NOTES ON DIFFUSION

Diffusion is one of the fundamental transport processes in environmental fluid mechanics.
Diffusion is random in nature and transport by diffusion occurs always from regions of high concentration to regions of low concentration.

There can be two different types of transport by diffusion:

1. TRANSPORT BY MOLECULAR DIFFUSION (due to random motion of the molecules)

   This type of transport obeys the Fick's law:

$$\boxed{J_i = -D\frac{\partial C}{\partial x_i}} \quad \left[\frac{Kg}{m^2 s}\right]$$

   and the mass flux is $\dot{m}_i = \int_A J_i \, dA$.

   The change in concentration of the diffusing mass over time is:

$$\boxed{\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x_i^2} = D\nabla^2 C}$$

2. TRANSPORT BY TURBULENT DIFFUSION (due to a non-uniform, time-dependent flow field)

   This type of transport allows mixing to occur at much faster rates than molecular diffusion alone.
   As a result turbulent diffusion coefficients are

typically orders of magnitude larger than the molecular diffusion coefficients.

In the case of turbulent diffusion, the Fick's law is not valid anymore, and the time evolution of concentration obeys the following equation:

$$\boxed{\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = D \frac{\partial^2 c}{\partial x_i^2}}$$

with $c(x_i, t) = \overline{c}(x_i) + \underbrace{c'(x_i, t)}_{\text{fluctuation of concentration}}$

$$u_i(x_i, t) = \overline{u}_i(x_i) + \underbrace{u_i'(x_i, t)}_{\text{fluctuation of velocity}}$$

REYNOLDS DECOMPOSITION

Following the same procedure used to derive the Reynolds-Averaged Navier-Stokes equations, an equation for the average concentration $\overline{c}$ can be obtained:

$$\frac{\partial \overline{c}}{\partial t} + \overline{u}_i \frac{\partial \overline{c}}{\partial x_i} = - \frac{\partial \overline{u_i' c'}}{\partial x_i} + \frac{\partial}{\partial x_i}\left(D \frac{\partial \overline{c}}{\partial x_i} \right)$$

molecular diffusion coefficient

where $\overline{u_i' c'}$ is an unknown term (analogous to the Reynolds stresses for velocity) that needs to be modeled.

The simplest model is based on the use of a Fick's law type for turbulent diffusion, which allows to write:

$$\boxed{\overline{u_i' c'} = -D_t \frac{\partial \overline{c}}{\partial x_i}}$$

with D_t = turbulent diffusion coefficient (analogous to the turbulent viscosity μ_T introduced to model the Reynolds stresses).

This yields:

$$\frac{\partial \overline{c}}{\partial t} + \overline{u_i} \frac{\partial \overline{c}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(D + D_t\right)\frac{\partial \overline{c}}{\partial x_i}\right]$$

The expression for D_t changes depending on the type of flow. In general form, D_t is proportional to the product of a characteristic velocity of the flow times a characteristic length of the flow:

$$D_t \propto u_{ref} \cdot l_{ref}$$

For instance, in a wide river with depth h and width $W \gg h$, an estimate of D_t can be:

$$D_t \propto u_* \cdot h$$

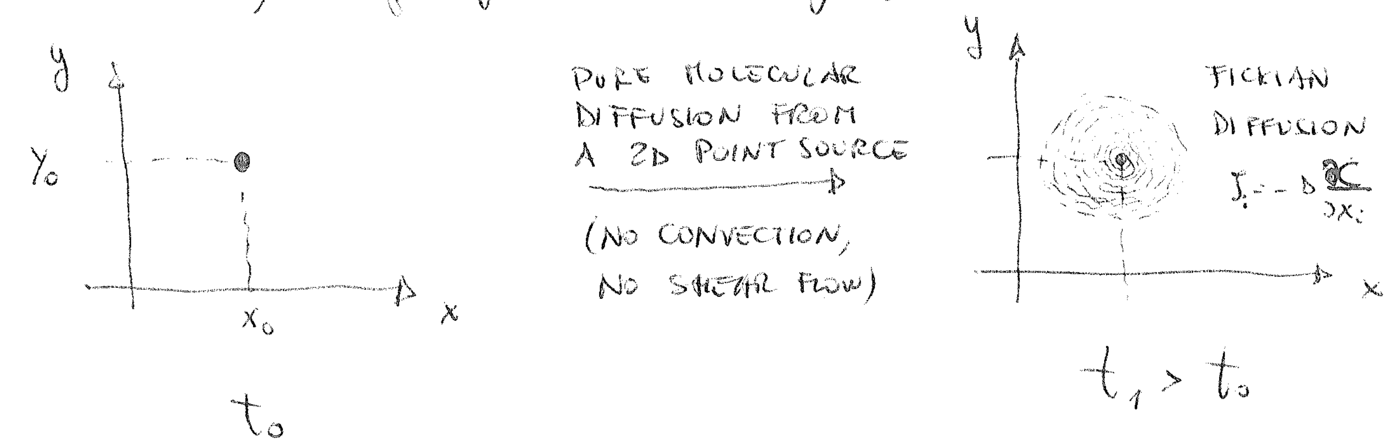
with $u_* = \sqrt{\frac{\tau_w}{\rho}}$ the shear velocity and τ_w the mean shear stress at the river bed.

How large is D_t compared to D? For air:

$$\underbrace{D_t \simeq 0.35 \ \frac{m^2}{s}}_{\text{turbulent diffusion}} \quad \text{vs} \quad \underbrace{D \cong 10^{-5} \ \frac{m^2}{s}}_{\text{molecular diffusion}}$$

It must be emphasized that turbulent diffusion is associated to turbulent convection phenomena, represented by the non-linear term $u_i \frac{\partial c}{\partial x_i}$ in the constitutive transport equation.
Turbulent convection is due to the presence of a non-uniform velocity field, and is of particular importance for shear flows, namely flows characterized by significant velocity gradients:

A



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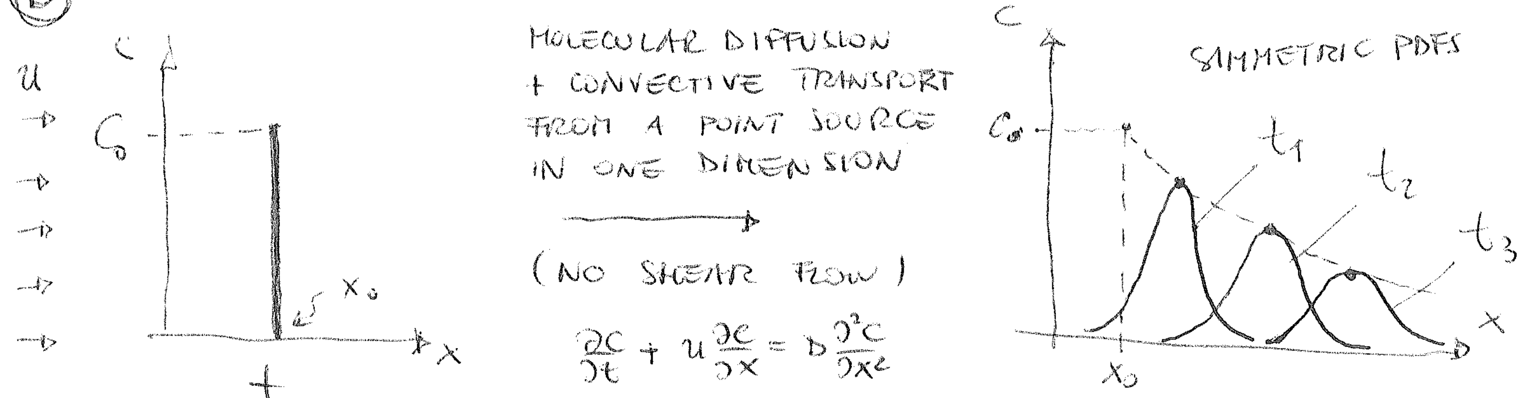

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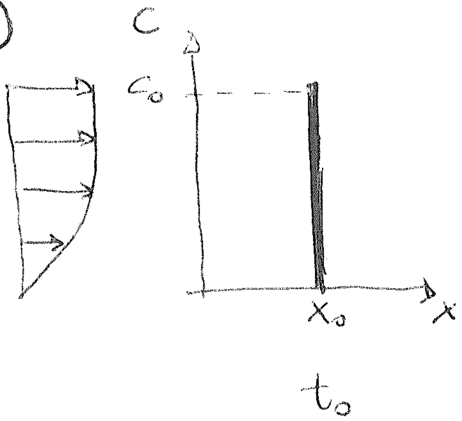
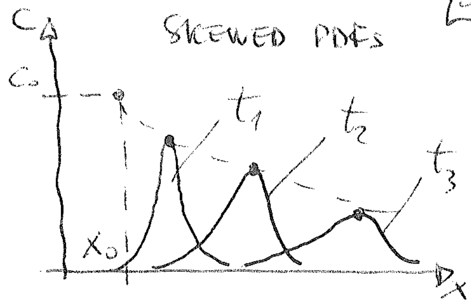


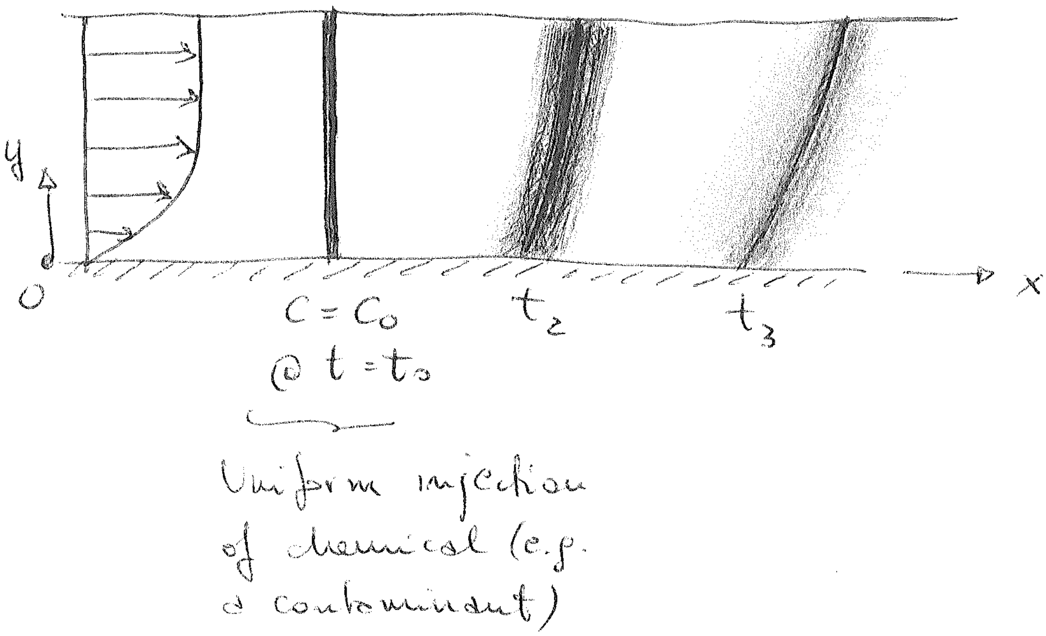
MOLECULAR DIFFUSION + CONVECTIVE DIFFUSION FROM A POINT SOURCE IN ONE DIMENSION

(SHEAR FLOW)



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

If the velocity profile is not uniform, e.g. in the vertical direction y, then there will be a velocity gradient $\frac{\partial u}{\partial y}$. This velocity gradient induces a non-uniform transport of concentration not only along x but also along y: This way concentration gradients in the vertical direction are created:



At time t_0, there is no vertical concentration gradient if the chemical is injected with uniform concentration. Therefore, there will be no net diffusive flux in the vertical direction.

Due to shear, the patch of injected chemical will be advected downstream and get stretched in the horizontal direction because of the different advection velocity in the shear profile. This is the situation at time t_2 for instance.

At this point, vertical concentration gradients have been created and a net diffusive flux in the vertical direction is established.

As the stretched-out patch travels downstream, the vertical concentration gradients will be smoothed out by diffusion and the patch will look like the one drawn at time t_3.

The combined process of convection and longitudinal diffusion is called <u>DISPERSION</u>.