Transport phenomena

2. Solving transport equations

2.1 From mass to heat and viscous stress transport

2.2 Homogenization of a cocktail (exact solution?)

2.3 Measuring a diffusion coefficient ?

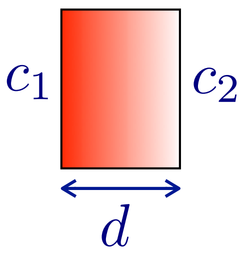
2.4 Depth of penetration

Transport phenomena

2. Solving transport equations

2.1 From mass to heat and viscous stress transport

mass:



Diffusion

$$\mathbf{j}_d = -D\boldsymbol{\nabla} c \;\rightarrow\; -D\,\frac{c_2 - c_1}{d}$$

Convection

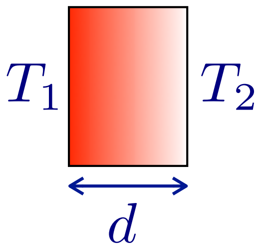
$$\mathbf{j}_c = c\,\mathbf{u}$$

$$\boxed{\frac{\partial c}{\partial t} + \mathbf{u}\cdot\boldsymbol{\nabla} c = D\,\Delta c + r}$$

[m^2.s^{-1}]

source/sink
eg: chemical reaction

heat:



Conduction: Fourrier's law

$$\boxed{\mathbf{j}_{cond} = -\kappa \boldsymbol{\nabla} T} \rightarrow \quad -\kappa \frac{T_2 - T_1}{d}$$

thermal flux [W.m^{-2}]

thermal conductivity [W.m^{-1}.K^{-1}]

Convection

$$\boxed{\mathbf{j}_{conv} = \rho C_p \, T \, \mathbf{u}}$$

density [kg.m^{-3}]

specific heat capacity [J.kg^{-1}.K^{-1}]

Heat equation:

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} T \right) = \kappa \Delta T + r$$

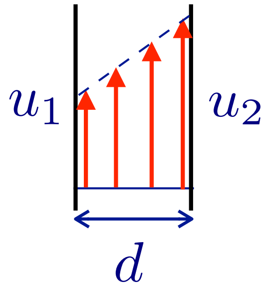
$$\boxed{\frac{\partial T}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} T = \alpha \Delta T + \frac{r}{\rho C_p}}$$

$$\boxed{\alpha = \kappa / \rho C_p}$$

thermal diffusivity [m^2.s^{-1}]

source/sink
eg: Joule effect

momentum:



"Conduction"

$$\boldsymbol{\sigma}_v = \eta(\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\mathbf{u}^{\mathrm{T}}) \;\rightarrow\; \eta\,\frac{u_2 - u_1}{d}$$

viscous stress [Pa]
~
flux of momentum

dynamic viscosity [Pa.s]
~
momentum "conductivity"

"Convection"

$$\rho\mathbf{u} \otimes \mathbf{u}$$

Navier & Stokes equation:

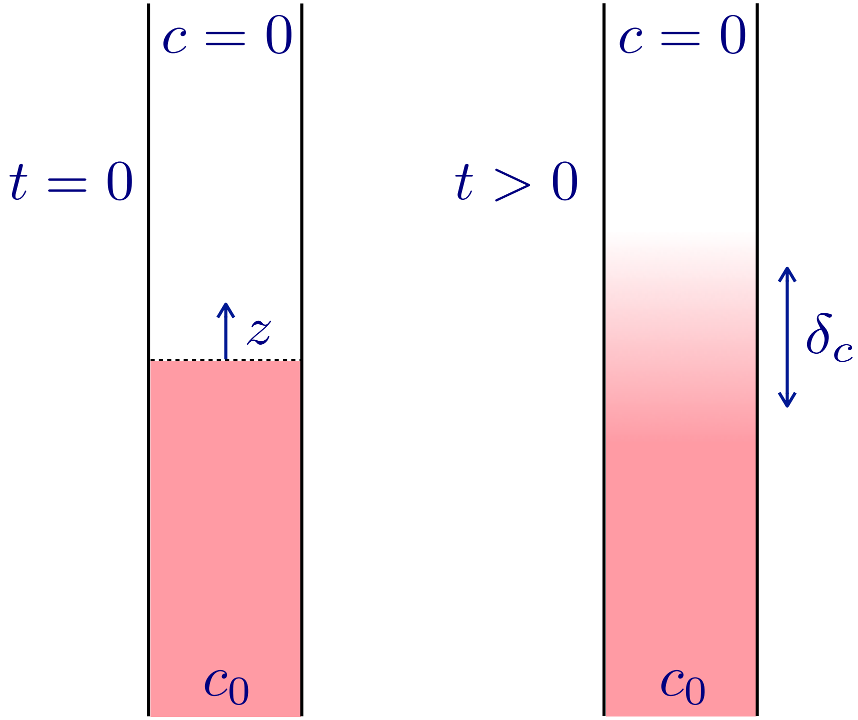
$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u} = \eta\,\Delta\mathbf{u} - \boldsymbol{\nabla}p + \rho\mathbf{g}$$

$$\boxed{\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u} = \nu\,\Delta\mathbf{u} - \frac{1}{\rho}\boldsymbol{\nabla}p + \mathbf{g}}$$

$$\nu = \eta/\rho$$

kinematic viscosity [m^2.s]
~
momentum "diffusion"

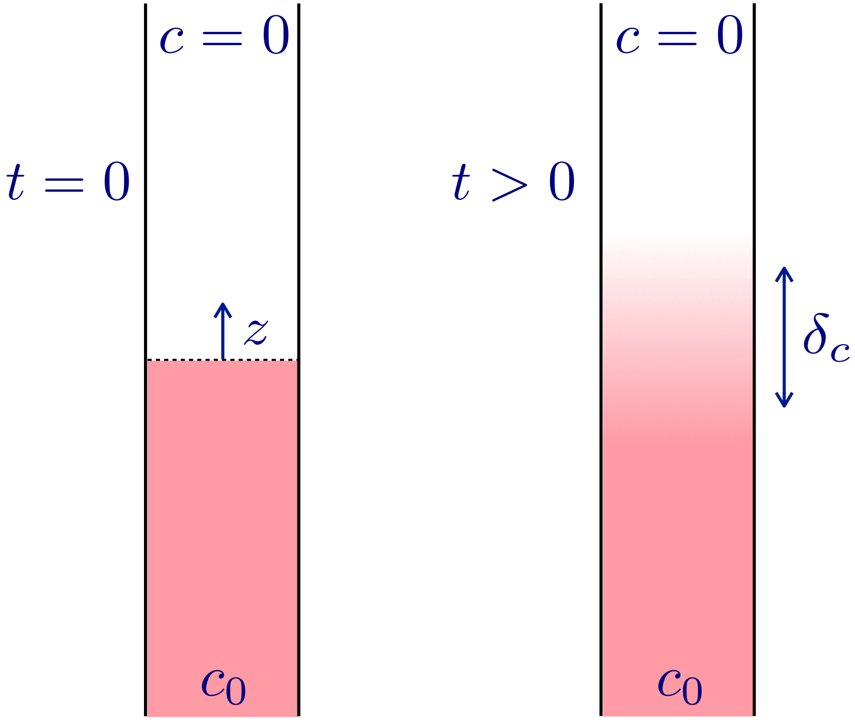
2.2 Homogenization of a cocktail



in scaling laws ?

exact solution ?

2.2 Homogenization of a cocktail



in scaling laws:

$$\delta_c \sim (Dt)^{1/2}$$

$$j_d \sim D \frac{c_0}{\delta_c} \sim \left(\frac{D}{t}\right)^{1/2} c_0$$

exact solution ?

$$\frac{\partial c}{\partial t} + \cancel{\mathbf{u}\cdot\boldsymbol{\nabla} c} = D \frac{\partial^2 c}{\partial x^2}$$

with

$$c(z = -\infty) = c_0$$
$$c(z = \infty) = 0$$

$$\frac{\partial c}{\partial t} + \cancel{\mathbf{u}\cdot\boldsymbol{\nabla}} c = D\,\frac{\partial^2 c}{\partial x^2}$$

new variable $\quad \xi = \dfrac{x}{2(Dt)^{1/2}} \quad \rightarrow \quad c\left(\dfrac{x}{2(Dt)^{1/2}}\right)?$

$$-\frac{x}{4D^{1/2}t^{3/2}}c'(\xi) = D\,\frac{1}{4Dt}c''(\xi)$$

$$c''(\xi) + \underbrace{\frac{x}{(Dt)^{1/2}}}_{\rightarrow\, 2\xi}c'(\xi) = 0$$

$$c''(\xi) + 2\xi c'(\xi) = 0$$

we define $\; g(\xi) = c'(\xi) \quad \rightarrow \quad g'(\xi) + 2\xi g(\xi) = 0$

$$\frac{dg}{g} = -2\xi d\xi$$

$$\ln(g) = -\xi^2 + cte$$

$$g(\xi) = A\exp(-\xi^2)$$

$$c(\xi) = A\int_0^{\xi} e^{-\omega^2} d\omega + B$$

$$x \to \infty \;\Rightarrow\; \xi \to \infty \;\Rightarrow\; c \to 0 \;\Rightarrow\; A\int_0^{\infty} e^{-\omega^2} d\omega + B = 0$$

$$\frac{\sqrt{\pi}}{2}$$

$$x \to -\infty \;\Rightarrow\; \xi \to -\infty \;\Rightarrow\; c \to c_0 \;\Rightarrow\; A\int_0^{-\infty} e^{-\omega^2} d\omega + B = c_0$$

$$\left(\begin{array}{l} \frac{\sqrt{\pi}}{2}A + B = 0 \\ \\ -\frac{\sqrt{\pi}}{2}A + B = c_0 \end{array} \right. \longrightarrow \left(\begin{array}{l} B = \frac{c_0}{2} \\ \\ A = -\frac{c_0}{\sqrt{\pi}} \end{array} \right.$$

$$c(x,t) = \frac{c_0}{2}\left(1 - \frac{2}{\sqrt{\pi}}\int_0^{\frac{x}{2(Dt)^{1/2}}} e^{-\omega^2} d\omega\right)$$

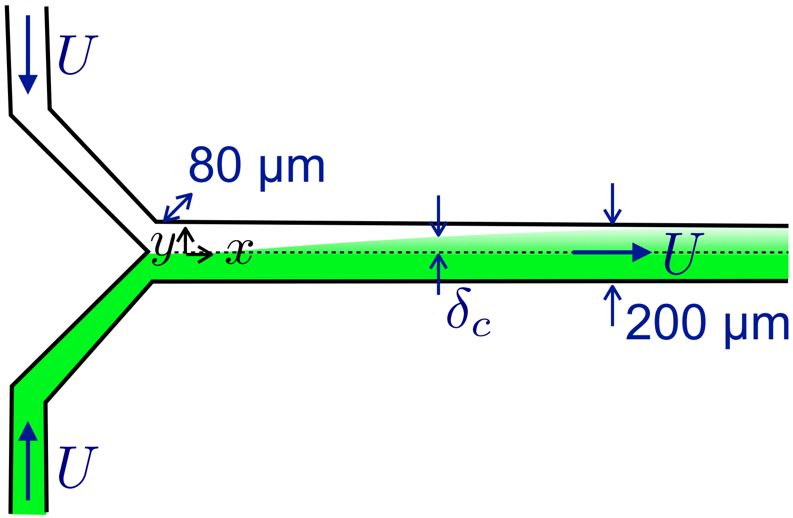
$$\boxed{c(x,t) = \frac{c_0}{2}\left(1 - \mathrm{erf}\left(\frac{x}{2(Dt)^{1/2}}\right)\right)}$$

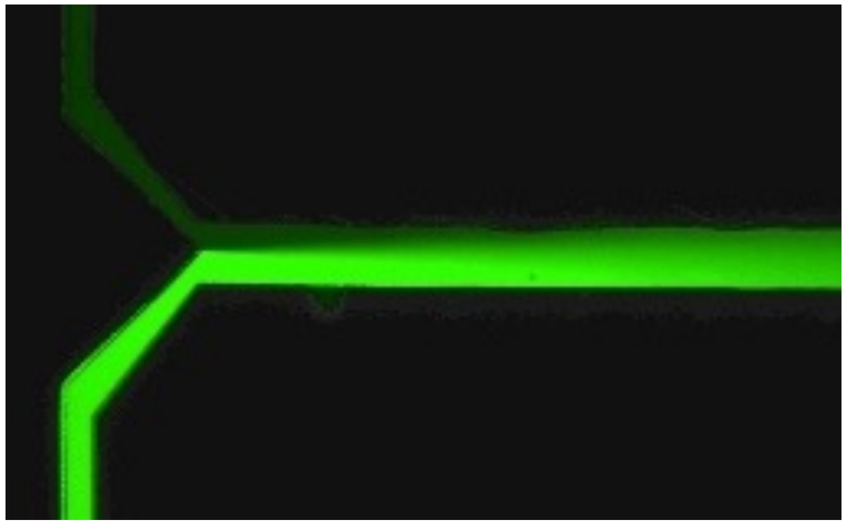
$$j_d = -D\frac{\partial c}{\partial x} = D\frac{c_0}{2}\frac{2}{\sqrt{\pi}}\frac{1}{2(Dt)^{1/2}}\exp\left(-\frac{x^2}{4Dt}\right)$$

$$j_d(x=0) = \frac{c_0}{2}\left(\frac{D}{\pi t}\right)^{1/2}$$

2.3 Measuring a diffusion coefficient ?

Y-junction in a microfluidic chip



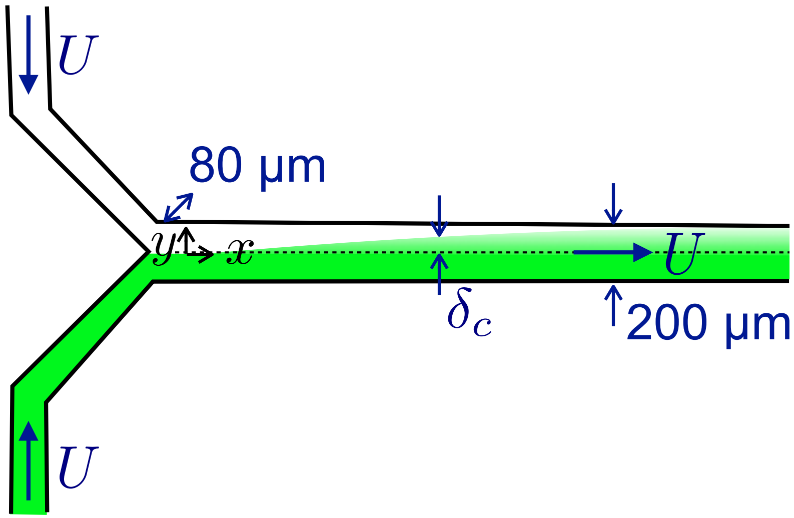


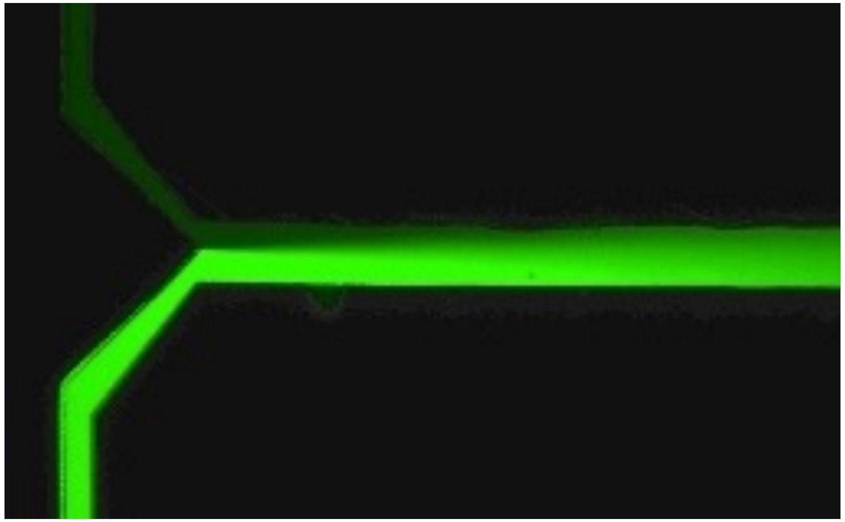
in scaling laws ?

exact solution ?

2.3 Measuring a diffusion coefficient ?

Y-junction in a microfluidic chip





in scaling laws:

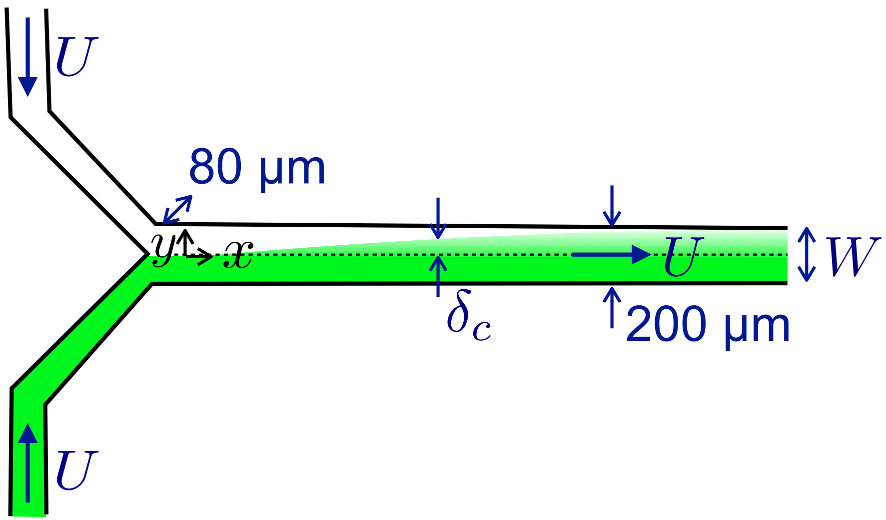
$$t \leftrightarrow \frac{c}{U}$$

$$\boxed{\delta_c \sim (Dt)^{1/2} \sim \left(D\frac{x}{U}\right)^{1/2}}$$

numerical estimate: $D \sim 4.10^{-10}$ m²/s $\quad U \sim 1$ mm/s $\quad x \sim 5$ cm

$\delta_c \sim 100$ µm

exact solution ?



we consider $\delta_c \ll W$

$$\Rightarrow \text{BCs:} \begin{cases} c(y=\infty)=0 \\ c(y=-\infty)=c_0 \end{cases}$$

$$\cancel{\frac{\partial c}{\partial t}} + \mathbf{u}\cdot\boldsymbol{\nabla} c = D\,\Delta c$$

steady flow

Hypothesis wall effects neglected: $\mathbf{u} = U\mathbf{e}_x \;\Rightarrow\; \mathbf{u}\cdot\boldsymbol{\nabla} c = U\dfrac{\partial c}{\partial x}$

$$U\frac{\partial c}{\partial x} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)$$

neglecting $\dfrac{\partial^2 c}{\partial x^2}$?

neglecting $\frac{\partial^2 c}{\partial x^2}$?

time to diffuse along x: $\tau_{diff} \sim \frac{x^2}{D}$ convection along x: $\tau_{conv} \sim \frac{x}{U}$

if $\tau_{conv} \ll \tau_{diff}$ convection dominates (along x)

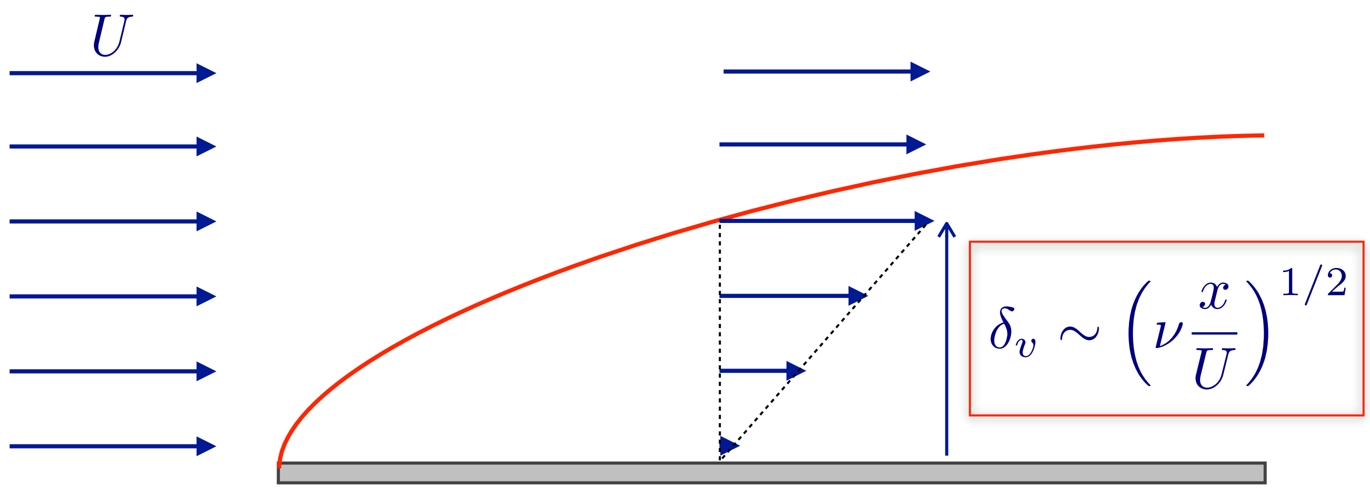
$$\frac{x}{U} \ll \frac{x^2}{D} \Leftrightarrow \boxed{Pe = \frac{Ux}{D} \gg 1 \quad \text{Peclet number}}$$

remains:

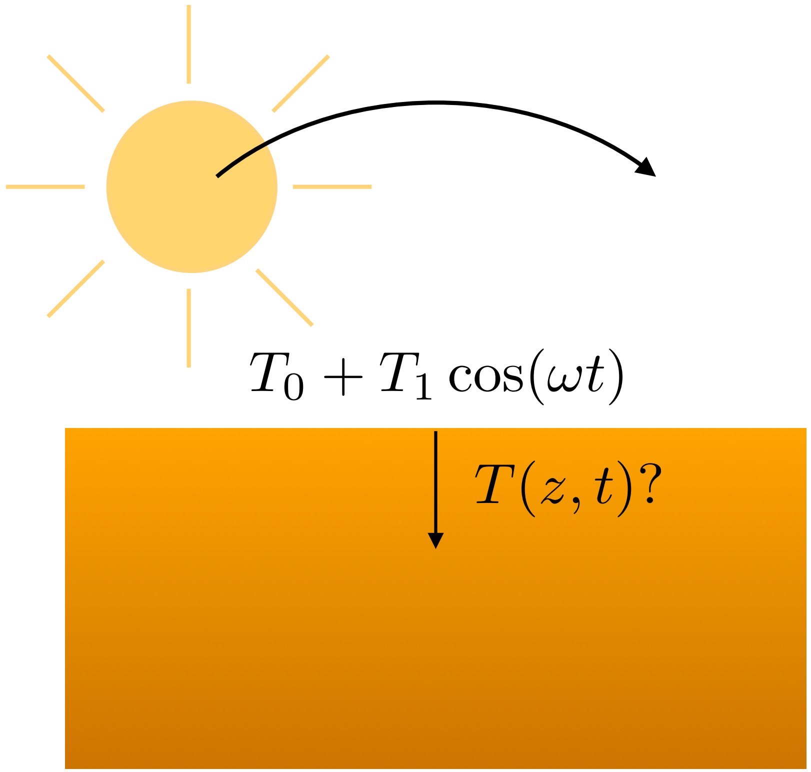
$$\frac{\partial c}{\partial x} = \frac{D}{U}\frac{\partial^2 c}{\partial y^2}$$ ⇒ same solution as before with $\xi = \frac{y}{2(Dx/U)^{1/2}}$

$$\boxed{c(x,y) = \frac{c_0}{2}\left(1 - \mathrm{erf}\left(\frac{y}{2(Dx/U)^{1/2}}\right)\right)}$$

Analogy boundary layer in fluids

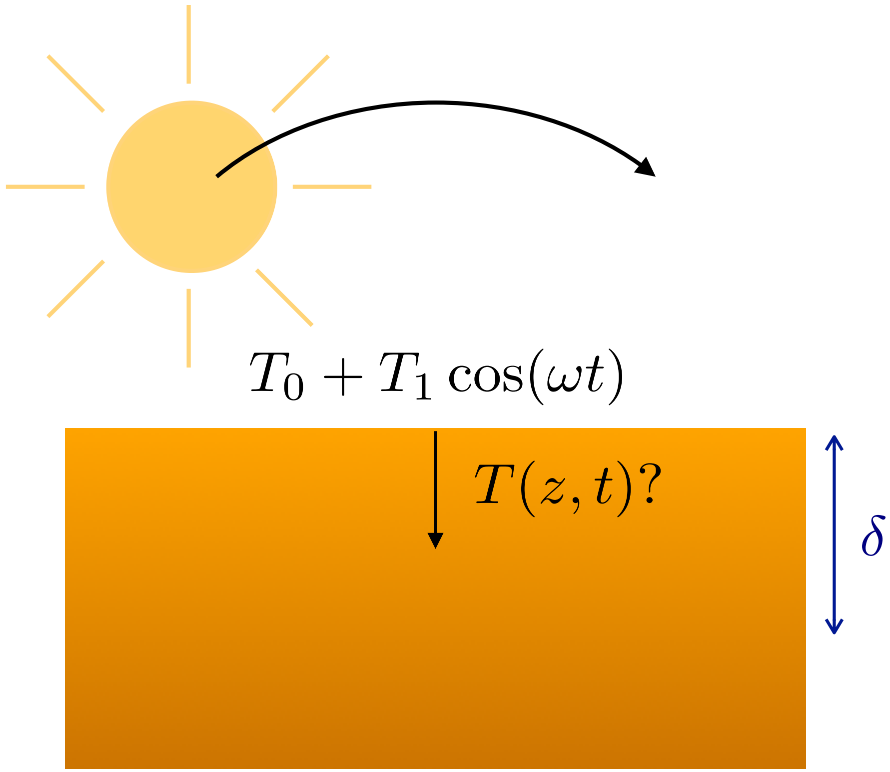


2.4 Measuring a diffusion coefficient ?



in scaling laws ?

2.4 Measuring a diffusion coefficient ?



in scaling laws ?

$$\frac{\partial T}{\partial t} = \alpha \, \frac{\partial^2 T}{\partial z^2}$$

$$\omega T \sim \alpha \, \frac{T}{\delta^2}$$

$$\boxed{\delta \sim (\alpha/\omega)^{1/2}}$$

Exact solution $$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial z^2}$$

Solution of the form $T(z,t) = \mathrm{Re}\left(T_0 + T^*(z)e^{i\omega t}\right)$?

$$\frac{\partial T}{\partial t} = i\omega T^*(z)e^{i\omega t} \qquad \frac{\partial^2 T}{\partial z^2} = T^{*\prime\prime}(z)e^{i\omega t}$$

$$T^{*\prime\prime}(z) - i\,\frac{\omega}{\alpha}T^* = 0$$

$$\frac{\omega}{\alpha}e^{i\frac{\pi}{2}}$$

$$\Rightarrow \quad \left(i\,\frac{\omega}{\alpha}\right)^{1/2} = \pm\sqrt{\frac{\omega}{\alpha}}e^{i\frac{\pi}{4}} = \pm\sqrt{\frac{\omega}{2\alpha}}(1+i)$$

$$T^*(z) = A\exp\left(\sqrt{\frac{\omega}{2\alpha}}(1+i)z\right) + B\exp\left(-\sqrt{\frac{\omega}{2\alpha}}(1+i)z\right)$$

$$T^*(z \to \infty) \text{ finite } \Rightarrow A = 0$$

$$T^*(z = 0) = T_1 \;\Rightarrow B = T_1$$

$$T(z,t) = \mathrm{Re}\left[T_0 + T_1 \exp\left(-\sqrt{\frac{\omega}{2\alpha}}\, z\right) e^{i\left(\omega t - \sqrt{\frac{\omega}{2\alpha}}\, z\right)}\right]$$

$$\boxed{T(z,t) = T_0 + T_1 \underbrace{\exp\left(-\sqrt{\frac{\omega}{2\alpha}}\, z\right)}_{\text{attenuation}} \cos\underbrace{\left(\omega t - \sqrt{\frac{\omega}{2\alpha}}\, z\right)}_{\text{phase lag}}}$$

attenuation depth $\boxed{\delta = \sqrt{\frac{\omega}{2\alpha}}}$

numerical estimate: $\alpha \sim 5.10^{-7}$ m²/s

$$\omega_{1\,day} = \frac{2\pi}{24 \times 3600} = 7.3\,10^{-5} \text{ rad/s} \;\Rightarrow\; \delta \sim 10 \text{ cm}$$

$$\omega_{1\,year} = 2.7\,10^{-7} \text{rad/s} \;\Rightarrow\; \delta \sim 2 \text{ m}$$