\tau = 0 \quad \forall z, \quad C_A = C_{A\infty}$

$\tau > 0 \quad z = 0, \quad C_A = C_{A0}$

$\tau > 0 \quad z - \infty, \quad C_A = C_{A\infty}$

2. Introduce new combined variable $\xi = \frac{z}{\sqrt{4D\tau}}$ and transform the problem. How did the equation and the conditions simplify?

$$\frac{\partial C_A}{\partial \tau} = D \frac{\partial^2 C_A}{\partial z^2}$$

kjerneregel: $\frac{\partial C_A}{\partial \tau} = \frac{\partial C_A}{\partial \xi} \frac{\partial \xi}{\partial \tau}$ og $\frac{\partial C_A}{\partial z} = \frac{\partial C_A}{\partial \xi} \frac{\partial \xi}{\partial z}$

$$\frac{\partial \xi}{\partial \tau} = \frac{z}{\sqrt{4D}} \frac{d}{d\tau} {}^{-1/2} = -\frac{1}{2} \frac{z}{\sqrt{4D}} \tau^{-3/2} = -\frac{1}{2} \underbrace{\frac{z}{\sqrt{4D\tau}}}_{=\xi} \cdot \frac{1}{\tau} = -\frac{\xi}{2} \Rightarrow \boxed{\frac{\partial C_A}{\partial \tau} = \frac{\partial C_A}{\partial \xi} \cdot \left(-\frac{\xi}{2\tau}\right)}$$

$$\frac{\partial \xi}{\partial z} = \frac{1}{\sqrt{4D\tau}} \Rightarrow \frac{\partial C_A}{\partial z} = \frac{\partial C_A}{\partial \xi} \cdot \frac{1}{\sqrt{4D\tau}}$$

$$\frac{\partial^2 C_A}{\partial z^2} = \frac{\partial}{\partial z}\left(\frac{\partial C_A}{\partial z}\right) = \frac{\partial}{\partial z}\left(\frac{\partial C_A}{\partial \xi} \frac{1}{\sqrt{4D\tau}}\right) = \frac{1}{\sqrt{4D\tau}} \underbrace{\frac{\partial}{\partial z}\left(\frac{\partial C_A}{\partial \xi}\right)}_{= \frac{\partial^2 C_A}{\partial z \partial \xi}}$$

Teorem: $\frac{\partial^2 C_A}{\partial z \partial \xi} = \frac{\partial^2 C_A}{\partial \xi \partial z} = \frac{\partial}{\partial \xi}\left(\frac{\partial C_A}{\partial z}\right)$

$$\Rightarrow \boxed{\frac{\partial^2 C_A}{\partial z^2} = \frac{1}{\sqrt{4D\tau}} \frac{\partial}{\partial \xi}\left(\frac{\partial C_A}{\partial \xi} \frac{1}{\sqrt{4D\tau}}\right) = \frac{1}{4D\tau} \frac{\partial^2 C_A}{\partial \xi^2}}$$

Den transformerte likningen blir:

$$\frac{\partial C_A}{\partial \xi} \cdot \left(-\frac{\xi}{2\tau}\right) = \cancel{D} \cdot \frac{1}{4\cancel{D}\tau} \frac{\partial^2 C_A}{\partial \xi^2}$$

$$\Rightarrow \underline{\underline{\frac{\partial^2 C_A}{\partial \xi^2} + 2\xi \frac{\partial C_A}{\partial \xi} = 0}}$$

Med BC:

$\xi = 0 \Rightarrow C_A = C_{A0}$

$\xi \to \infty \Rightarrow C_A = C_{A\infty}$

3. Solution to this diffusion problem is an error function.
   a. Find out about the properties of error function.
   b. Find the relations describing the concentration profile and the flux
   c. Discuss how this problem differ from the stead-state diffusion through a thin film

a) Errorfunksjonen er en odde funksjon

b) Løser uttrykket fra 2. :

La $u = \frac{\partial C}{\partial \xi} \Rightarrow \frac{du}{d\xi} + 2\xi u = 0$

$$\frac{du}{d\xi} = -2\xi u$$

$$\frac{1}{u}du = -2\xi d\xi \qquad /\text{int}$$

$$\ln(u) = -\xi^2 + k_0$$

$$u = \underbrace{e^{k_0}}_{= K_1} \cdot e^{-\xi^2}$$

$$u = K_1 e^{-\xi^2} \qquad /u = \frac{\partial C_A}{\partial \xi}, \text{int}$$

$$\int \partial C_A = \int K_1 e^{-\xi^2} \partial \xi$$

$$\Rightarrow C_A = K_1 \underbrace{\int_0^{\xi} e^{-\xi^2} d\xi}_{= \frac{\sqrt{\pi}}{2}\text{erf}(\xi)} + K_2$$

Insert BC

$$\xi = 0, \quad \text{erf}(0) = 0 \Rightarrow C_A = K_2 = C_{A0} \Rightarrow K_2 = C_{A0}$$

$$\xi \to \infty, \quad \text{erf}(\infty) = 1 \Rightarrow C_A = K_1 \frac{\sqrt{\pi}}{2} \underbrace{\text{erf}(\infty)}_{=1} + C_{A0} = C_{A\infty}$$

$$C_A = K_1 \frac{\sqrt{\pi}}{2} + C_{A0} = C_{A\infty}$$

$$K_1 = \frac{C_{A\infty} - C_{A0}}{\frac{\sqrt{\pi}}{2}}$$

$$\Rightarrow C_A = (C_{A\infty} - C_{A0}) \frac{2}{\sqrt{\pi}} \int_0^{\xi} e^{-\xi^2} d\xi + C_{A0}$$

$$\Rightarrow \underline{\underline{\frac{C_A - C_{A0}}{C_{A\infty} - C_{A0}} = \text{erf}(\xi)}}$$

Subst. $z = \xi\sqrt{4D\tau}$

$$\frac{dz}{\partial \xi} = \sqrt{4D\tau}$$

$$d\xi = \frac{dz}{\sqrt{4D\tau}}$$

$$J_{A,z} = -D\frac{\partial C_A}{\partial z} = -D\frac{\partial}{\partial z}\left[(C_{A\infty} - C_{A0})\frac{2}{\sqrt{\pi}} \int_0^{\xi} e^{-\xi^2} d\xi + C_{A0}\right]$$

$$= -D(C_{A\infty} - C_{A0}) \frac{2}{\sqrt{\pi}} \frac{1}{\sqrt{4D\tau}} \frac{d}{dz} \int_0^{\xi} e^{-\frac{z^2}{4D\tau}} d\xi$$

$$\underline{\underline{J_{A,z} = \sqrt{\frac{D}{\pi\tau}}(C_{A0} - C_{A\infty}) e^{-\frac{z^2}{4D\tau}}}}$$

c) Ved å sette $z=0$,

$$J_{A,z=0} = \sqrt{\frac{D}{\pi \tau}}\,(C_{A0} - C_{A\infty})$$

Steady-state film

$$J_A = -D\,\frac{C_{AL} - C_{A0}}{L} = D\,\frac{C_{A0} - C_{AL}}{L}$$

Får tilsvarende drivkraft, men ulike koeffisienter.

2

A) Equimolar counter-diffusion of compounds A and B

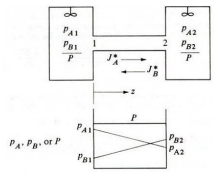


FIGURE 6.2-1. *Equimolar counterdiffusion of gases A and B.*

Consider the following problem:

- Two gases A nad B in two large chambers at constant total pressure
- Concentrations in chambers are uniform
- The chambers are connected with a tube where molecules of A diffuse into the right, since the total P is constant, equal net moles of B must diffuse into the left.

1. Derive the relation between the fluxes of A and B and the diffusion coefficients D_{AB} and D_{BA}
2. How will that simplify the relation for total flux of A?

1) $N = N_A + N_B = 0 \Rightarrow N_A = -N_B$

$$dC_A = -dC_B$$

Fick's lov:

$$J_A = -D_{AB}\,\frac{dC_A}{dz}$$

$$\Rightarrow N_A = J_A = -D_{AB}\,\frac{dC_A}{dz}$$

$$N_B = J_B = -D_{BA}\,\frac{dC_B}{dz} = D_{BA}\,\frac{dC_A}{dz}$$

$$N_A = -N_B$$

$$-D_{AB}\,\frac{dC_A}{dz} = -D_{BA}\,\frac{dC_A}{dz}$$

$$\Rightarrow D_{AB} = D_{BA}$$

2) Total flux of A:

$$N_A = -c\,D_{AB}\frac{dx_A}{dz} + \frac{c_A}{c}\cancel{N}^{=0}$$

$$N_A = -D_{AB}\frac{dc_A}{dz} \qquad , \; c_A = \frac{n_A}{V} = \frac{P_A}{RT}$$

$$N_A = -\frac{D_{AB}}{RT}\frac{dP_A}{dz}$$

$$N_A = -\frac{D_{AB}}{RT}\cdot\frac{P_{A2}-P_{A1}}{z_2-z_1}$$

B) Diffusion of compound A through stagnant non diffusing compound B

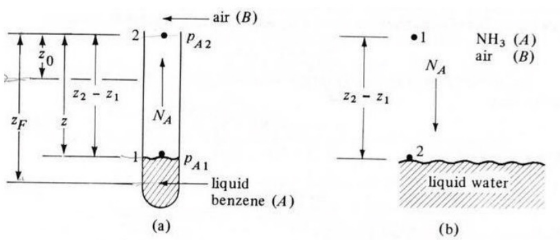


FIGURE 6.2.-2. *Diffusion of A through stagnant, nondiffusing B: (a) benzene evaporating into air, (b) ammonia in air being absorbed into water.*

Consider the 2 examples of this type of problem:

a) Pure liquid evaporates from the bottom of a narrow tube where a large amount of inert is passed at the top. The inert B is not soluble in the liquid and so it is not diffusing to/from the interface.
b) A compound is absorbed into water from a gas mixture. The other compounds in the gas phase are not soluble in water and so they are not diffusing to/from the interface.

1. Derive relation for the total flux.
2. Derive general relation for the total flux of A for diffusion of compound A through stagnant non diffusing compound B
3. Derive a relation for the total flux of A if the solution is very dilute.

1) $J_A = -D_{AB}\frac{dc_A}{dz} + \frac{c_A}{c}N$

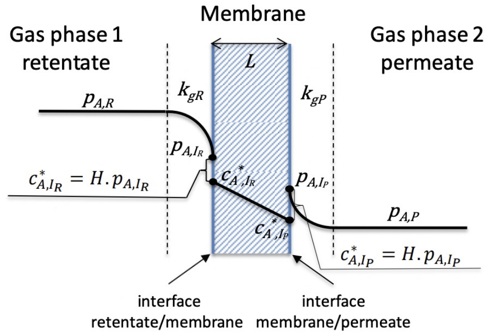
No diffusion of B

2) $N = N_A + N_B \Rightarrow J_A = -D_{AB}\frac{dc_A}{dz} + \frac{c_A}{c}(N_A+N_B) = -D_{AB}\frac{dc_A}{dz} + \frac{c_A}{c}N_A$

3) dilute $\Rightarrow c_A \ll c$, $\frac{c_A}{c} \approx 0$

$$\Rightarrow J_A = -D_{AB}\frac{dc_A}{dz}$$

$\boxed{3}$



Consider the following mass transfer problem:

1) Two gases are separated by a membrane of the thickness L
2) Solute A diffuses from gas phase 1 through the membrane into gas phase 2
3) Assume steady state and equilibrium at the interfaces where the solubility of A in the membrane is described by Henrys law

1. Derive an expression for the overall mass transfer coefficient
2. Derive an expression for the flux of solute A through the membrane in terms of the overall mass transfer coefficient

Fluxes

To retentate through film

$$N_{A,R} = k_{gR}(p_{A,R} - p_{AI,R})$$

$$N_{A,M} = \frac{D_A}{L}(C^*_{AI,r} - C^*_{AI,p})$$

$$N_{A,P} = k_{gP}(P_{AI,P} - P_{A,P})$$

$$N_{Ar} = k_{gR}(P_{Ar} - P_{AI_r})$$
$$\parallel$$
$$N_{AM} = \frac{D_A}{L}(C^*_{AI_r} - C^*_{AI_p})$$
$$\parallel$$
$$N_{AP} = k_gP(P_{AI_p} - P_{A_p})$$

$N_A = N_{AR} = N_{Am} = N_{AP}$

Se pptx

$$\Rightarrow N_A\left(\frac{1}{k_{gR}} + \frac{1}{D_A \cdot H} + \frac{1}{k_{gp}}\right) = P_{AR} - P_{AP}$$

$$\Rightarrow N_A = \frac{P_{AR} - P_{AP}}{\frac{1}{k_{gR}} + \frac{L}{D_A H} + \frac{1}{k_{gP}}} = \frac{P_{AR} - P_{AP}}{\frac{1}{k_{gR}} + \frac{L}{P_A'} + \frac{1}{k_{gP}}}$$

membrane permeability

$P_A' = D_A \cdot H$

Henry's law: $C = HP$

$$\Rightarrow N_{A,m} = \frac{D_A H}{L}(P_{AI,R} - P_{AI,P})$$

$$N_{A,R} = k_{gR}(p_{A,R} - p_{Ai,R}) \Rightarrow \frac{N_{A,R}}{k_{gR}} = P_{A,R} - P_{AI,R}$$

$$N_{A,m} = \frac{D_A H}{L}(P_{AI,R} - P_{AI,P}) \Rightarrow \frac{N_{A,M}}{L/D_A H} = P_{AI,R} - P_{AI,P}$$

$$N_{A,P} = k_{gP}(P_{AI,P} - P_{A,P}) \Rightarrow \frac{N_{A,P}}{k_g P} = P_{AIP} - P_{AP}$$

Sum up, Steady state: $N_{A,R} = N_{A,I} = N_{A,P} = N_A$

$$\Rightarrow N_A\left(\frac{1}{k_{gR}} + \frac{L}{D_A H} + \frac{1}{k_{gP}}\right) = P_{A,R} - P_{A,P}$$

$$\Rightarrow N_A = \frac{P_{A,R} - P_{A,P}}{\frac{1}{k_{gR}} + \frac{L}{D_A H} + \frac{1}{k_{gP}}}$$

K_g : Overall mass transfer coefficient

$$K_g = \frac{1}{\frac{1}{k_{gR}} + \frac{L}{D_A H} + \frac{1}{k_{gP}}}$$

$$\Rightarrow N_A = K_g (P_{A,R} - P_{A,P})$$