# Lecture 17: Diffusion

Logistics: - HW3 Thursday is last chance !

- HW6 due Thursday

Last time: - Solute mass balance

$$\boxed{\phi \frac{\partial c}{\partial t} + \nabla \cdot [qc - \underline{\underline{D}}_H \nabla c] = -\phi k c}$$

Advective: $qc$

Diffusive: $-\underline{\underline{D}}_H \nabla c$ mol. Diff. + Dispersion

Reactive: $-\phi k c$

- Scaling

$$\frac{\partial c'}{\partial t'} + \nabla' \cdot \left[ \underbrace{\frac{t_c}{t_A}}_{\Pi_1} q' c' - \underbrace{\frac{t_c}{t_D}}_{\Pi_2} \underline{\underline{D}}_H' \nabla' c' \right] = - \underbrace{\frac{t_c}{t_R}}_{\Pi_3} c'$$

- Characteristic time scales:

advective: $t_A = \dfrac{x_c}{q_c/\phi} = \dfrac{x_c}{v_c}$

diffusive: $t_D = \dfrac{\phi x_c^2}{D_c}$

reactive: $t_R = \dfrac{1}{k}$

- Peclet number: $Pe = \dfrac{t_D}{t_A} = \dfrac{q_c x_c}{D_c}$

$Da = \dfrac{t_r}{t_R}$

Today: Diffusion

# Diffusion

$$\frac{\partial c'}{\partial t'} + \nabla'\cdot\left[\underbrace{\frac{t_D}{t_A}}_{Pe} \underline{q}'c' - \cancelto{1}{\frac{t_D}{t_D}} \underline{\underline{D}}'_H \nabla' c'\right] = -\underbrace{\frac{t_D}{t_R}}_{\frac{t_D}{t_A}\frac{t_A}{t_R} = Pe\,Da} c'$$

choose diff. time scale: $t_c = t_D$

$$\frac{\partial c'}{\partial t'} + \nabla'\cdot\left[ Pe\ \underline{q}'c - D'_H \nabla' c' \right] = -Pe\,Da\ c'$$

if $Pe \ll 1$ and $Da \sim 1$

limit equation$_1$

$$\boxed{\frac{\partial c'}{\partial t'} - \nabla'\cdot\left[\cancelto{1}{\underline{\underline{D}}'_H} \nabla' c'\right] = 0}$$

$$\frac{\partial c'}{\partial t'} - \nabla\cdot\nabla c = 0 \qquad \nabla^2 c$$

dim.less diffusion equation

redimensionalize: $c' = \frac{c}{c_c}$ ....

$$\phi \frac{\partial c}{\partial t} - \nabla\cdot\left[\underline{\underline{D}}_H \nabla c\right] = 0$$

note: if $\underline{q} = 0$ $\quad \underline{\underline{D}}_H = 0 \qquad \underline{\underline{D}}_H = \phi D_m \underline{\underline{I}} + \cancelto{0}{\underline{\underline{D}}_H}$

$$\Rightarrow \quad \boxed{\frac{\partial c}{\partial t} - \nabla\cdot\left[D_m \nabla c\right] = 0} \quad \text{diff. eqn.}$$

similar equns:

heat ~~transfer~~ conduction : $\underbrace{\rho c_p}_{\text{heat storage}} \frac{\partial T}{\partial t} - \nabla \cdot [\kappa \nabla T] = 0$

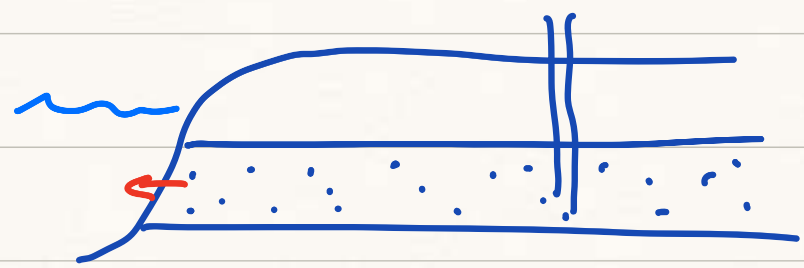
slightly compressible flow: $\underbrace{S \frac{\partial h}{\partial t}}_{\text{storage}} \underbrace{- \nabla \cdot [K \nabla h]}_{\text{incompressible flow}} = 0$

## Diffusion of solute out of aquifer

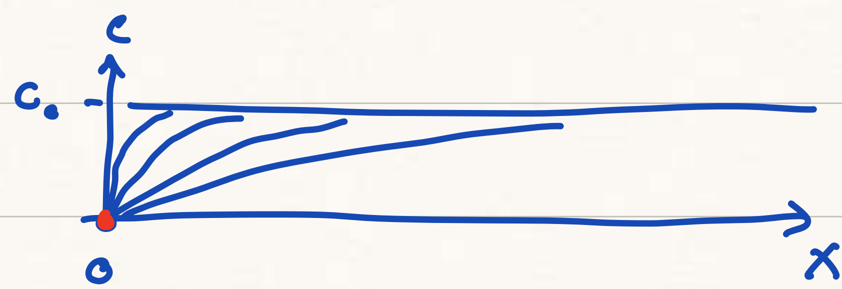
PDE: $\frac{\partial c}{\partial t} - D_m \frac{\partial^2 c}{\partial x^2} = 0 \qquad x \in [0, \infty)$

BC: $c(0,t) = 0$

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



Q: How fast does this concentration front propagate?




How do we scale problem?

No obvious length scale, because we have half-space
external

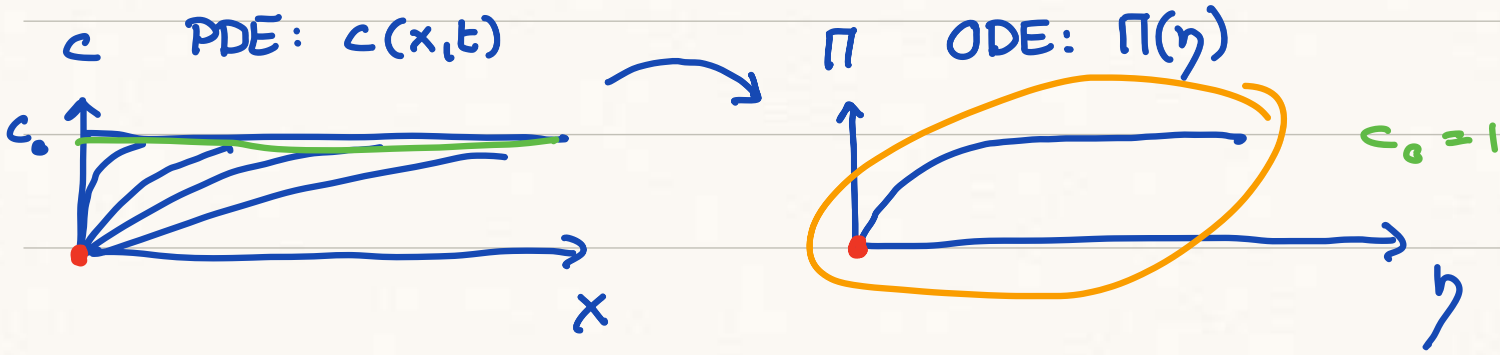
Internal length scale: $\sqrt{D_m \underline{t}} \left\{ \sqrt{\frac{m^2}{s} s} = m \right.$

What about $x' = \frac{x}{\sqrt{D_m t}}$ ?

We are not just scaling with parameters, but with another independent variable

$\Rightarrow$ results in a new independent variable !

$$\boxed{\eta = \frac{x}{\sqrt{4Dt}}}$$ Boltzmann variable




By introducing $\eta \sim \frac{x}{\sqrt{t}}$ we reduce PDE to an ODE

$\eta$ is called the similarity variable and solution is said to be self-similar

Q: What is the ODE ?

First : $c' = \frac{c}{c_0}$ $\quad 0 \leq c' \leq 1$ $\quad$ IC: $c' = 1$

Solution : $c'(x,t) = \Pi(\eta(x,t))$ $\quad \Pi(\eta)$

substitute into PDE

Transform derivatives:

$$\frac{\partial c'}{\partial t} = \frac{\partial}{\partial t}(\Pi(\eta(x,t)) = \frac{d\Pi}{d\eta}\frac{\partial \eta}{\partial t}$$ chain rule

$$\eta = \frac{x}{\sqrt{4D_m t}}$$

$$\frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{4D_m t}} \qquad \frac{\partial \eta}{\partial t} = -\frac{\eta}{2t}$$

$$\frac{\partial^2 c'}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{d\Pi}{d\eta}\frac{\partial \eta}{\partial x}\right) = \left(\frac{\partial \eta}{\partial x}\right)^2 \frac{d^2\Pi}{d\eta^2} = \frac{1}{4D_m t}\frac{d^2\Pi}{d\eta^2}$$

Substitute into PDE:

$$\frac{\partial c'}{\partial t} - D_m\frac{\partial^2 c'}{\partial x^2} = -\frac{\eta}{2\cancel{t}}\frac{d\Pi}{d\eta} - \frac{\cancel{D_m}}{4\cancel{D_m}\cancel{t}}\frac{d^2\Pi}{d\eta^2} = 0$$

ODE: $\boxed{\frac{d^2\Pi}{d\eta^2} + 2\eta\frac{d\Pi}{d\eta} = 0}$

BC: $\boxed{\Pi(0) = 0 \qquad \lim_{\eta\to\infty} \Pi = 1}$

Self-Similar ODE

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

IC of PDE $t \to 0$ $\eta \to \infty$ (x finite)

Solve ODE:

1) substitute: $u \equiv \frac{d\Pi}{d\eta} \Rightarrow \frac{du}{d\eta} + 2\eta u = 0$

2) separate variables: $\frac{du}{u} = -2\eta \, d\eta$

$$\ln u = -\eta^2 + a$$

$$u = b\, e^{-\eta^2}$$

3) re substitute: $\frac{d\Pi}{d\eta} = b e^{-\eta^2}$

4) separate variables: $d\Pi = b\, e^{-\eta^2} d\eta$

$$\Pi(\eta) = b \int_0^{\eta} e^{-z^2} dz$$

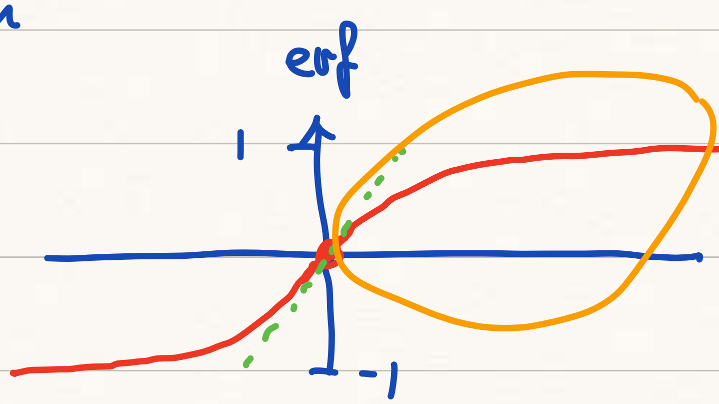
$z$ = dummy variable

integral does not have analytic solu.

$\Rightarrow$ give it a name and move on

5) Identify error function

$$\boxed{\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-z^2} dz}$$




Properties:

- $\mathrm{erf}(-x) = -\,\mathrm{erf}(x)$ "point symmetric"

- $\mathrm{erf}(0) = 0$
- $\mathrm{erf}(x) \approx x \qquad |x| \ll 1$
- $\lim_{x \to \infty} \mathrm{erf}(x) = 1 , \qquad \lim_{x \to -\infty} \mathrm{erf}(x) = -1$

Therefore: $\Pi(\eta) = b \frac{\sqrt{\pi}}{2} \mathrm{erf}(\eta)$

BC: $\lim_{\eta \to \infty} \Pi(\eta) = b \frac{\sqrt{\pi}}{2} = 1 \quad \Rightarrow \quad b = \frac{2}{\sqrt{\pi}}$

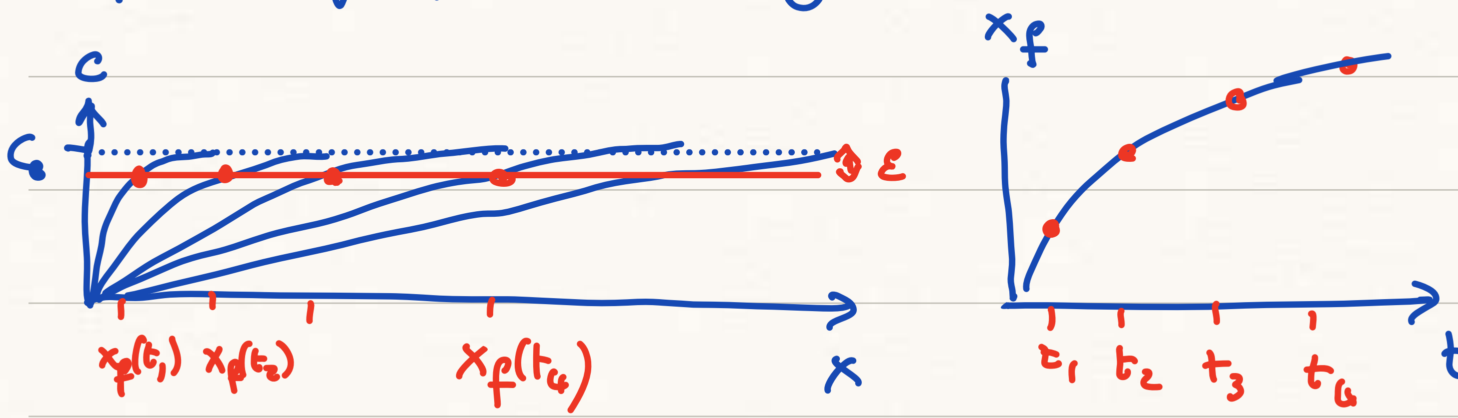
Self-similar solu: $\boxed{\Pi(\eta) = \mathrm{erf}(\eta)}$

6) Resubstitute: $c = c_0 c' \qquad \eta = \frac{x}{\sqrt{4Dt}}$

Transient concentration evolution

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

# Speed of front propagation




Note: infinitesimal changes propagate
<u>infinitely</u> fast!

Finite changes, $\Delta c = \varepsilon > 1$, propagate with
<u>finite</u> velocity.

Define front as location where c has changed by ε from its initial value $c_0$

$$c(x_f, t) = c_0 - \varepsilon c_0 = c_0 (1-\varepsilon)$$

$$\downarrow$$

$$\cancel{c_0} \operatorname{erf}\left(\frac{x_f}{\sqrt{4Dt}}\right) = \cancel{c_0}(1-\varepsilon)$$

inverse error function

$$\frac{x_f}{\sqrt{4Dt}} = \operatorname{erf}^{-1}(1-\varepsilon) = \alpha(\varepsilon) = \text{const}$$

$$\Rightarrow \quad \boxed{x_f = \alpha(\varepsilon)\sqrt{4Dt}}$$

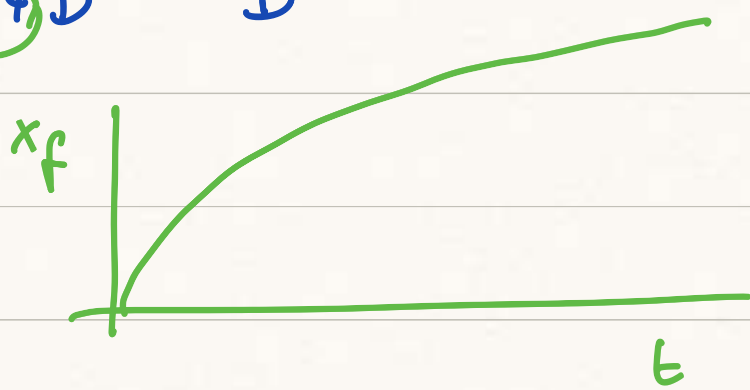
Concentration perturbation propagates as $\sqrt{t}$

$$x_f \sim \sqrt{t}$$

This matches our diffusive time scale

$$x_c = x_f = \alpha(\varepsilon)\sqrt{4Dt_D}$$

$$t_D = \frac{x_c^2}{\alpha(\varepsilon)\,4D} \sim \frac{x_c^2}{D}$$




$$\frac{\partial c}{\partial t} \underbrace{- \nabla\cdot[D_m \nabla c]}_{\text{know}} = 0$$

new