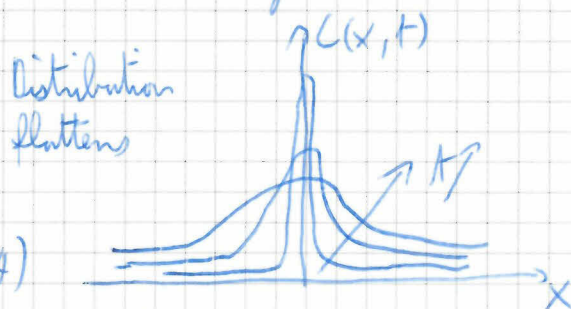




Solution of the D.E. (various initial and boundary conditions)

① Point source (1D)

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



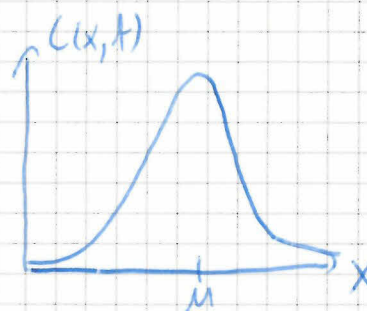
Compare with Normal distribution: $\frac{1}{\sqrt{2\pi}\sigma} e^{-x^2/2\sigma^2} = N(0, \sigma)$

Variance $2Dt \rightarrow 0$ for $t \rightarrow 0$ (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)

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



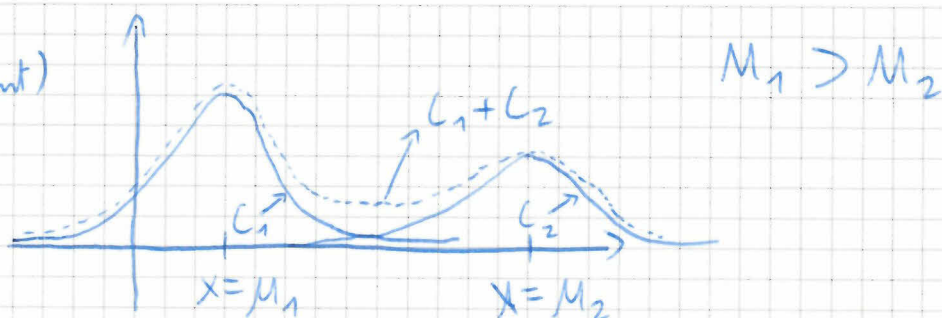
The distribution has a maximum when the argument of the exponential is zero.

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



②

③ Two sources (point)



C_1 solution for source 1, C_2 for source 2

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

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

$$\frac{\partial (C_1 + C_2)}{\partial t} \stackrel{?}{=} 0 \quad \frac{\partial^2 (C_1 + C_2)}{\partial x^2}$$

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

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.

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

N = number of sources



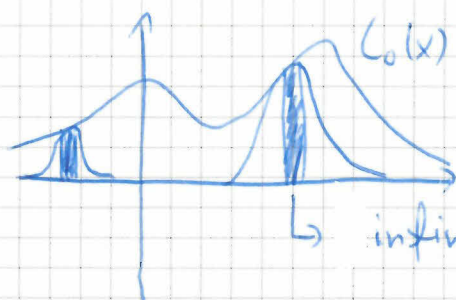
3

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:

$$\sum_i \rightarrow \int \quad (\text{integral over source position})$$

$$\frac{M_i}{A} \rightarrow C_0(\xi) d\xi \quad \left[\begin{array}{l} \xi \text{ integration variable} \\ \hookrightarrow M/L^3 \hookrightarrow L \\ \hookrightarrow M/L^2 \end{array} \right] \text{ same dimension}$$



Each of them evolves like a point source.

We thus have the solution

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

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

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

$$\begin{aligned} \frac{\partial C(x, t)}{\partial t} &= \frac{\partial}{\partial t} \int_{-\infty}^{\infty} C_0(\xi) \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-\xi)^2}{4Dt}} d\xi = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} \left(C_0(\xi) \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-\xi)^2}{4Dt}} \right) d\xi \\ &= \int_{-\infty}^{\infty} C_0(\xi) D \frac{\partial^2}{\partial x^2} \left[\frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-\xi)^2}{4Dt}} \right] d\xi = D \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} C_0(\xi) \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-\xi)^2}{4Dt}} d\xi \\ &\quad \text{solution of the V.E.} = D \frac{\partial^2}{\partial x^2} C(x, t) \quad \square \end{aligned}$$



4

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

$$\text{We have } \lim_{t \rightarrow 0} C(x, t) = \int_{-\infty}^{\infty} C_0(z) \lim_{t \rightarrow 0} \frac{e^{-(x-z)^2/4Dt}}{\sqrt{4\pi Dt}} dz$$

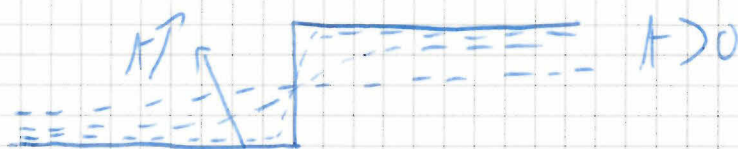
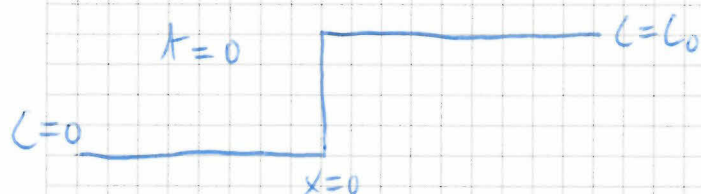
point source solution

$$= \int_{-\infty}^{\infty} C_0(z) \delta(x-z) dz$$

$$= \lim_{\varepsilon \rightarrow 0} \int_{x-\varepsilon/2}^{x+\varepsilon/2} C_0(z) \frac{1}{\varepsilon} dz = C_0(x) \frac{\varepsilon}{\varepsilon} = C_0(x)$$

$C_0(z)$ becomes constant over an infinitely small domain

⑥ Example of continuous I.C.: gate opening



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

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

result independent

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



We get

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

$$= \int_0^{\infty} C_0 \frac{1}{\sqrt{4\pi Dt}} e^{-(x-\xi)^2/4Dt} d\xi$$

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

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

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

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

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

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

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

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

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

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

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



6

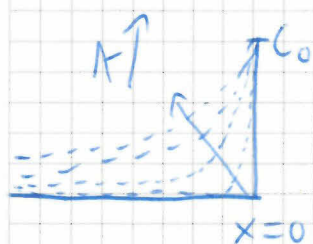
As a final solution, we thus get

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

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

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

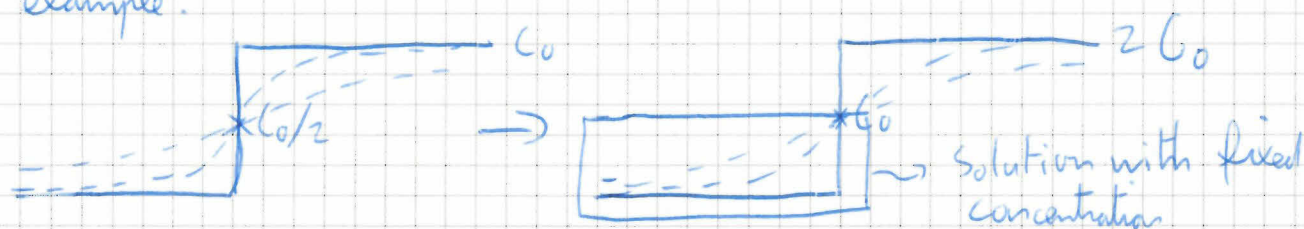
⑦ Fixed boundary concentration



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

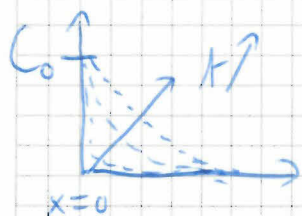
$$C(x, t=0) = C_0 \theta(x) \quad (\text{I.C.})$$

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



The solution with fixed boundary concentration is thus

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



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

↳ mirror transformation $x \rightarrow -x$

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



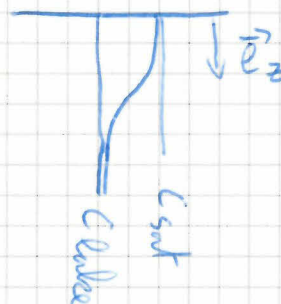
⑧ Oxygen diffusion in lake

Concentration in o

As in exercise set 2

lake surface
 $\downarrow \vec{e}_z$

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



$$C_o(z) = C_l + \Theta(-z)(C_{sat} - C_l)$$

$$C(z) = C_{sat} - (C_{sat} - C_l) \operatorname{erf}\left(\frac{z}{\delta\sqrt{t}}\right) \quad (\text{see exercise set 2})$$

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

$$z=\infty \Rightarrow \operatorname{erf} \rightarrow 1 \text{ and } C(\infty) = C_{lake} \quad (\text{concentration deep in the lake})$$

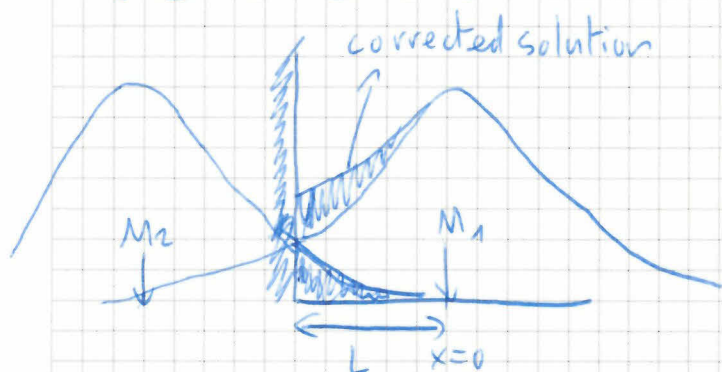
Comparison with the previous solution yields

$$\delta\sqrt{t} \sim \sqrt{4\kappa t} \Rightarrow \delta \sim \sqrt{2\kappa t}$$

characteristic thickness of transition layer



9) Reflecting boundaries "Method of images"



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

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

Problem: at the wall we need zero flux

Solution: take also a virtual source $C_2(x,t) = \frac{M_2}{A} \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x+2L)^2}{4Dt}}$
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 $C(x,t) = \frac{M}{A\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} e^{-\frac{(x+2nL)^2}{4Dt}}$

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