ICEA

Università degli Studi di Padova

LESSON 5: 2D AND 3D DIFFUSION

Let's see the fundamental solution in case of 2D diffusion. In this case the concentration is defined as following:

$$c = \lim_{\substack{\Delta x \to 0 \\ \Delta y \to 0}} \frac{\Delta M}{\Delta x \Delta y} \qquad [\mathrm{kg/m^2}]$$

and the problem of diffusion becomes:

$$\begin{cases} \dfrac{\partial c}{\partial t} - D\left(\dfrac{\partial^2 c}{\partial x^2} + \dfrac{\partial^2 c}{\partial y^2}\right) = 0 \\ c(x, y, 0) = M\delta(x)\delta(y) \qquad x, y = 0 \\ c(x, y, t) = 0 \qquad x, y \to \pm\infty \end{cases}$$

$\longrightarrow$ <u>Initial condition</u>

$\longrightarrow$ <u>Boundary conditions</u>

N.B. The hypotheses are the same of the 1D case:

- Still fluid, i.e. $\boldsymbol{u} = 0$
- Incompressible fluid, i.e. $\nabla \cdot \boldsymbol{u} = 0$
- Mass conservation, i.e. $\mathrm{d}M/dt = 0$

2D DIFFUSION

The problem can be solved thanks to the linearity of the process, which allows to express c as following:

$$c(x,y,t) = c_1(x,t)\, c_2(y,t)$$

Then:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial t}(c_1\, c_2) = c_1 \frac{\partial c_2}{\partial t} + c_2 \frac{\partial c_1}{\partial t}$$

$$\frac{\partial c}{\partial x} = c_1 \cancelto{0}{\frac{\partial c_2}{\partial x}} + c_2 \frac{\partial c_1}{\partial x} = c_2 \frac{\partial c_1}{\partial x} \longrightarrow \frac{\partial^2 c}{\partial x^2} = c_2 \frac{\partial^2 c_1}{\partial x^2}$$

$$\frac{\partial c}{\partial x} = c_1 \frac{\partial c_2}{\partial y} + c_2 \cancelto{0}{\frac{\partial c_1}{\partial y}} = c_1 \frac{\partial c_2}{\partial y} \longrightarrow \frac{\partial^2 c}{\partial y^2} = c_1 \frac{\partial^2 c_2}{\partial y^2}$$

By replacing the derivatives, the diffusion equation reads:

2D DIFFUSION

$$\frac{\partial c}{\partial t} - D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) = c_1 \frac{\partial c_2}{\partial t} + c_2 \frac{\partial c_1}{\partial t} - D\left(c_2 \frac{\partial^2 c_1}{\partial x^2} + c_1 \frac{\partial^2 c_2}{\partial y^2}\right) = 0$$

$$\longrightarrow \quad c_2 \underbrace{\left[\frac{\partial c_1}{\partial t} - D\frac{\partial^2 c_1}{\partial x^2}\right]}_{0} + c_1 \underbrace{\left[\frac{\partial c_2}{\partial t} - D\frac{\partial^2 c_2}{\partial y^2}\right]}_{0} = 0 \qquad \forall c_1, c_2$$

It means that the following equations have to be solved:

$$\begin{cases} \dfrac{\partial c_1}{\partial t} - D\dfrac{\partial^2 c_1}{\partial x^2} = 0 \\ c_1(x,0) = M_1\delta(x) \qquad x = 0 \\ c_1(x,t) = 0 \qquad x \to \pm\infty \end{cases} \qquad \begin{cases} \dfrac{\partial c_2}{\partial t} - D\dfrac{\partial^2 c_2}{\partial y^2} = 0 \\ c_2(y,0) = M_2\delta(y) \qquad y = 0 \\ c_2(y,t) = 0 \qquad y \to \pm\infty \end{cases}$$

Fundamental solution of 1D diffusion

$$\begin{cases} c_1 = \dfrac{k_1}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}} \\ c_2 = \dfrac{k_2}{\sqrt{4\pi D t}}\, e^{-\frac{y^2}{4Dt}} \end{cases}$$

2 Gaussian distribution along x and y axes

Since $c = c_1\, c_2$, we find:

$$c = \frac{k_1}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}} \cdot \frac{k_2}{\sqrt{4\pi D t}}\, e^{-\frac{y^2}{4Dt}} = \frac{k_1 k_2}{4\pi D t}\, e^{-\frac{x^2+y^2}{4Dt}}$$

$k_1 k_2 = ?$

The value of $k_1 k_2$ is determined by the mass conservation:

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

$$\widehat{c_1} = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}} \qquad \widehat{c_2} = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{y^2}{4Dt}}$$

$$M = k_1 k_2 \int_{-\infty}^{+\infty} \cancelto{1}{\widehat{c_1}(x,t)\, \mathrm{d}x} \int_{-\infty}^{+\infty} \cancelto{1}{\widehat{c_2}(y,t)\, \mathrm{d}y}$$

$$M = k_1 k_2$$

Finally:

$$c(x,y,t) = \frac{M}{4\pi D t}\, e^{-\frac{x^2+y^2}{4Dt}}$$

2D concentration distribution

$$c(x,y,t) = \frac{M}{4\pi t\sqrt{D_x D_y}}\, e^{-\left(\frac{x^2}{4D_x t}+\frac{y^2}{4D_y t}\right)}$$

2D concentration distribution in anysotropic condition ($D_x \neq D_y$)

Similarly for **3D diffusion**:

$$c(x,y,z,t) = \frac{M}{(4\pi D t)^{3/2}}\, e^{-\frac{x^2+y^2+z^2}{4Dt}}$$

3D concentration distribution

$$c(x,y,z,t) = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}}\, e^{-\left(\frac{x^2}{4D_x t}+\frac{y^2}{4D_y t}+\frac{z^2}{4D_z t}\right)}$$

3D concentration distribution in anysotropic condition ($D_x \neq D_y \neq D_z$)

ADVECTION + LONGITUDINAL DIFFUSION

$$\begin{cases} \dfrac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c = D\, \nabla^2 c \\ c(x,0) = 0 \qquad x > 0 \\ c(x,0) = c_0 \qquad x \le 0 \end{cases}$$

Step distribution

Assumptions:

- 1D flow, i.e., $\boldsymbol{u} = (u_0, 0, 0)$
- Uniform flow, i.e., $u_0 = \text{const}$
- Incompressible fluid, i.e., $\nabla \cdot \boldsymbol{u} = 0$
- Mass conservation, i.e., $\mathrm{d}M/dt = 0$
- Diffusion only along x, i.e., $\dfrac{\partial^2 c}{\partial y^2}, \dfrac{\partial^2 c}{\partial z^2} = 0$

By expanding the A-D equation:

$$\frac{\partial c}{\partial t} + \left(\underbrace{\cancel{u_x}}_{u_0} \frac{\partial c}{\partial x} + \underbrace{\cancel{u_y}}_{0} \frac{\partial c}{\partial y} + \underbrace{\cancel{u_z}}_{0} \frac{\partial c}{\partial z} \right) = D \left(\frac{\partial^2 c}{\partial x^2} + \underbrace{\cancel{\frac{\partial^2 c}{\partial y^2}}}_{0} + \underbrace{\cancel{\frac{\partial^2 c}{\partial z^2}}}_{0} \right)$$

And then:

$$\frac{\partial c}{\partial t} + u_0 \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2}$$

The differential equation needs of being simplified by traslating the reference system with velocity u_0. The new reference system is (ξ, t), being ξ defined as: $\xi(x,t) = x - u_0 t$.

In the new reference system:

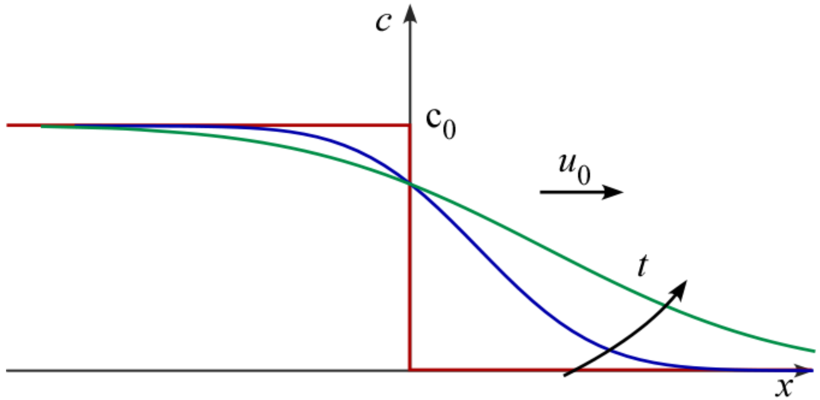
$$\frac{\partial c}{\partial t} - \cancel{u_0 \frac{\partial c}{\partial \xi}} + \cancel{u_0 \frac{\partial c}{\partial \xi}} = D\frac{\partial^2 c}{\partial \xi^2} \longrightarrow \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial \xi^2}$$

1D Diffusion equation

Triavially:

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

$$\longrightarrow c(x,t) = \frac{c_0}{2}\operatorname{erfc}\left(\frac{x - u_0 t}{\sqrt{4Dt}}\right)$$

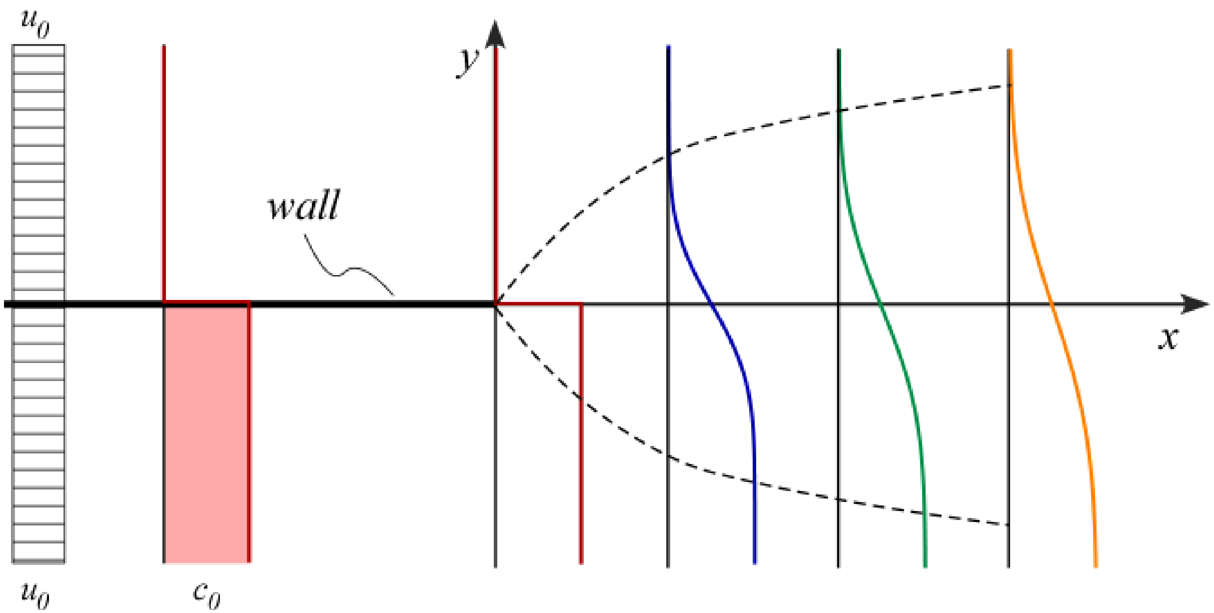


$$c(x,t) \qquad\qquad c(\xi(x,t),t)$$

$$\frac{\partial c(x,t)}{\partial t} \longrightarrow \frac{dc(\xi,t)}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial \xi}\frac{\partial \xi}{\partial t} = \frac{\partial c}{\partial t} - u_0\frac{\partial c}{\partial \xi}$$

$$\frac{\partial c(x,t)}{\partial x} \qquad \frac{\partial c(\xi,t)}{\partial x} = \frac{\partial c}{\partial \xi}\frac{\partial \xi}{\partial x} = \frac{\partial c}{\partial \xi}$$

ADVECTION + TRANSVERSAL DIFFUSION



Assumptions:

- Steady flow, i.e. $c(x,y,t) = c(x,y)$
- Uniform flow, i.e., $\boldsymbol{u} = (u_0, 0, 0)$
- Incompressible fluid, i.e., $\nabla \cdot \boldsymbol{u} = 0$
- Mass conservation, i.e., $\mathrm{d}M/dt = 0$

The differential equation which rules the problem is:

$$\cancel{\frac{\partial c}{\partial t}}_{0} + u_0 \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} + D \frac{\partial^2 c}{\partial y^2} \longrightarrow \underbrace{u_0 \frac{\partial c}{\partial x}}_{\textit{Longitudinal Advection}} = \underbrace{D \frac{\partial^2 c}{\partial x^2}}_{\textit{Longitudinal Diffusion}} + \underbrace{D \frac{\partial^2 c}{\partial y^2}}_{\textit{Transversal Diffusion}}$$

ADVECTION + TRANSVERSAL DIFFUSION

We have two length scales along x-axis:

- $L_D = \sqrt{Dt}$ → Longitudinal Diffusion
- $L_U = u_0 t$ → Longitudinal Advection

In our application $L_U \gg L_D$, i.e., $u_0 t \gg \sqrt{Dt}$.

Indeed, given a period of time t, the distance travel by the solute due to the advection is:

$$L_x = u_0 t \longrightarrow t = L_x / u_0$$

By equaling the advection with the diffusive length after the period of time t, we find:

$$u_0 t = \sqrt{Dt} \longrightarrow L_x = \sqrt{D\, L_x / u_0}$$

$$\longrightarrow \sqrt{\frac{D}{u_0 L_x}} = 1$$

$D \approx 2 \cdot 10^{-9}\ m^2/s$

$u_0 \approx 0.1 - 1.0\ m/s$

It is true until $\frac{D}{u_0} = L_x$ → $L_x = 10^{-9}$ m!!!!
If $L_x \gg 10^{-9}$ m longitudinal diffusion is negligible!

I can express the ratio into the square root as following:

$$\frac{D}{u_0 L_x} = \frac{D}{\nu}\frac{\nu}{u_0 L_x} \longrightarrow \frac{D}{u_0 L_x} = \frac{1}{Sc}\frac{1}{Re}$$

$\nu \approx 10^{-6}\ m^2/s$
Kinematic viscosity of water

Where: - $Sc = \nu/D$ is the Schmidt Number
- $Re = u_0 L_x/\nu$ is the Reynolds Number

The differential equation can then be simplified and it reads:

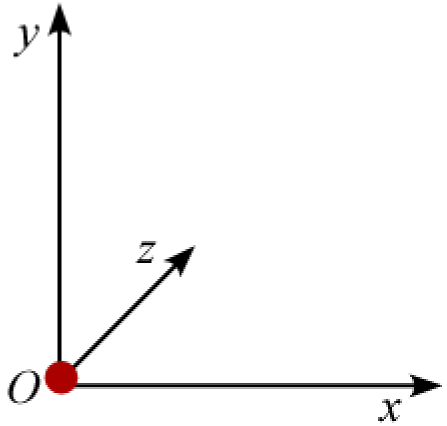
$$u_0 \frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial y^2} \xrightarrow{\tau = x/u_0} \frac{\partial c}{\partial \tau} = D\frac{\partial^2 c}{\partial y^2}$$

<u>1D Diffusion equation</u>

If we consider the following initial condition:

$$\begin{cases} c(x,y) = 0 & y > 0, x = 0 \rightarrow \tau = 0 \\ c(x,y) = c_0 & y \leq 0, x = 0 \rightarrow \tau = 0 \end{cases}$$

Then: $$c(\tau, y) = \frac{c_0}{2}\operatorname{erfc}\left(\frac{y}{\sqrt{4D\tau}}\right) \longrightarrow c(x,y) = \frac{c_0}{2}\operatorname{erfc}\left(\frac{y}{\sqrt{4D\,x/u_0}}\right)$$



Assumptions:

- Constant Mass Rate in O, i.e., $\frac{\mathrm{d}M}{dt} = \dot{M}(0,0,0)$
- Uniform flow, i.e., $\boldsymbol{u} = (u_0, 0, 0)$
- Incompressible fluid, i.e., $\nabla \cdot \boldsymbol{u} = 0$
- Stationary process, i.e., $c(x, y, z, t) = c(x, y, z)$

The differential equation of the problem is:

$$\frac{\partial c}{\partial t} + u_0 \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} + D \frac{\partial^2 c}{\partial y^2} + D \frac{\partial^2 c}{\partial z^2}$$

Being advection predominant on diffusion along x, the equation can be simplified in:

$$\frac{\partial c}{\partial t} + u_0 \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial y^2} + D \frac{\partial^2 c}{\partial z^2}$$

The diffusion can be described by discretizing the time of the process. Indeed:

ADVECTION + 3D DIFFUSION

- $t_0 = 0 \rightarrow t_1 = t_0 + \Delta t$: a first amount of mass ΔM is injected in *O,* and it starts to diffuse along *y* and *z* as 2D diffusion problem.
- $t_1 \rightarrow t_2 = t_1 + \Delta t$: a second amount of mass ΔM is injected in *O,* and it starts to diffuse along *y* and *z* as 2D diffusion problem. The first ΔM moves along x of $u_0 t$ and the solute spreads along *y* and *z.*

It is worth noting that: $\mathrm{d}M = \dot{M}\mathrm{d}t = \dot{M}\dfrac{\mathrm{d}x}{u_0}$

This definition of $\mathrm{d}M$ into 2D diffusion yelds:

$$\hat{c}(y,z,t) = \frac{\mathrm{d}M}{4\pi D\mathrm{d}t}\, e^{-\frac{y^2+z^2}{4D\mathrm{d}t}} = \frac{\dot{M}\mathrm{d}x}{u_0}\frac{1}{4\pi D\mathrm{d}t}\, e^{-\frac{y^2+z^2}{4D\mathrm{d}t}}$$

$$\hat{c} = \lim_{\substack{\Delta y\to 0\\ \Delta z\to 0}} \frac{\Delta M}{\Delta y \Delta z}$$

Being $c = \hat{c}\,/\mathrm{d}x$, we find:

$$c(x,y,z,t) = \frac{\dot{M}\cancel{\mathrm{d}x}}{u_0\cancel{\mathrm{d}x}}\frac{1}{4\pi D\mathrm{d}t}\, e^{-\frac{y^2+z^2}{4D\mathrm{d}t}} = \frac{\dot{M}}{u_0}\frac{1}{4\pi D\mathrm{d}t}\, e^{-\frac{y^2+z^2}{4D\mathrm{d}t}}$$

ADVECTION + 3D DIFFUSION

The flow is uniform, then: $u_0 = \frac{\mathrm{d}x}{\mathrm{d}t} \xrightarrow{\int} \frac{x}{t}$

That into 2D diffusion equation yelds:

$$c(x,y,z,t) = \frac{\dot{M}\,\mathrm{d}t}{4\pi D \mathrm{d}t \mathrm{d}x}\, e^{-\frac{y^2+z^2}{4D\mathrm{d}t}}$$

By replacing $\mathrm{d}t$ and $\mathrm{d}x$ with t and x, finally we have:

$$c(x,y,z,t) = \frac{\dot{M}}{4\pi D x}\, e^{-\frac{y^2+z^2}{4Dt}}$$

$$\longrightarrow \quad c(x,y,z) = \frac{\dot{M}}{4\pi D x}\, e^{-\frac{y^2+z^2}{4Dx}u_0}$$