Introduction.

Flux : $\dfrac{\text{amount of substance removed}}{\text{time} \cdot (\text{area})}$.

↳ we assume that the flux is proportional to the substance concentration.

↳ $N = K \cdot C_s$

where K is the mass transfer coefficient.

Tambien se puede definir el flux como

$$N = \mathcal{D}\,\frac{C}{L} \quad \Big\}\ \text{Fick's law.}$$

La corriente está dada por el producto

$$\vec{N} \cdot A\hat{n} = \text{Current.}$$

Ficks' Law:

The flux of a sustance throug a traverse area A is given by

$$\vec{J} = A\vec{j}$$

where j is the current density: particles per unit time per unit area.

He purposed that

$$\vec{j} = -\mathcal{D}\nabla C$$

where $\mathcal{D}$ is a coefficient dependent on the substance.

$$\Rightarrow J = -A\mathcal{D}\nabla C.$$

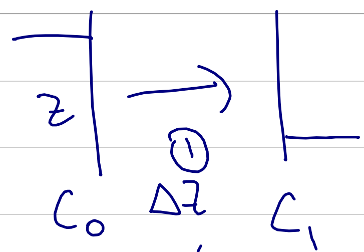
By conservation of mass

$$\frac{\partial C}{\partial t} + \nabla\cdot\vec{J} = 0$$

From where we get:

$$\frac{\partial C}{\partial t} = -\nabla\left(-A\mathcal{D}\nabla C\right) = \mathcal{D}\left(\nabla^2 C + \nabla A \nabla C\right)$$

Argumento Físico:



¿Cuál es el perfil de concentración en la región 1 de largo l?

Tenemos que

$$A\left(j(z) - j(z+\Delta z)\right) = 0$$

El lado derecho es cero, debido a que no hay acumulación.

Dividiendo por el volumen de la región, tenemos

$$V = A\cdot\Delta z$$

$$\Rightarrow -\left(\frac{j(z+\Delta z) - j(z)}{\Delta z}\right) = 0 .$$

En el límite $\Delta z \to 0$

$$-\frac{dj}{dz} = 0 . \quad ;$$

De acuerdo con Fick, $j = -D\frac{dc}{dz}$

$$\Rightarrow +D\frac{d^2c}{dz^2} = 0$$

$$C(z) = \left(\frac{C_l - C_1}{l}\right)z + C_1$$

$$\Rightarrow C = az + b$$

$C(0) = b = C_1$; $c(l) = al + b = C_l$

$\Rightarrow$

Membrane diffusion.

$$\frac{\partial c}{\partial t} = \mathcal{D}\frac{\partial^2 c}{\partial z^2} \qquad \xi = \frac{z}{\sqrt{4Dt}}$$

$$\frac{d\xi}{dt} = \frac{z}{\sqrt{4D}} \cdot -\frac{1}{2} t^{-3/2} -$$

$$= -\frac{z}{2t\sqrt{4Dt}}$$

$$\frac{\partial c}{\partial t} = \frac{\partial c}{\partial \xi} \cdot \frac{\partial \xi}{\partial t} = \mathcal{D} \cdot \frac{\partial}{\partial z} \cdot \frac{\partial c}{\partial \xi} \cdot \frac{\partial \xi}{\partial z}$$

$$= \mathcal{D}\frac{\partial^2 c}{\partial \xi^2}\left(\frac{\partial \xi}{\partial z}\right)^2$$

$$\Rightarrow \frac{\partial c}{\partial \xi} \cdot \left(-\frac{1}{2t\sqrt{4Dt}} \cancel{z} \quad - \right) = \mathcal{D}\frac{\partial^2 c}{\partial \xi^2}\frac{z^2}{4Dt}$$

$$\Rightarrow \frac{\partial c}{\partial \xi} = -\frac{2\mathcal{D}tz}{\sqrt{4Dt}} \cdot \frac{\partial^2 c}{\partial \xi^2}$$

$$\frac{\partial c}{\partial \xi} = -2\mathcal{D}t\xi\frac{\partial^2 c}{\partial \xi^2}$$

Integro differential form

$$\frac{\partial^2 \psi}{\partial \xi^2} = -\left(c_+(\xi) - c_-(\xi)\right)$$

$$\psi' - \psi'(0) = -\int_0^{\xi} d\xi' \left(c_+(\xi') - c_-(\xi')\right)$$

$\psi' = 0$ therefore

$$\psi' = -\int_0^{\xi} d\xi' \left(c_+(\xi') - c_-(\xi')\right) < 0$$

We can write the diffusion system as

$$\frac{\partial c_+}{\partial t} = \mathcal{D}_+\left(\frac{\partial^2 c_+}{\partial \xi^2} - \frac{\partial c_+}{\partial \xi}\cdot\frac{\partial \psi}{\partial \xi} - c_+\frac{\partial^2 \psi}{\partial \xi^2}\right)$$

$$\rightarrow \frac{\partial c_+}{\partial t} = \mathcal{D}_+\left(\frac{\partial^2 c_+}{\partial \xi^2} + \frac{\partial c_+}{\partial \xi}\int_0^{\xi} d\xi' \left(c_+(\xi') - c_-(\xi')\right)\right.$$

$$\left. + c_+\left(c_+(\xi) - c_-(\xi)\right)\right)$$

$$\frac{\partial c_-}{\partial t} = \mathcal{D}_-\left(\frac{\partial^2 c_-}{\partial \xi^2} - \frac{\partial c_-}{\partial \xi}\int_0^{\xi} d\xi' \left(c_+(\xi') - c_-(\xi')\right)\right.$$

$$\left. - c_-\left(c_+(\xi) - c_-(\xi)\right)\right)$$

we get the following system:

$$\frac{\partial C_+}{\partial t} = D_+ \left[\left(\frac{\partial^2 C_+}{\partial \xi^2} \right) + \frac{\partial C_+}{\partial \xi} \int_0^{\xi} d\xi' \left(C_+(\xi) - C_-(\xi) \right) + C_+(\xi) \left(C_+(\xi) - C_-(\xi) \right) \right]$$

$$\frac{\partial C_-}{\partial t} = D_- \left[\left(\frac{\partial^2 C_-}{\partial \xi^2} \right) - \frac{\partial C_-}{\partial \xi} \int_0^{\xi} d\xi' \left(C_+(\xi) - C_-(\xi) \right) - C_+(\xi) \left(C_+(\xi) - C_-(\xi) \right) \right]$$

Discretization

$$\frac{\partial C_+}{\partial t} = \frac{C_+^{n+1} - C_+^{n}}{\Delta t}$$

$$\int_0^{\xi} d\xi' \left(C_+(\xi) - C_-(\xi) \right) = \sum_{i=1}^{\xi_j} \Delta\xi \cdot \left(C_+(i \cdot \Delta\xi) - C_-(i \cdot \Delta\xi) \right)$$