ICEA

Università degli Studi di Padova

LESSON 3: FUNDAMENTAL SOLUTION OF DIFFUSION

FUNDAMENTAL SOLUTION

It is useful to study diffusion by dimensional analysis. From the definition of Diffusivity:

$$D = \frac{L^2}{T} \longrightarrow L \propto \sqrt{DT}$$

Now, we express the problem by the following non-dimensional parameter:

$$\eta = \frac{x}{\sqrt{4Dt}}$$

$\sqrt{4Dt}$ → *Length scale of the problem*

It is worth noting that: $\eta = \eta(x,t)$

And then:

$$\frac{\partial \eta}{\partial x} = \frac{\partial}{\partial x}\left(\frac{x}{\sqrt{4Dt}}\right) = \frac{1}{\sqrt{4Dt}}$$

$$\frac{\partial \eta}{\partial t} = \frac{\partial}{\partial t}\left(\frac{x}{\sqrt{4Dt}}\right) = -\frac{4D}{2}\frac{1}{4Dt}\underbrace{\frac{x}{\sqrt{4Dt}}}_{\eta} = -\frac{1}{2t}\eta$$

The concentration can be expressed as:

$$c = M\, f(x, t, D) \longrightarrow c = \frac{M}{\sqrt{4Dt}}\, g(\eta)$$

This term preserves the physical meaning of c

Now, let's analyze the differential equation:

$$\underbrace{\frac{\partial c}{\partial t}}_{a} = D\, \underbrace{\frac{\partial^2 c}{\partial x^2}}_{b}$$

a

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial t}\left(\frac{M}{\sqrt{4Dt}}\, g(\eta)\right) = -\frac{1}{2t}\frac{M}{\sqrt{4Dt}} g(\eta) + \frac{M}{\sqrt{4Dt}}\frac{\partial g(\eta)}{\partial t}$$

$$\frac{\partial c}{\partial t} = -\frac{1}{2t}\frac{M}{\sqrt{4Dt}} g(\eta) + \frac{M}{\sqrt{4Dt}}\frac{\mathrm{d}g}{\mathrm{d}\eta}\frac{\partial \eta}{\partial t} = -\frac{1}{2t}\frac{M}{\sqrt{4Dt}} g(\eta) - \frac{1}{2t}\eta\frac{M}{\sqrt{4Dt}}\frac{\mathrm{d}g}{\mathrm{d}\eta}$$

$$\frac{\partial \eta}{\partial t} = -\frac{1}{2t}\eta$$

$$\longrightarrow \frac{\partial c}{\partial t} = -\frac{1}{2t}\frac{M}{\sqrt{4Dt}}\left(g(\eta) + \eta\frac{\mathrm{d}g}{\mathrm{d}\eta}\right)$$

b

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right)$$

$$\frac{\partial c}{\partial x} = \frac{M}{\sqrt{4Dt}}\frac{\partial g(\eta)}{\partial x}$$

$$\frac{\partial c}{\partial x} = \frac{M}{\sqrt{4Dt}}\frac{\mathrm{d}g}{\mathrm{d}\eta}\frac{\partial \eta}{\partial x} = \frac{M}{\sqrt{4Dt}}\frac{1}{\sqrt{4Dt}}\frac{\mathrm{d}g}{\mathrm{d}\eta}$$

$$\frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{4Dt}}$$

$$\longrightarrow \frac{\partial c}{\partial x} = \frac{M}{4Dt}\frac{\mathrm{d}g}{\mathrm{d}\eta}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{M}{4Dt}\frac{\mathrm{d}g}{\mathrm{d}\eta}\right)$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{M}{4Dt}\frac{\partial}{\partial x}\left(\frac{\mathrm{d}g}{\mathrm{d}\eta}\right) = \frac{M}{4Dt}\frac{\mathrm{d}^2 g}{\mathrm{d}\eta^2}\frac{\partial \eta}{\partial x}$$

$$\longrightarrow \frac{\partial^2 c}{\partial x^2} = \frac{M}{4Dt}\frac{1}{\sqrt{4Dt}}\frac{\mathrm{d}^2 g}{\mathrm{d}\eta^2}$$

The solutions of (a) and (b) in the 1-D Diffusion equation yield:

$$-\frac{1}{2\cancel{t}}\frac{\cancel{M}}{\cancel{\sqrt{4Dt}}}\left(g(\eta)+\eta\frac{\mathrm{d}g}{\mathrm{d}\eta}\right)=\cancel{D}\frac{\cancel{M}}{4\cancel{Dt}}\frac{1}{\cancel{\sqrt{4Dt}}}\frac{\mathrm{d}^2g}{\mathrm{d}\eta^2}$$

$$\longrightarrow \quad \frac{\mathrm{d}^2g}{\mathrm{d}\eta^2}+2\eta\frac{\mathrm{d}g}{\mathrm{d}\eta}+2g=0$$

Ordinary Differential Equation

The latter equation is easily solved, by integrating the following expression:

$$\frac{\mathrm{d}^2g}{\mathrm{d}\eta^2}+2\frac{\mathrm{d}}{\mathrm{d}\eta}(\eta g)=0$$

$$\int\frac{\mathrm{d}^2g}{\mathrm{d}\eta^2}\mathrm{d}\eta+2\int\frac{\mathrm{d}}{\mathrm{d}\eta}(\eta g)\,\mathrm{d}\eta=-k_1$$

$$\longrightarrow \quad \frac{\mathrm{d}g}{\mathrm{d}\eta}+2\,\eta g+k_1=0$$

The <u>symmetry</u> of c (and then of $g(\eta)$) allows to determine the constant k_1:

$$\left.\frac{\partial c}{\partial x}\right|_{x=0} = 0 \rightarrow \left.\frac{\partial g}{\partial \eta}\right|_{\eta=0} = 0 \quad \xrightarrow{\text{yields}} \quad \cancel{\frac{\mathrm{d}g}{\mathrm{d}\eta}}^{0} + 2\,\cancel{\eta}^{0} g + k_1 = 0 \quad \longrightarrow \quad k_1 = 0$$

And then:

$$\frac{\mathrm{d}g}{\mathrm{d}\eta} + 2\,\eta g = 0$$

Separating the variables and integrating, the latter equation reads:

$$-\eta\,\mathrm{d}\eta = \frac{1}{2}\frac{\mathrm{d}g}{g} \quad \xrightarrow{\int} -\int \eta\,\mathrm{d}\eta = \frac{1}{2}\int \frac{\mathrm{d}g}{g}$$

$$-\cancel{\frac{1}{2}}\eta^2 = \cancel{\frac{1}{2}}\ln g + k \quad \xrightarrow{\text{exp}} \quad g = k_2\, e^{-\eta^2}$$

The constant k_2 is determined by the mass conservation:

$$M = \int_{-\infty}^{+\infty} c \, \mathrm{d}x = \int_{-\infty}^{+\infty} \frac{M}{\sqrt{4Dt}} k_2 \, e^{-\eta^2} \, \mathrm{d}x$$

By changing the integration variable ($x \rightarrow \eta$), the mass conservation reads:

$$\cancel{M} = \cancel{M} \int_{-\infty}^{+\infty} \frac{1}{\cancel{\sqrt{4Dt}}} k_2 \, e^{-\eta^2} \, \cancel{\sqrt{4Dt}} \, \mathrm{d}\eta$$

$$\eta = \frac{x}{\sqrt{4Dt}} \longrightarrow \mathrm{d}\eta = \frac{\mathrm{d}x}{\sqrt{4Dt}}$$

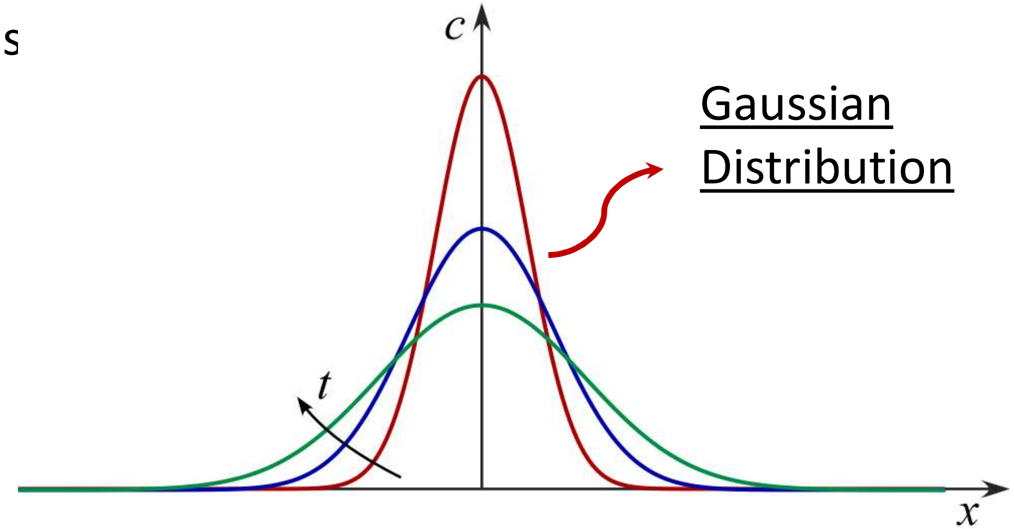
$$k_2 \int_{-\infty}^{+\infty} e^{-\eta^2} \, \mathrm{d}\eta = 1 \longrightarrow k_2 = \frac{1}{\sqrt{\pi}}$$

Remarkable integral: $\int_{-\infty}^{+\infty} e^{-\eta^2} \, \mathrm{d}\eta = \sqrt{\pi}$

Finally, the solution of the diffusion equation is

$$c = \frac{M}{\sqrt{4Dt}} \frac{1}{\sqrt{\pi}} e^{-\eta^2}$$

$$\longrightarrow \quad c = \frac{M}{\sqrt{4\pi Dt}} \, e^{-\frac{x^2}{4Dt}}$$



The solution can be analyzed by statistical moments:

$$\mathcal{M}_0 = \int_{-\infty}^{+\infty} c \, \mathrm{d}x = M$$ → Mass solute

$$\mathcal{M}_1 = \int_{-\infty}^{+\infty} c \, x \, \mathrm{d}x = \mu \, \mathcal{M}_0$$ → μ is the centroid of solute distribution

$$\mathcal{M}_2 = \int_{-\infty}^{+\infty} (x-\mu)^2 \, c \, \mathrm{d}x = \sigma^2 \, \mathcal{M}_0$$ → σ^2 is the variance of solute distribution

Let's analyze the statistical moment of 1st order, in particular μ:

$$\mu = \frac{1}{\mathcal{M}_0} \int_{-\infty}^{+\infty} c \, x \mathrm{d}x$$

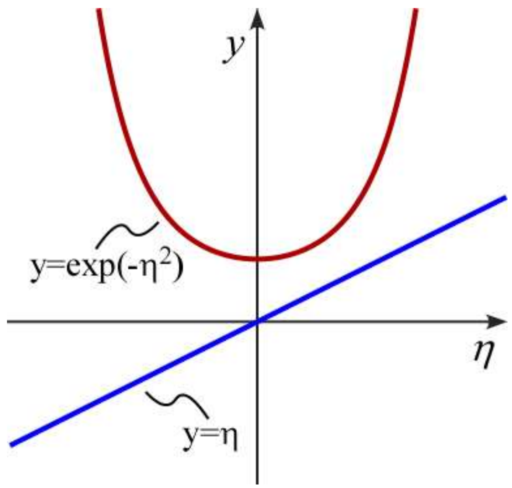
$$\mu = \frac{1}{\cancel{M}} \int_{-\infty}^{+\infty} \frac{\cancel{M}}{\sqrt{4\pi D t}} \, e^{-\frac{x^2}{4Dt}} \, x \, \mathrm{d}x = \int_{-\infty}^{+\infty} \frac{\eta}{\sqrt{\pi}} \, e^{-\eta^2} \sqrt{4Dt} \, \mathrm{d}\eta$$

$$\eta = \frac{x}{\sqrt{4Dt}} \longrightarrow \mathrm{d}\eta = \frac{\mathrm{d}x}{\sqrt{4Dt}}$$

$$\mu = \sqrt{\frac{4Dt}{\pi}} \int_{-\infty}^{+\infty} \eta \, e^{-\eta^2} \, \mathrm{d}\eta$$

In general: $\mathcal{M}_n = \int_{-\infty}^{+\infty} (x-\mu)^n \, c \, \mathrm{d}x = \sigma^2 \, \mathcal{M}_0$

PROPERTIES OF FUNDAMENTAL SOLUTION



$$\eta\, e^{-\eta^2} = |\eta|\, e^{-\eta^2}$$

$\eta \geq 0$ $\quad$ $\eta < 0$

Odd function

→ $\mu = 0$

Let's analyze the statistical moment of 2nd order, in particular σ^2:

$$\sigma^2 = \frac{1}{\mathcal{M}_0}\int_{-\infty}^{+\infty} (x-\mu)^2\, c\, \mathrm{d}x = \frac{1}{M}\int_{-\infty}^{+\infty} \frac{M}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}}\, x^2\, \mathrm{d}x$$

$$\eta = \frac{x}{\sqrt{4Dt}} \longrightarrow \mathrm{d}\eta = \frac{\mathrm{d}x}{\sqrt{4Dt}}$$

$$\sigma^2 = \frac{4Dt}{\sqrt{4\pi D t}}\int_{-\infty}^{+\infty} \eta^2\, e^{-\eta^2}\sqrt{4Dt}\, \mathrm{d}\eta = \frac{4Dt}{\sqrt{\pi}}\frac{\sqrt{\pi}}{2}$$

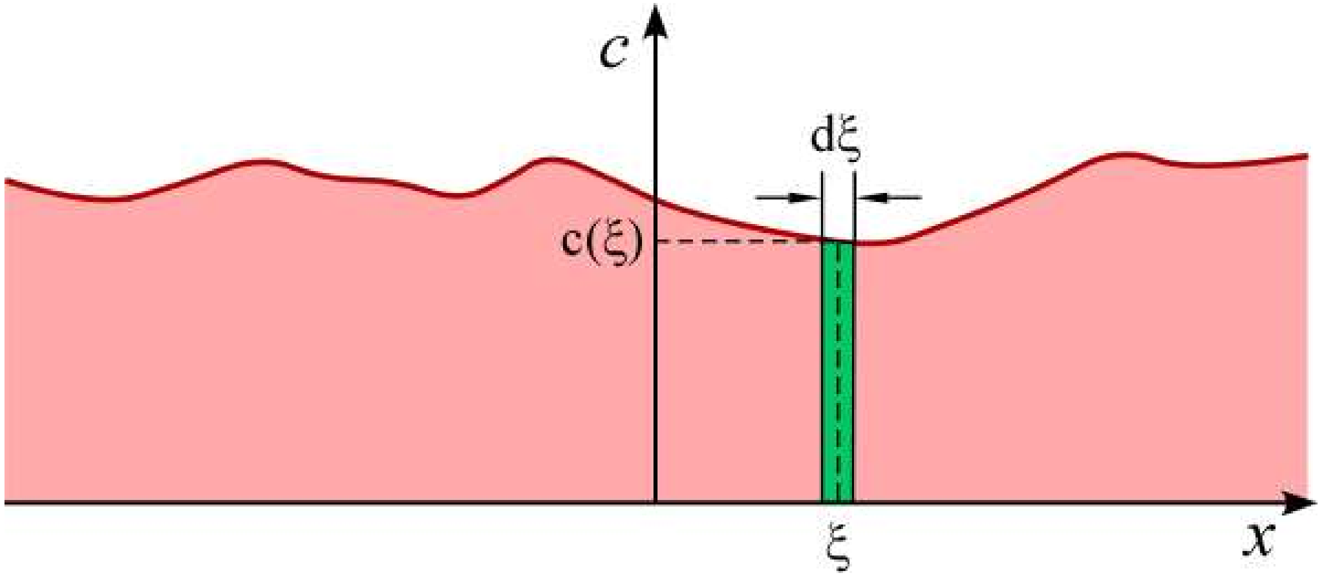
Remarkable integral: $\int_{-\infty}^{+\infty} \eta^2 e^{-\eta^2}\, \mathrm{d}\eta = \frac{\sqrt{\pi}}{2}$

→ $\sigma^2 = 2Dt$

Variance linearly increases with time: $\frac{\mathrm{d}\sigma^2}{\mathrm{d}t} = 2D$

GENERAL PROBLEM

Let's consider the following problem:



Initial distribution of solute concentration

$$c(x,0) = c_0(x)$$

The solution is due to the superposition principle. In particular, we analyze the small green area, that can be approximated as:

$$c_0(\xi)\mathrm{d}\xi$$

Central value of c_0 ← → *width*

→ We assume that $c_0(\xi)$ is uniform in dξ

When $\mathrm{d}\xi \rightarrow 0$, the area becomes a slug release of mass $\mathrm{d}M$. Indeed:

$$\mathrm{d}M = c_0(\xi)\mathrm{d}\xi\,\mathrm{d}y\,\mathrm{d}z \quad (\mathrm{d}y = 1,\ \mathrm{d}z = 1) \longrightarrow \widehat{c_0}(x) = \mathrm{d}M\delta(x-\xi)$$

Lumped injection of mass

The solution is the same of the one shown previously (fundamental solution), that is:

$$\hat{c}(x,t,\xi) = \frac{\mathrm{d}M}{\sqrt{4\pi D t}}\, e^{-\frac{(x-\xi)^2}{4Dt}}$$

Contribution due to $\mathrm{d}\xi$

Therefore the solution for $c_0(x)$ is the convolution of the fundamental case along the whole domain. Formally, it reads:

$$\longrightarrow \quad c(x,t) = \int_{-\infty}^{+\infty} \hat{c}(x,t,\xi)\,\mathrm{d}\xi = \frac{1}{\sqrt{4\pi D t}} \int_{-\infty}^{+\infty} c_0(\xi)\, e^{-\frac{(x-\xi)^2}{4Dt}}\,\mathrm{d}\xi$$

Also in this case the mass is conserved. Indeed:

$$M = \int_{-\infty}^{+\infty} c(x,t)\,\mathrm{d}x = \int_{-\infty}^{+\infty} \left[\frac{1}{\sqrt{4\pi D t}} \int_{-\infty}^{+\infty} c_0(\xi)\, e^{-\frac{(x-\xi)^2}{4Dt}} \mathrm{d}\xi\right] \mathrm{d}x$$

$$M = \int_{-\infty}^{+\infty} \frac{c_0(\xi)}{\sqrt{4\pi D t}} \left[\int_{-\infty}^{+\infty} e^{-\frac{(x-\xi)^2}{4Dt}}\,\mathrm{d}x\right] \mathrm{d}\xi$$

$$\eta = \frac{x-\xi}{\sqrt{4Dt}} \longrightarrow \mathrm{d}\eta = \frac{\mathrm{d}x}{\sqrt{4Dt}}$$

$$M = \int_{-\infty}^{+\infty} \frac{c_0(\xi)}{\cancel{\sqrt{4Dt}}\sqrt{\pi}} \left[\cancel{\sqrt{4Dt}} \int_{-\infty}^{+\infty} e^{-\eta^2}\,\mathrm{d}\eta\right] \mathrm{d}\xi$$

$$\int_{-\infty}^{+\infty} e^{-\eta^2}\,\mathrm{d}\eta = \sqrt{\pi}$$

$$M = \int_{-\infty}^{+\infty} \frac{c_0(\xi)}{\cancel{\sqrt{\pi}}} \cancel{\sqrt{\pi}}\,\mathrm{d}\xi = \int_{-\infty}^{+\infty} c_0(\xi)\mathrm{d}\xi$$

That is:

$$M = \int_{-\infty}^{+\infty} c(x,t)\,\mathrm{d}x = \int_{-\infty}^{+\infty} c_0(\xi)\mathrm{d}\xi$$

The mass is constant with time varying