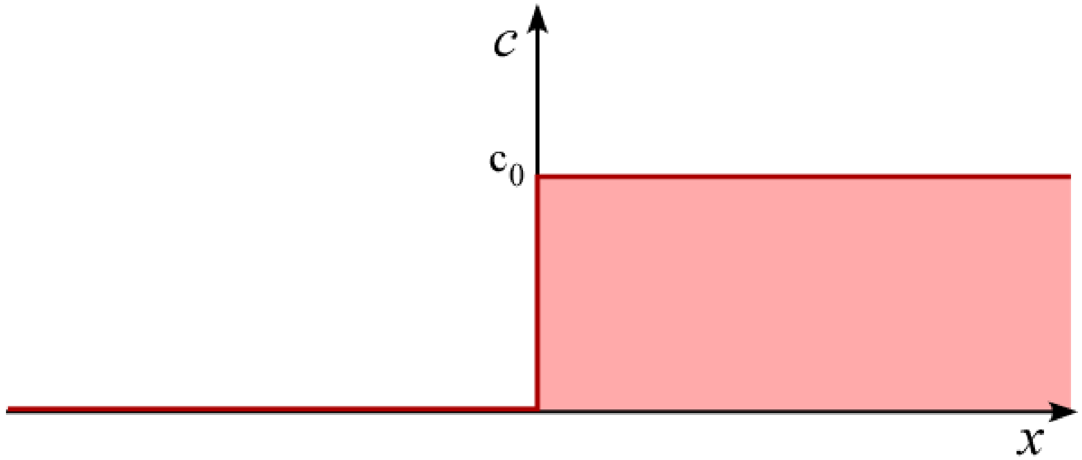
ICEA

UNIVERSITÀ DEGLI STUDI DI PADOVA

# LESSON 4: REMARKABLE CASES OF DIFFUSION

Let's analyze the following case at $t = 0$:




$$c(x,0) = \begin{cases} 0 & x < 0 \\ c_0 & x \geq 0 \end{cases}$$

In this case, the convolution of the fundamental solution reads:

$$c(x,t) = \frac{c_0}{\sqrt{4\pi D t}} \int_0^{+\infty} e^{-\frac{(x-\xi)^2}{4Dt}} \, \mathrm{d}\xi$$

The solution of the integral requires the change of the integration variable $\xi$ with $\eta$, that is defined as:

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

It is worth noting that: $\mathrm{d}\eta = -\dfrac{\mathrm{d}\xi}{\sqrt{4Dt}}$

And then the extremities of integration become:

$$\xi = 0 \quad \longrightarrow \quad \eta = \frac{x}{\sqrt{4Dt}}$$

$$\xi \to +\infty \quad \longrightarrow \quad \eta \to -\infty$$

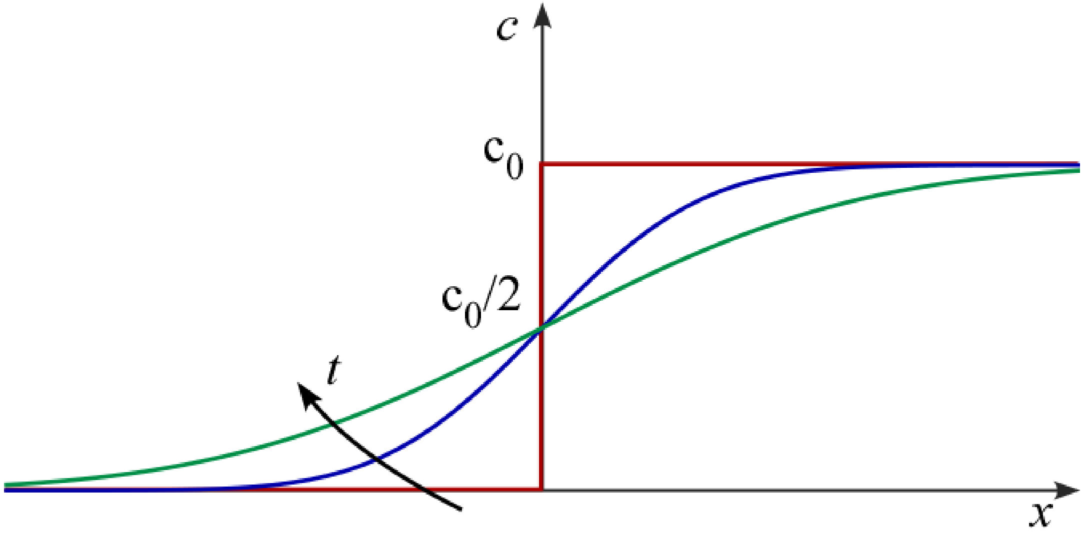
The integral reads:

$$c(\eta,t) = -\frac{c_0}{\cancel{\sqrt{4Dt}}\sqrt{\pi}}\cancel{\sqrt{4Dt}}\int_{\frac{x}{\sqrt{4Dt}}}^{-\infty} e^{-\eta^2}\,\mathrm{d}\eta$$

$$c(\eta,t) = \frac{c_0}{\sqrt{\pi}}\int_{-\infty}^{\frac{x}{\sqrt{4Dt}}} e^{-\eta^2}\,\mathrm{d}\eta = \frac{c_0}{\sqrt{\pi}}\left[\underbrace{\int_{-\infty}^{0} e^{-\eta^2}\,\mathrm{d}\eta}_{\frac{\sqrt{\pi}}{2}} + \underbrace{\int_{0}^{\frac{x}{\sqrt{4Dt}}} e^{-\eta^2}\,\mathrm{d}\eta}_{\frac{\sqrt{\pi}}{2}\,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right)}\right]$$

Finally, the equation infers in the following:

$$c(x,t) = \frac{c_0}{2}\left[1 + \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right]$$




Nothing that:

$$c(0,t) = \frac{c_0}{2}$$

$$c(\infty,t) = c_0$$

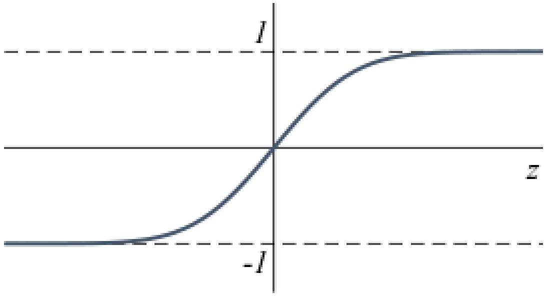
$$c(-\infty,t) = 0$$

*Error function* $\mathrm{erf}(z)$ *is defined as:* $\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-\eta^2}\,\mathrm{d}\eta$

*Properties:* $\mathrm{erf}(-z) = -\mathrm{erf}(z)$

$\mathrm{erf}(0) = 0$

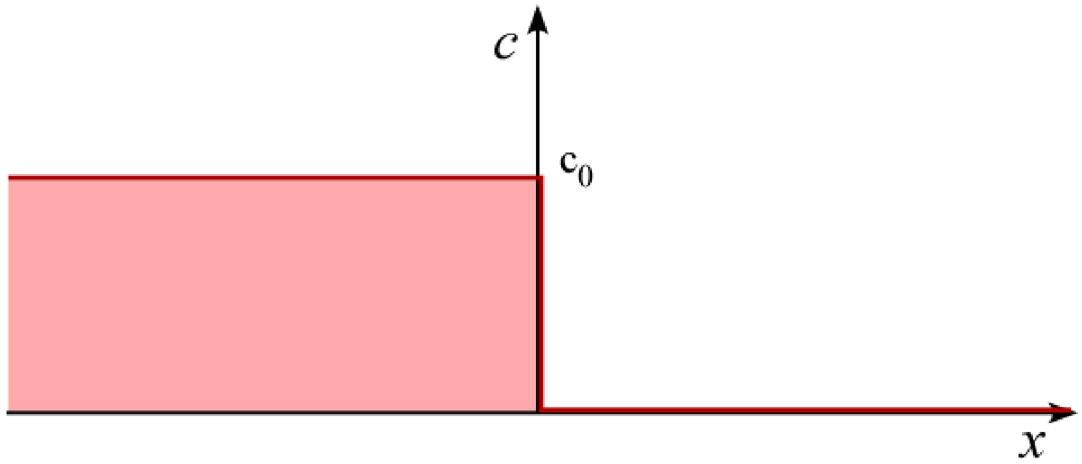
$\mathrm{erf}(\pm\infty) = \pm 1$



# STEP DISTRIBUTION OF CONCENTRATION

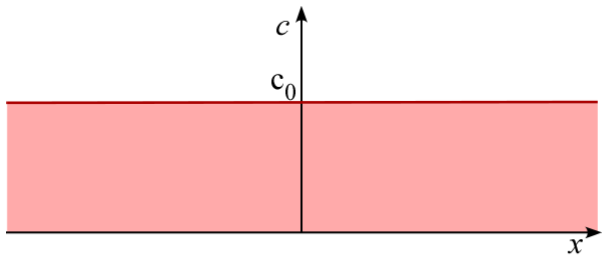


For the step of concentration on the left side of the domain at $t = 0$




$$c(x,0) = \begin{cases} c_0 & x \le 0 \\ 0 & x > 0 \end{cases}$$

the solution is due to the superposition of the following cases:

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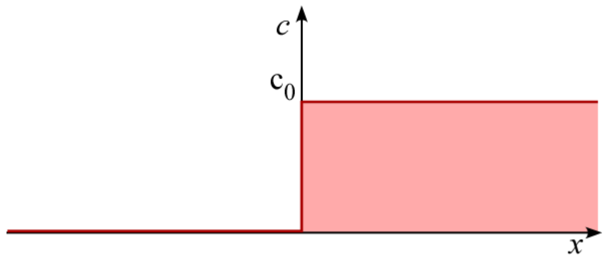



$$c(x,t) = c_0$$

$$c(x,t) = \frac{c_0}{2}\left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right]$$

# STEP DISTRIBUTION OF CONCENTRATION



That is: $c(x,t) = c_0 - \dfrac{c_0}{2}\left[1 + \mathrm{erf}\left(\dfrac{x}{\sqrt{4Dt}}\right)\right] = \dfrac{c_0}{2}\left[1 - \mathrm{erf}\left(\dfrac{x}{\sqrt{4Dt}}\right)\right]$

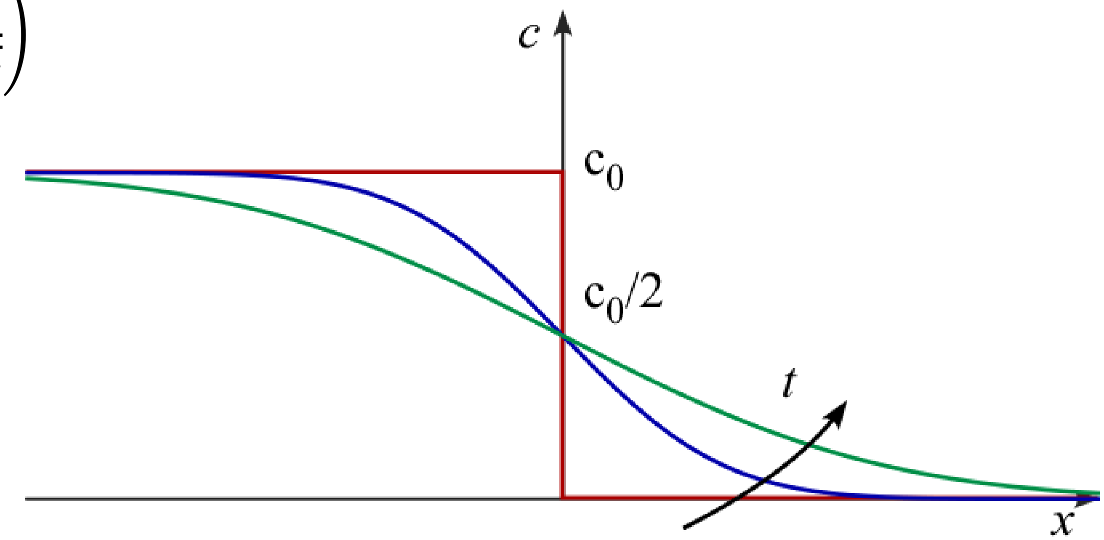
$$\longrightarrow \quad c(x,t) = \frac{c_0}{2}\,\mathrm{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)$$

Noting that:

$$c(0,t) = \frac{c_0}{2}$$

$$c(\infty,t) = 0$$

$$c(-\infty,t) = c_0$$




*Complementary Error function* $\mathrm{erfc}(z)$ *is:* $\mathrm{erfc}(z) = \dfrac{2}{\sqrt{\pi}}\displaystyle\int_z^{\infty} e^{-\eta^2}\,\mathrm{d}\eta$

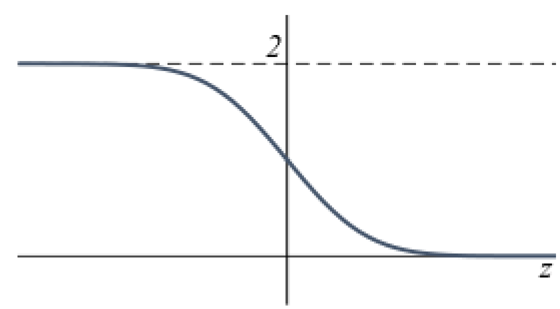
*Properties:*

$\mathrm{erfc}(z) = 1 - \mathrm{erf}(z)$

$\mathrm{erfc}(0) = 1$

$\mathrm{erfc}(+\infty) = 0$

$\mathrm{erf}(-\infty) = 2$

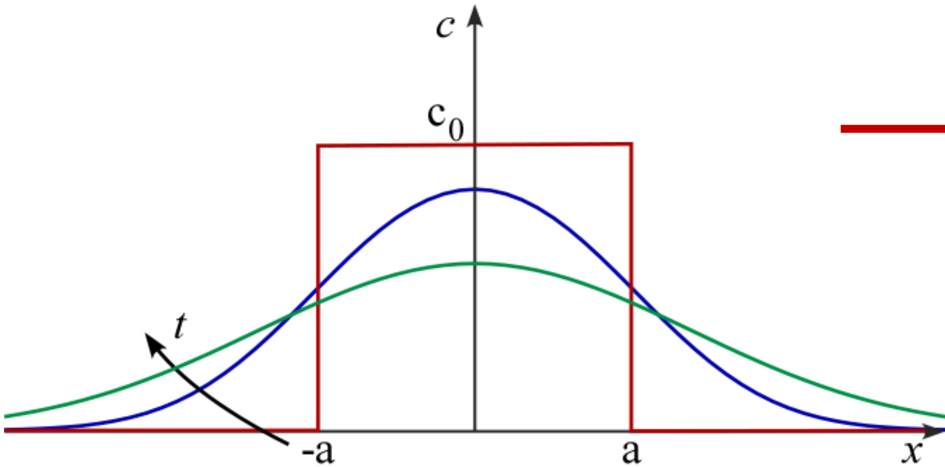


# INNER STEP



The solution of $c(x,t)$, starting from the inner step of concentration, is given by the difference of two steps of concentration:

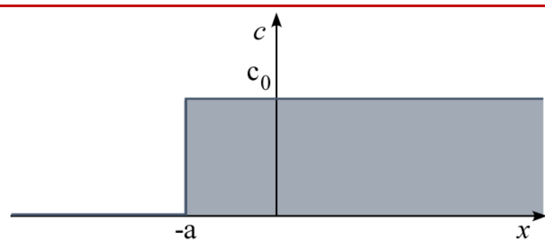
$$c(x,t)=\frac{c_0}{2}\left[\cancel{1}+\mathrm{erf}\left(\frac{a+x}{\sqrt{4Dt}}\right)\right]-\frac{c_0}{2}\left[\cancel{1}+\mathrm{erf}\left(\frac{x-a}{\sqrt{4Dt}}\right)\right]=\frac{c_0}{2}\left[\mathrm{erf}\left(\frac{a+x}{\sqrt{4Dt}}\right)-\mathrm{erf}\left(\frac{x-a}{\sqrt{4Dt}}\right)\right]$$




$$\longrightarrow \quad c(x,t)=\frac{c_0}{2}\left[\mathrm{erf}\left(\frac{a+x}{\sqrt{4Dt}}\right)+\mathrm{erf}\left(\frac{a-x}{\sqrt{4Dt}}\right)\right]$$

Noting that:

$$c(0,t)=c_0\,\mathrm{erf}\left(\frac{a}{\sqrt{4Dt}}\right)$$




$$c(x,t)=\frac{c_0}{2}\left[1+\mathrm{erf}\left(\frac{a+x}{\sqrt{4Dt}}\right)\right]$$

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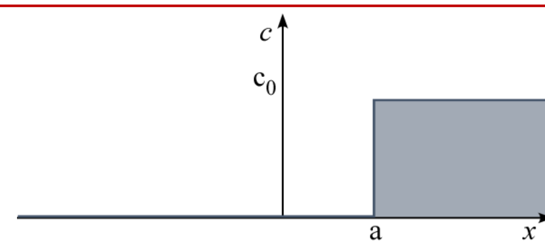


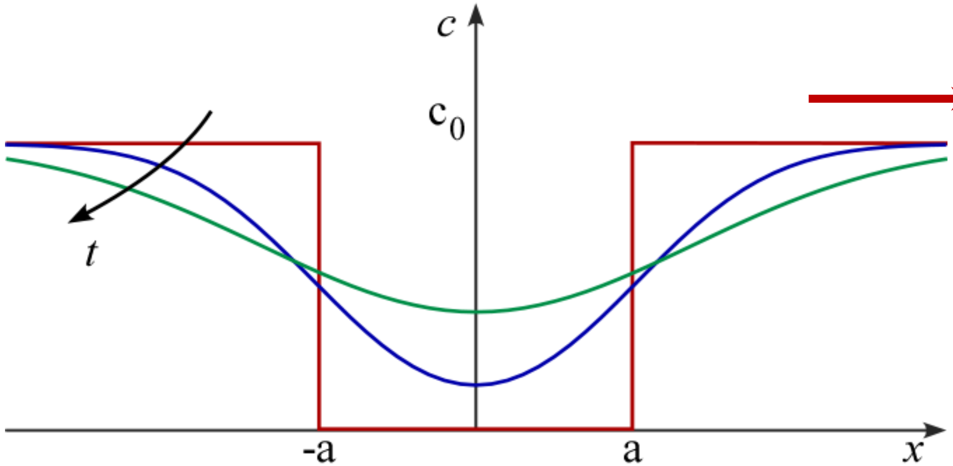

$$c(x,t)=\frac{c_0}{2}\left[1+\mathrm{erf}\left(\frac{x-a}{\sqrt{4Dt}}\right)\right]$$

# EXTERNAL STEPS



The solution of $c(x,t)$, starting from external steps of concentration, is given by the sum of two steps of concentration:

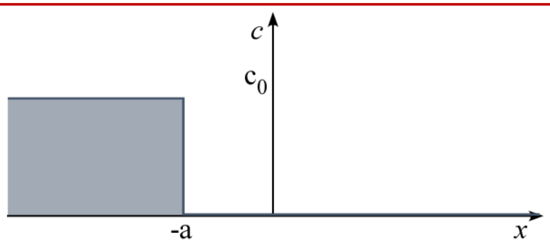
$$c(x,t)=\frac{c_0}{2}\operatorname{erfc}\left(\frac{a+x}{\sqrt{4Dt}}\right)+\frac{c_0}{2}\left[1+\operatorname{erf}\left(\frac{x-a}{\sqrt{4Dt}}\right)\right]=\frac{c_0}{2}\operatorname{erfc}\left(\frac{a+x}{\sqrt{4Dt}}\right)+\frac{c_0}{2}\left[1-\operatorname{erf}\left(\frac{a-x}{\sqrt{4Dt}}\right)\right]$$




$$c(x,t)=\frac{c_0}{2}\left[\operatorname{erfc}\left(\frac{a+x}{\sqrt{4Dt}}\right)+\operatorname{erfc}\left(\frac{a-x}{\sqrt{4Dt}}\right)\right]$$

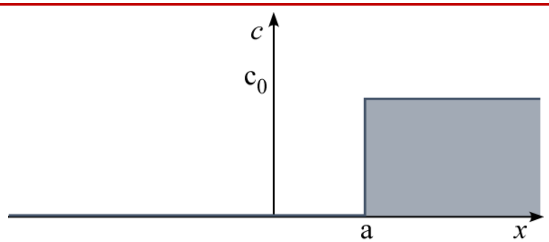
Noting that:

$$c(0,t)=c_0\operatorname{erfc}\left(\frac{a}{\sqrt{4Dt}}\right)$$




$$c(x,t)=\frac{c_0}{2}\operatorname{erfc}\left(\frac{a+x}{\sqrt{4Dt}}\right)$$

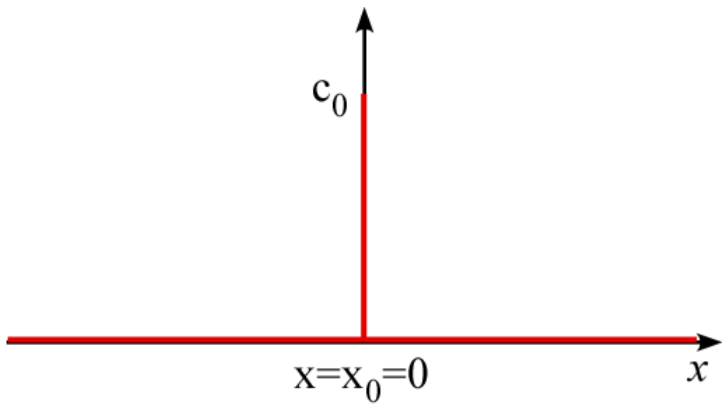
+




$$c(x,t)=\frac{c_0}{2}\left[1+\operatorname{erf}\left(\frac{x-a}{\sqrt{4Dt}}\right)\right]$$

# SOURCE POINT

Let's analyze the case in which  constant concentration is maintained in a source point:




$$c(x,0) = \begin{cases} \dfrac{\partial c}{\partial t} = D\,\dfrac{\partial^2 c}{\partial x^2} \\ c(x,0) = 0 \qquad x \neq x_0 = 0 \\ c(x_0,t) = c_0 \qquad x = x_0 = 0 \end{cases}$$

*Concentration is constant with time varying*

Formally the solution is similar to the fundamental one:

$$c = c_0\, f(\eta)$$

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

$$\longrightarrow \quad f(\eta) = ?$$

Let's see the terms in the Diffusion equation: $\underset{a}{\dfrac{\partial c}{\partial t}} = D \underset{b}{\dfrac{\partial^2 c}{\partial x^2}}$

a $$\frac{\partial c}{\partial t} = c_0 \frac{\partial f(\eta)}{\partial t} = c_0 \frac{\mathrm{d}f}{\mathrm{d}\eta}\frac{\partial \eta}{\partial t} \longrightarrow \frac{\partial c}{\partial t} = -\frac{c_0}{2t}\eta\frac{\mathrm{d}f}{\mathrm{d}\eta}$$

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

b $$\frac{\partial^2 c}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right) = \frac{\partial}{\partial x}\left(c_0 \frac{\partial f(\eta)}{\partial x}\right) = c_0 \frac{\partial}{\partial x}\left(\frac{\mathrm{d}f}{\mathrm{d}\eta}\frac{\partial \eta}{\partial x}\right)$$

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

$$\frac{\partial^2 c}{\partial x^2} = \frac{c_0}{\sqrt{4Dt}}\frac{\partial}{\partial x}\left(\frac{\mathrm{d}f}{\mathrm{d}\eta}\right) = \frac{c_0}{\sqrt{4Dt}}\frac{\partial \eta}{\partial x}\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{\mathrm{d}f}{\mathrm{d}\eta}\right) \longrightarrow \frac{\partial^2 c}{\partial x^2} = \frac{c_0}{4Dt}\frac{\mathrm{d}^2 f}{\mathrm{d}\eta^2}$$

By replacing the two terms into the diffusion equation, it reads:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

$$-\frac{\cancel{c_0}}{2\cancel{t}}\eta\frac{\mathrm{d}f}{\mathrm{d}\eta} = \cancel{D}\frac{\cancel{c_0}}{\cancel{4}\cancel{D}\cancel{t}}\frac{\mathrm{d}^2 f}{\mathrm{d}\eta^2} \longrightarrow \frac{\mathrm{d}^2 f}{\mathrm{d}\eta^2} + 2\eta\frac{\mathrm{d}f}{\mathrm{d}\eta} = 0$$

<u>Ordinary Differential Equation (ODE)</u>

ODE can be easily solved by integrating twice, i.e.:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}\eta^2} + 2\eta\frac{\mathrm{d}f}{\mathrm{d}\eta} = 0 \quad \xrightarrow{\int} \quad \frac{\mathrm{d}f}{\mathrm{d}\eta} = k_1 e^{-\eta^2}$$

$$\frac{\mathrm{d}f}{\mathrm{d}\eta} = k_1 e^{-\eta^2} \quad \xrightarrow{\int} \quad f(\eta) = k_1\int_0^\eta e^{-\xi^2}\mathrm{d}\xi + k_2$$

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-\eta^2}\,\mathrm{d}\eta$$

$$\longrightarrow \quad f(\eta) = k_1\frac{\sqrt{\pi}}{2}\mathrm{erf}(\eta) + k_2$$

The two constants of integration are determined by the BCs of the problem. Indeed:

1) $x = 0 \quad \rightarrow \quad c = c_0 \quad \longrightarrow \quad \eta = \dfrac{x}{\sqrt{4Dt}} = 0 \quad \rightarrow \quad \dfrac{c}{c_0} = f(\eta) = 1$

Then:

$$f(0) = k_1\frac{\sqrt{\pi}}{2}\underbrace{\mathrm{erf}(0)}_{0} + k_2 = 1 \quad \longrightarrow \quad k_2 = 1$$

2) $\lim_{x\to\pm\infty} c = 0 \longrightarrow \lim_{\eta\to\pm\infty} f(\eta) = 0$

Then:

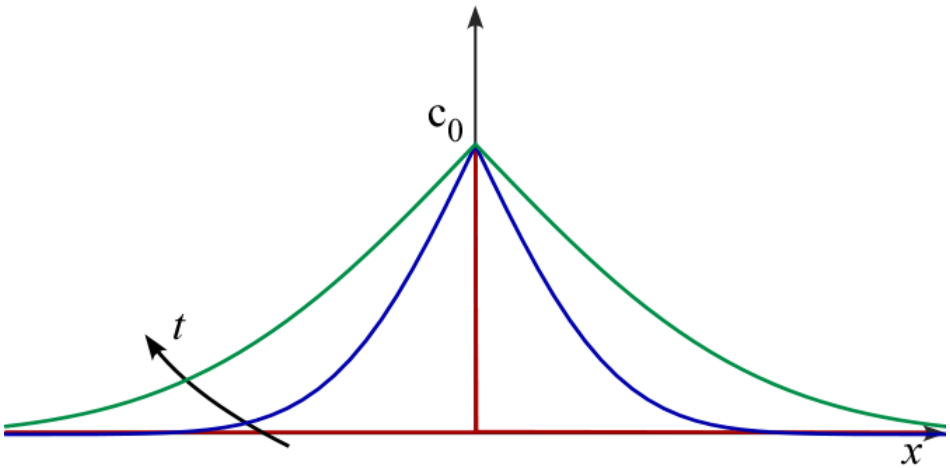
$$f = k_1 \frac{\sqrt{\pi}}{2}\operatorname{erf}(\pm\infty) + 1 = k_1 \frac{\sqrt{\pi}}{2}(\pm 1) + 1 = 0$$

a) $k_1 \frac{\sqrt{\pi}}{2} + 1 = 0 \longrightarrow k_1 = -\frac{2}{\sqrt{\pi}} \qquad \eta, x \geq 0$

b) $-k_1 \frac{\sqrt{\pi}}{2} + 1 = 0 \longrightarrow k_1 = \frac{2}{\sqrt{\pi}} \qquad \eta, x < 0$

Finally, the solution is:

$$\longrightarrow \begin{cases} c(x,t) = c_0\left[1 - \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right] = c_0 \operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) & x \geq 0 \\ c(x,t) = c_0\left[1 - \operatorname{erf}\left(\frac{|x|}{\sqrt{4Dt}}\right)\right] = c_0 \operatorname{erfc}\left(\frac{|x|}{\sqrt{4Dt}}\right) & x < 0 \end{cases}$$




Let's calculate the mass of the system, which varies with time varying.

$$M = \int_{-\infty}^{+\infty} c(x,t)\,\mathrm{d}x = 2\,c_0 \int_0^{+\infty} \mathrm{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)\mathrm{d}x$$

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

$$M = 2c_0\sqrt{4Dt}\int_0^{+\infty}\mathrm{erfc}(\eta)\mathrm{d}\eta \longrightarrow M = 1.1284\,c_0\sqrt{4Dt}$$

$$M \propto \sqrt{t}$$

Moreover, the mass rate is:

$$\frac{\mathrm{d}M}{\mathrm{d}t} = 1.1284\,c_0\sqrt{4D}\,\frac{\mathrm{d}\sqrt{t}}{\mathrm{d}t} = 1.1284\,c_0\sqrt{4D}\,\frac{1}{2\sqrt{t}} \longrightarrow \dot{M} = 0.5642\,c_0\sqrt{\frac{4D}{t}}$$

# SOURCE POINT



The general case of source point of a solute is described by the following system of equations:

$$c(x,0) = \begin{cases} \dfrac{\partial c}{\partial t} = D\,\dfrac{\partial^2 c}{\partial x^2} & \\ c(x,0) = 0 & x = 0 \\ c(0,t) = c_0(t) & x = 0 \end{cases}$$

The solution is determined by Taylor's series expansion: $t = \tau + \mathrm{d}\tau \quad \rightarrow \quad c(t) = c(\tau + \mathrm{d}\tau)$

Then, when $x$ if fixed: $$c_0(\tau + \mathrm{d}\tau) = c_0(\tau) + \left.\frac{\mathrm{d}c_0}{\mathrm{d}\tau}\right|_\tau \mathrm{d}\tau + O(\mathrm{d}\tau^2)$$

the solution for source point with $c_0$ constant in $\mathrm{d}\tau$ is:

$$\mathrm{d}c(x,\tau) = \left.\frac{\mathrm{d}c_0}{\mathrm{d}\tau}\right|_\tau \mathrm{d}\tau \,\mathrm{erfc}\left(\frac{|x|}{\sqrt{4D(t-\tau)}}\right) \longrightarrow$$

*$c$ profile observed at $\mathrm{d}\tau$ after the injection of $\frac{\mathrm{d}c_0}{\mathrm{d}\tau}\mathrm{d}\tau$*

$\mathrm{d}\tau = t - \tau$

By integrating the latter between $[0,t]$, we find the solution:

$$\longrightarrow \quad c(x,t) = \int_0^t \frac{\mathrm{d}c_0}{\mathrm{d}\tau}\,\mathrm{erfc}\left(\frac{|x|}{\sqrt{4D(t-\tau)}}\right)\mathrm{d}\tau$$