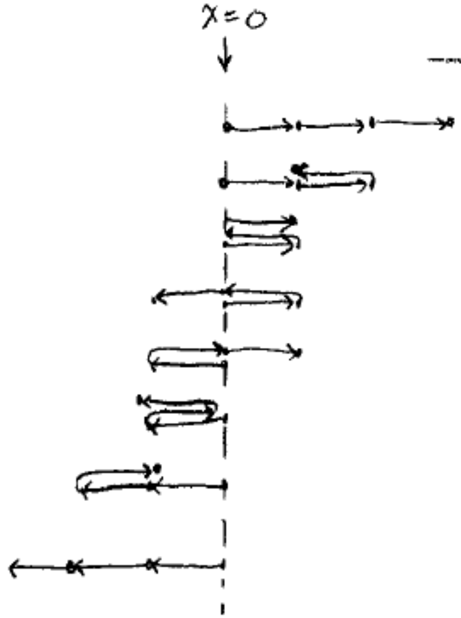
MICROSCOPIC ORIGIN



$\{x_1, x_2, x_3\}$, cm	$x_2 \times k_3$, cm	
1, 2, 3	+2	0
1, 2, 1	-2	
1, 0, 1	0	0
1, 0, -1	0	
-1, 0, 1	0	0
-1, 0, -1	0	
-1, -2, -1	-2	0
-1, -2, -3	+2	

$\langle x_2 k_3 \rangle = 0$

$$\langle x_3 \rangle = \frac{1}{8} \sum x_3 = 0$$

$$\langle (x_3)^2 \rangle = \frac{1}{8} \sum (x_3)^2 = \frac{1}{8} \cdot 24 = 3$$

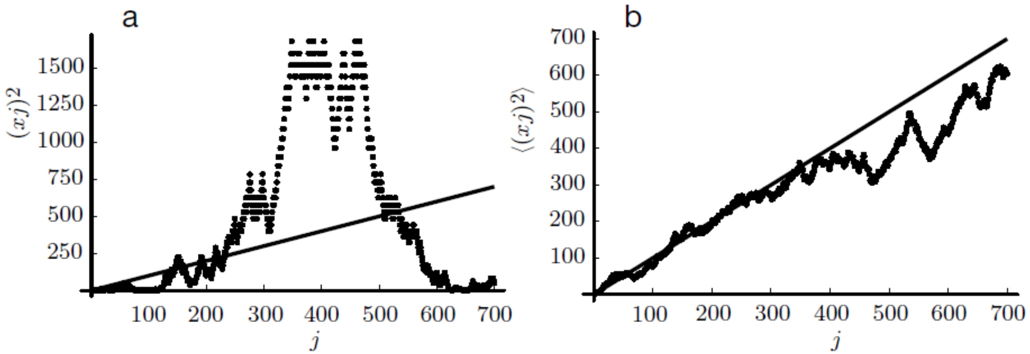
$$\langle (x_N)^2 \rangle = \langle (x_{N-1} + k_N L)^2 \rangle = \langle (x_{N-1})^2 \rangle + 2L\langle x_{N-1} k_N \rangle + L^2 \langle (k_N)^2 \rangle.$$

Position after Nth step

$$\langle (x_N)^2 \rangle = NL^2.$$

$$N = t/\Delta t \qquad D = L^2/2\Delta t \quad \Rightarrow \quad \langle (x_N)^2 \rangle = 2Dt$$

One dimensional random walk



Thirty walks

Figure 4.5: (Mathematical functions.) (**a**) Squared deviation $(x_j)^2$ for a single, one-dimensional random walk of 700 steps. Each step is one unit long. The solid line shows j itself; the graph shows that $(x_j)^2$ is not at all the same as j. (**b**) As (a), but this time the dots represent the *average* $\langle (x_j)^2 \rangle$ over thirty such walks. Again the solid line shows j. This time $\langle (x_j)^2 \rangle$ does resemble the idealized diffusion law (Equation 4.4).

From: Nelson

Discuss how do we get information out of SINGLE walk?

Fick’s Law

Question: What is the flux of solute particles if there is concentration gradient in the sample? And so, how does the concentration profile evolve with time?

Point to ponder: Does concentration gradient make particles diffuse faster?

What’s your guess?

Model to try: All that the particles are doing is randomly walking. Not interacting with each other in any other way except banging against each other and randomly choosing new direction from Boltzmann’s distribution.

Fick's first law states that the rate of diffusion for a chemical species in a solution increases with the difference in concentration between two adjacent regions.

Fick's second law states that the movement of the species dramatically decreases with the distance from the region of higher concentration.

...Adolf Eugen Fick (1829–1901), a 26-year-old physician, published his first paper in the physical sciences and an abstracted translation in English about the diffusion of chemical species in aqueous solutions.

3. ADOLF FICK

We now arrive at this year 1855 which we are now celebrating, when Adolf Fick, only 26 years old, proposed the quantitative laws of diffusion. At that time, Fick was an anatomy demonstrator in Zürich. It is quite interesting to note that these basic equations are not due to a Chemist or a Physicist, but to a Physiologist! But Fick was a man with a large scientific culture, not only in medicine, but also in mathematics and physics. In 1856, he published a monograph entitled "Medical Physics", the first book of this kind, where he discussed biophysical problems, such as the mixing of air in the lungs, the work of the heart, the heat economy of the human body, the mechanics of muscular contraction, the hydrodynamics of the blood circulation, etc…Fick's name remains well known in the history of cardiology.

Let us come back to our main purpose by quoting the first lines of Fick's paper published in the Philosophical Magazine, (a paper translated from the original one in Poggendorff's Annalen) [3] : " A few years ago, Graham published an extensive investigation on the diffusion of salts in water, in which he more especially compared the diffusibility of different salts. It appears to me a matter of regret, however, that in such an exceedingly valuable and extensive investigation, *the development of a fundamental law*, for the operation of diffusion in a single element of space, was neglected, and *I have therefore endeavoured to supply this omission*."

..from **One and a Half Century of Diffusion: Fick, Einstein, before and beyond**

Jean Philibert

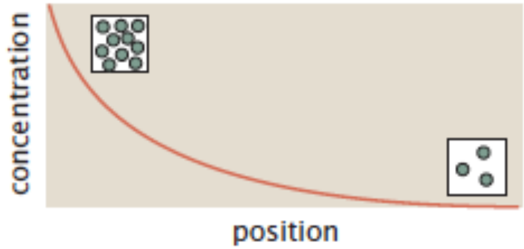
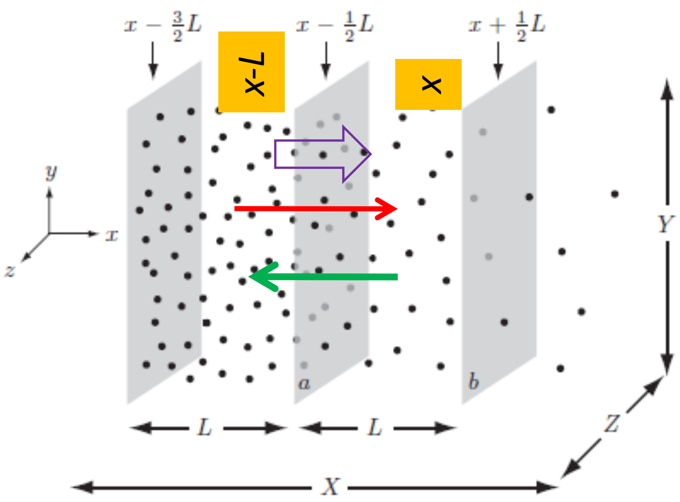


Figure 13.10: Example of a concentration profile. The plot shows the variation of the concentration with distance along some spatial domain, illustrating the idea of a position-dependent concentration.

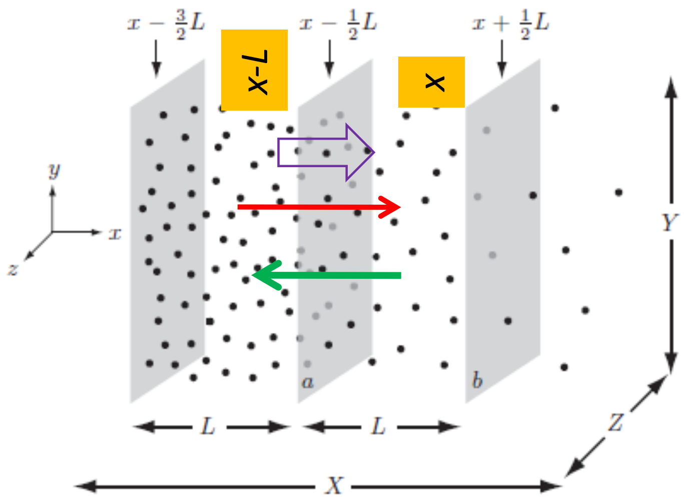


1. In each bin half of the particles go to left bin and half to the bin on right every Δt
2. Get the no. of particles crossing left to right
3. Make bins really narrow
4. From number profile to concentration profile
5. Find expression for flux or the number of particles per unit area goinf from left to right

Nelson p128-133

$$\boxed{j = -D\frac{\mathrm{d}c}{\mathrm{d}x}. \quad \text{Fick's law}}$$

Diffusion constant same definition as last derivation



Remember?

$$\frac{dy}{dx} = \lim_{\delta x \to 0} \frac{\delta y}{\delta x} = \lim_{\delta x \to 0} \frac{f(x+\delta x) - f(x)}{\delta x}$$

Total no. Of particles going Left to right (to the bin centred at x)

$$\frac{1}{2}(N(x-L) - N(x))$$

Making L really thin…. $N(x-L) - N(x) \to -L\dfrac{\mathrm{d}\langle N(x)\rangle}{\mathrm{d}x}.$

From number profile to concentration profile.. $c = N/(LYZ)$

Flux has dimensions $\mathbb{T}^{-1}\mathbb{L}^{-2}$

Number of particles crossing a cross-sectional area per unit area per unit time

$$j = \frac{1}{YZ \times \Delta t} \times \boxed{\frac{1}{2} \times L \times \left(-\frac{\mathrm{d}}{\mathrm{d}x} LYZc(x)\right)} = -\frac{1}{\Delta t}\frac{L^2}{2} \times \frac{\mathrm{d}c}{\mathrm{d}x}.$$

$$\boxed{j = -D\frac{\mathrm{d}c}{\mathrm{d}x}. \quad \text{Fick's law}}$$

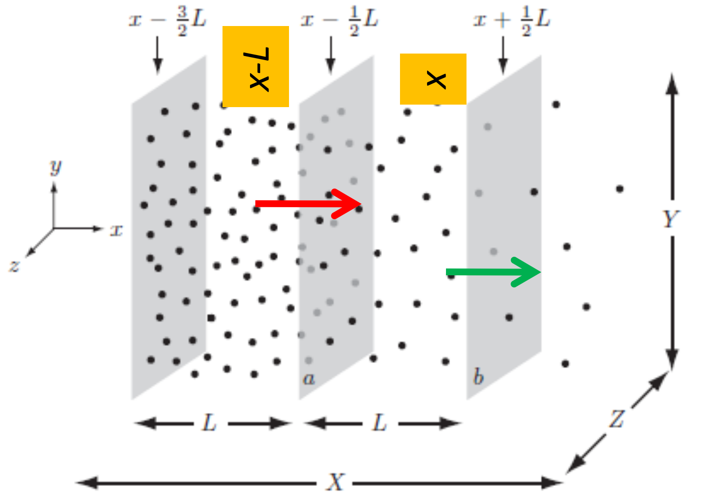
Diffusion equation:…….how does the concentration profile evolve in time?

$$\frac{\mathrm{d}}{\mathrm{d}t}N(x) = \left(YZj(x-\tfrac{L}{2}) - YZj(x+\tfrac{L}{2})\right).$$

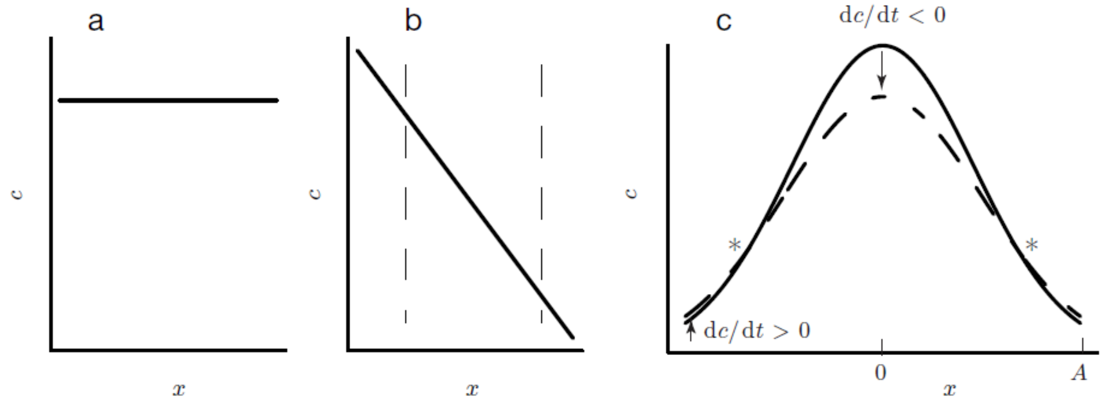
$$\frac{\mathrm{d}c}{\mathrm{d}t} = -\frac{\mathrm{d}j}{\mathrm{d}x}$$

$$\boxed{j = -D\frac{\mathrm{d}c}{\mathrm{d}x}. \qquad \text{Fick's law}}$$

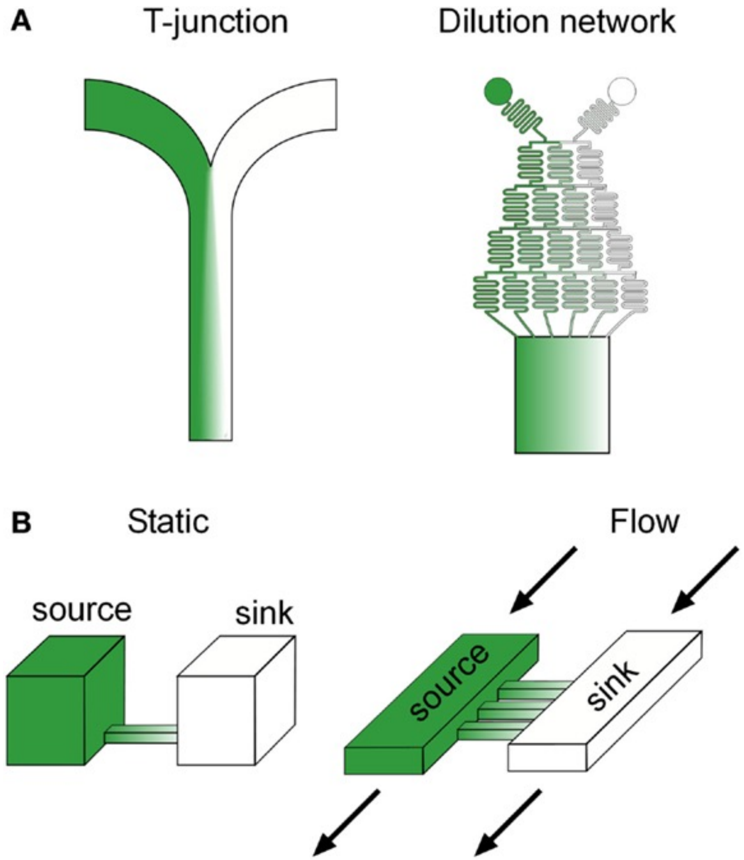
$$\boxed{\frac{\mathrm{d}c}{\mathrm{d}t} = D\frac{\mathrm{d}^2c}{\mathrm{d}x^2}. \qquad \text{diffusion equation}}$$



What does this mean?



How will these profiles evolve?



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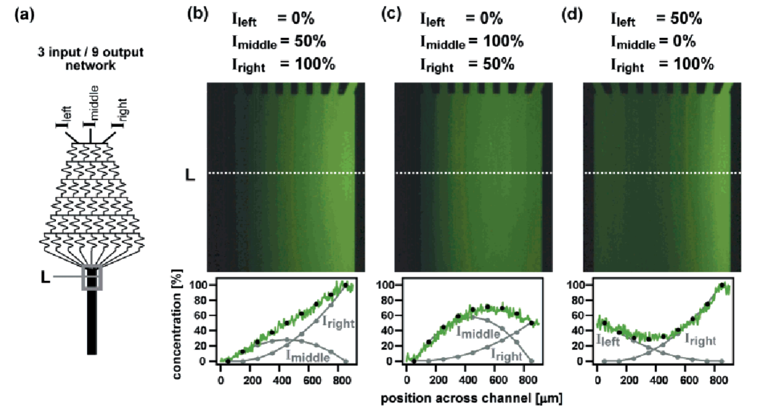

Fluorescence micrographs showing (b) linear and (c, d) parabolic gradients of fluorescein in solution. The microfluidic

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$$\boxed{j = -D\frac{\mathrm{d}c}{\mathrm{d}x}. \qquad \textbf{Fick's law}}$$

$$\boxed{\frac{\mathrm{d}c}{\mathrm{d}t} = D\frac{\mathrm{d}^2c}{\mathrm{d}x^2}. \qquad \textbf{diffusion equation}}$$

Cannot calculate exact fluxes and concentration evolution without "D".

What is D for particles in solution?

$$D = \frac{k_B T}{6\pi\eta a}$$

$a \rightarrow$ Radius of the Particle

$\eta \rightarrow$ Viscosity of the medium

HOW? : later