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Département fédéral de l'intérieur DFI
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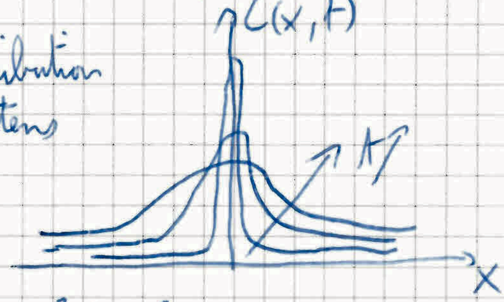
Solution of the D.E. (various initial and boundary conditions)

1 Point source (1D)

$$C(x,t) = \frac{M}{A\sqrt{4\pi D t}}\, e^{-x^2/4Dt} \qquad (*)$$



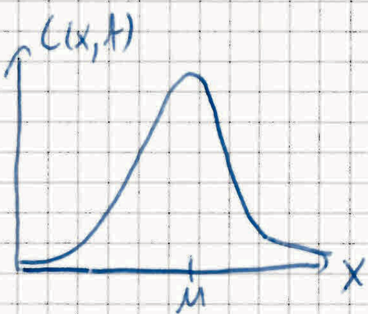
Compare with Normal distribution: $\frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-x^2/2\sigma^2} = N(0,\sigma)$

Variance $2Dt \to 0$ for $t \to 0$ (in this limit the distribution becomes a δ Dirac distribution)

It is of course easy to verify that $(*)$ satisfies the diffusion equation $\frac{\partial C}{\partial t} = D\,\frac{\partial^2 C}{\partial x^2}$ by computing derivatives of the solution.

2 Source located at $x = \mu$ (point)

$$C(x,t) = \frac{M}{A\sqrt{4\pi D t}}\, e^{-(x-\mu)^2/4Dt}$$

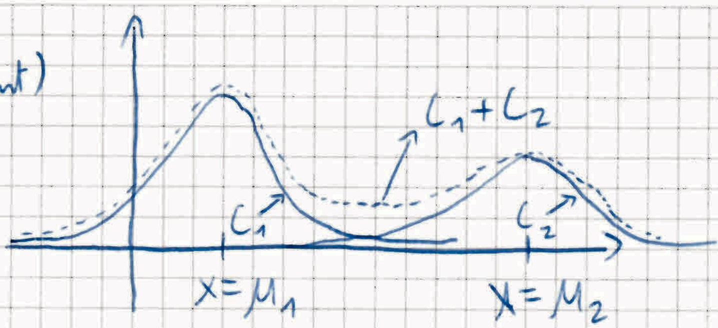


The distribution has a maximum when the argument of the exponential is zero.

Again easy to verify that it is solution of the diffusion equation.

3) Two sources (point)

$M_1 > M_2$



C_1 solution for source 1, C_2 for source 2

We have $C_{1,2} = \dfrac{M_{1,2}}{A\sqrt{4\pi D t}} e^{-(x-\mu_{1,2})^2/4Dt}$

If C_1 and C_2 are solutions of the D.E. then $C_1 + C_2$ is also solution.

$$\frac{\partial (C_1 + C_2)}{\partial t} \stackrel{?}{=} D \frac{\partial^2 (C_1 + C_2)}{\partial x^2}$$

$$\Rightarrow \underbrace{\left(\frac{\partial C_1}{\partial t} - D\frac{\partial^2 C_1}{\partial x^2}\right)}_{=0} + \underbrace{\left(\frac{\partial C_2}{\partial t} - D\frac{\partial^2 C_2}{\partial x^2}\right)}_{=0} \stackrel{?}{=} 0$$

The initial condition is also verified by $C(x,t) = C_1(x,t) + C_2(x,t)$

$$C(x, t=0) = \frac{M_1}{A}\delta(x-\mu_1) + \frac{M_2}{A}\delta(x-\mu_2)$$

4) Several sources (point)

Direct generalization of the previous case.

$$C(x,t) = \sum_{i=1}^{N} \frac{M_i}{A\sqrt{4\pi D t}} e^{-(x-\mu_i)^2/4Dt}$$

N = number of sources

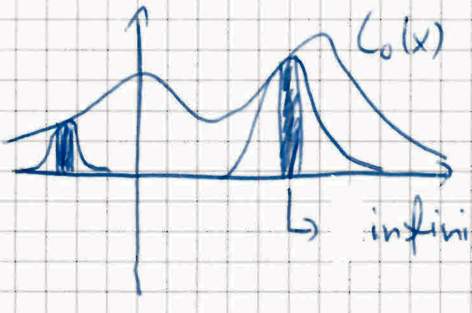
5 Continuous I.C. $C(x, t=0) = C_0(x)$ (general case)

In the limit of ∞ many sources we can do the following transformations to the preceding case:

$\sum_i \rightarrow \int$ (integral over source position)

$\dfrac{M_i}{A} \rightarrow C_0(\xi)\, d\xi$ $\quad \xi$ integration variable

$\dfrac{M_i}{A} \hookrightarrow M/L^2$; $C_0(\xi) \hookrightarrow M/L^3$, $d\xi \hookrightarrow L$, $C_0(\xi)\,d\xi \hookrightarrow M/L^2$ — same dimension



Each of them evolves like a point source.

$\hookrightarrow$ infinitesimal point source

We thus have the solution

$$C(x,t) = \int_{-\infty}^{\infty} C_0(\xi) \frac{1}{\sqrt{4\pi D t}} e^{-(x-\xi)^2/4Dt}\, d\xi \qquad (**)$$

⚠ Do not confuse x (resulting concentration at x) and ξ (integration variable)

We verify now that $(**)$ is solution of the D.E.

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial t}\int_{-\infty}^{\infty} C_0(\xi)\frac{1}{\sqrt{4\pi Dt}} e^{-(x-\xi)^2/4Dt}\, d\xi = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} C_0(\xi)\frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-\xi)^2}{4Dt}}\, d\xi$$

$$= \int_{-\infty}^{\infty} C_0(\xi)\, D \frac{\partial^2}{\partial x^2}\Big[\underbrace{\frac{e^{-(x-\xi)^2/4Dt}}{\sqrt{4\pi Dt}}}_{\text{solution of the D.E.}}\Big]\, d\xi = D\frac{\partial^2}{\partial x^2}\int_{-\infty}^{\infty} C_0(\xi)\frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-\xi)^2}{4Dt}}\, d\xi$$

$$= D\frac{\partial^2}{\partial x^2} C(x,t) \qquad \blacksquare$$

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We then verify that the continuous initial condition $C(x, t=0) = C_0(x)$ is satisfied by $(\ast\ast)$.

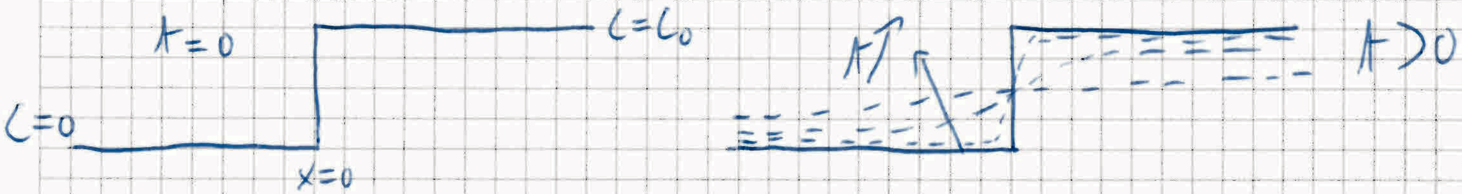
We have
$$\lim_{t\to 0} C(x,t) = \int_{-\infty}^{\infty} C_0(\xi) \lim_{t \to 0} \underbrace{\frac{e^{-(x-\xi)^2/4Dt}}{\sqrt{4\pi D t}}}_{\text{point source solution}} d\xi$$

$$= \int_{-\infty}^{\infty} C_0(\xi)\, \delta(x-\xi)\, d\xi$$

$$= \lim_{\varepsilon \to 0} \int_{x-\varepsilon/2}^{x+\varepsilon/2} C_0(\xi) \frac{1}{\varepsilon} d\xi = C_0(x) \frac{\varepsilon}{\varepsilon} = C_0(x) \quad \blacksquare$$

$C_0(\xi)$ becomes constant over an infinitely small domain

⑥ Example of continuous I.C.: gate opening



$$C(x, t=0) = C_0(x) = C_0\, \theta(x)$$

$$\theta(n) = \begin{cases} 0 & n<0 \\ 1/2 & n=0 \\ 1 & n>0 \end{cases} \quad \text{or} \quad \begin{cases} 0 & n<0 \\ 1 & n\geq 0 \end{cases}$$

(different conventions) result independent

We use the general formula for a continuous I.C to compute the solution.

We get

$$C(x,t) = \int_{-\infty}^{\infty} \underbrace{C_0\,\theta(\xi)}_{C_0(\xi)} \frac{1}{\sqrt{4\pi D t}}\, e^{-(x-\xi)^2/4Dt}\, d\xi$$

$$= \int_{0}^{\infty} C_0 \frac{1}{\sqrt{4\pi D t}}\, e^{-(x-\xi)^2/4Dt}\, d\xi$$

↳ independent of the convention chosen for $\theta(\xi)$

We make the change of variables $\alpha = x - \xi \Rightarrow d\alpha = -d\xi$

If $\xi = 0$ then $\alpha = x$

$\xi = \infty$ then $\alpha = -\infty$

$$\Rightarrow C(x,t) = -\int_{x}^{-\infty} C_0 \frac{1}{\sqrt{4\pi D t}}\, e^{-\alpha^2/4Dt}\, d\alpha$$

We then make the change $B = \alpha/\sqrt{4Dt} \Rightarrow d\alpha = \sqrt{4Dt}\, dB$

If $\alpha = -\infty$ then $B = -\infty$

$\alpha = x$ then $x/\sqrt{4Dt}$

$$\Rightarrow C(x,t) = -\int_{x/4Dt}^{-\infty} C_0 \frac{1}{\sqrt{\pi}}\, e^{-B^2}\, dB$$

$$= \underbrace{-C_0 \int_{0}^{-\infty} \frac{1}{\sqrt{\pi}}\, e^{-B^2}\, dB}_{C_0 \int_0^{\infty} \frac{1}{\sqrt{\pi}} e^{-\tilde{B}^2} d\tilde{B}} \underbrace{- C_0 \int_{x/\sqrt{4Dt}}^{0} \frac{1}{\sqrt{\pi}}\, e^{-B^2}\, dB}_{\frac{C_0}{2}\,\mathrm{erf}(x/4Dt)}$$

$$= C_0 \frac{\sqrt{\pi}}{2} \frac{1}{\sqrt{\pi}} + \frac{C_0}{2}\,\mathrm{erf}(x/4Dt)$$

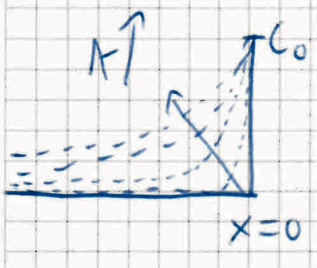
As a final solution, we thus get

$$C(x,t) = \frac{C_0}{2}\left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right] \quad \text{with } \operatorname{erf}(x) = \int_0^x \frac{2}{\sqrt{\pi}} e^{-\beta^2} d\beta$$

Remark on the gate opening: at the gate ($x=0$), the concentration remains constant:

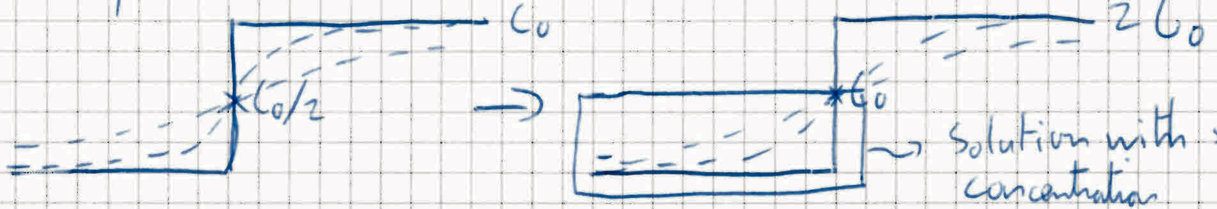
$$C(x=0,t) = C_0/2 \quad \forall t \quad \text{since } \operatorname{erf}(0) = 0.$$

7 Fixed boundary concentration



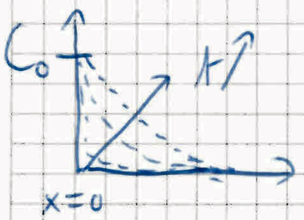
$$C(x=0,t) = C_0 \quad \forall t \quad \text{(B.C.)}$$
$$C(x,t=0) = C_0\,\theta(x) \quad \text{(I.C.)}$$

To find the solution, we consider a gate as in the previous example.



The solution with fixed boundary concentration is thus

$$C(x,t) = C_0\left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right]$$



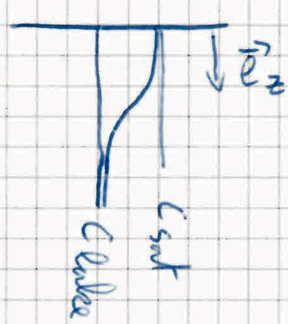
$$C'(x,t) = C_0\left[1 - \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right]$$

↳ ~~xxxx~~ transformation $x \to -x$

$$\operatorname{erf}(-x) = \int_0^{-x} \frac{2}{\sqrt{\pi}} e^{-\beta^2} d\beta = -\int_0^x \frac{2}{\sqrt{\pi}} e^{-\beta^2} d\beta = -\operatorname{erf}(x)$$

8 Oxygen diffusion in lake

Concentration in O



As in exercise set 2 $\quad \downarrow \vec e_z$ lake surface

Concentration in Oxygen goes down from C_{sat} to C_{lake} from the surface.

$$C_0(z) = C_\ell + \Theta(-z)(C_{sat} - C_\ell)$$

$$C(z) = C_{sat} - (C_{sat} - C_\ell)\,\mathrm{erf}\left(\frac{z}{\delta\sqrt{2}}\right)$$ (see exercise set 2)

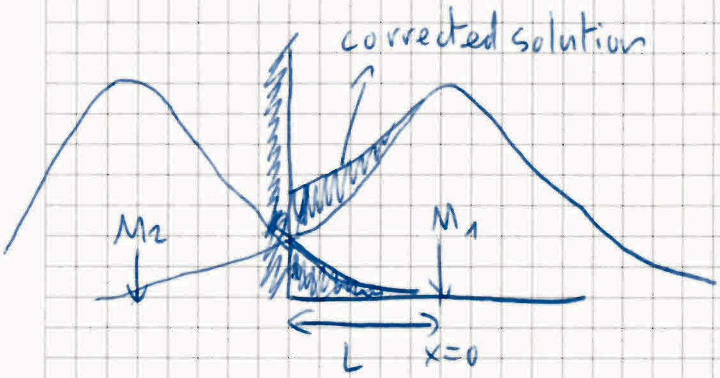
$z = 0 \Rightarrow C(0) = C_{sat}$

$z = \infty \Rightarrow \mathrm{erf} \to 1$ and $C(\infty) = C_{lake}$ (concentration deep in the lake)

Comparison with the previous solution yields

$$\delta\sqrt{2} \sim \sqrt{4Dt} \Rightarrow \underbrace{\delta}_{\text{characteristic thickness of transition layer}} \sim \sqrt{2Dt}$$

(9) Reflecting boundaries "Method of images"



B.C. : $\left.\frac{\partial C}{\partial x}\right|_{x=-L} = 0$

$$C_1(x,t) = \frac{M_1}{A} \frac{1}{\sqrt{4\pi D t}} e^{-x^2/4Dt}$$

Problem: at the wall we need zero flux

Solution: take also a virtual source $C_2(x,t) = \frac{M_2}{A}\frac{1}{\sqrt{4\pi D t}} e^{-\frac{(x+2L)^2}{4Dt}}$
with $M_1 = M_2$

C_1 and C_2 are solution of the D.E.

$$J = -D \frac{\partial C}{\partial x} \quad \text{Fick's law}$$

$$J_1(x=-L) = -J_2(x=-L)$$

$\Rightarrow$ $C_1 + C_2$ is solution of the D.E. and satisfies the reflecting B.C.

(10) Two walls: similar $C(x,t) = \frac{M}{A\sqrt{4\pi D t}} \sum_{m=-\infty}^{\infty} e^{-(x+2mL)^2/4Dt}$

↳ At each reflection we need a source that has diffused over an additional $2L$.