# LESSON 12: ESTIMATION OF $K_x$

# ESTIMATION OF $K_x$

There are several methods to correctly estimate the dispersion coefficient $K_x$ in the Gaussian zone:

i. Empirical Formulas
ii. Chatwin Method
iii. Moments Method

*These Methods have been described in the exercise lesson*

iv. Calibration Method
v. Velocity Field Method
vi. Graphic Method

# EMPIRICAL FORMULAS

The literature provides several formulas based on the multiple regression analysis of experimental data.

- McQuivey & Keefer (1974):

$$K_x = 0.058\,\frac{Q}{i_b B}$$

- Liu (1977):

$$K_x = \alpha\,\frac{U^2}{z_0 u_*} \qquad \alpha = 0.18\left(\frac{u_*}{U}\right)^{3/2}$$

- Seo & Cheong (1998)

$$K_x = 5.195\,z_0 u_*\left(\frac{B}{z_0}\right)^{0.62}\left(\frac{u_*}{U}\right)^{1.428}$$

- Kashelipour & Falconer (2002):

$$K_x = 10.612\,z_0 u_*\left(\frac{u_*}{U}\right)$$

# CHATWIN METHOD



Chatwin rearranges the fundamental solution proposed by Taylor for 1D Fickian type process as following:

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

$$e^{\frac{(x-Ut)^2}{4K_x t}} = \frac{M}{A\sqrt{4\pi K_x}} \frac{1}{C\sqrt{t}}$$

$$R = \frac{M}{A\sqrt{4\pi K_x}}$$

ln

$$\frac{(x-Ut)^2}{4K_x t} = \ln\frac{R}{C\sqrt{t}} \longrightarrow \frac{(x-Ut)^2}{4K_x} = t\ln\frac{R}{C\sqrt{t}}$$

And then:

$$\frac{x}{2\sqrt{K_x}} - \frac{U}{2\sqrt{K_x}}t = \sqrt{t\ln\frac{R}{C\sqrt{t}}} = C^*$$

*Fictitious concentration*

# CHATWIN METHOD

Often the amount of mass M is unknown. In this case it is useful rewritting the term R:

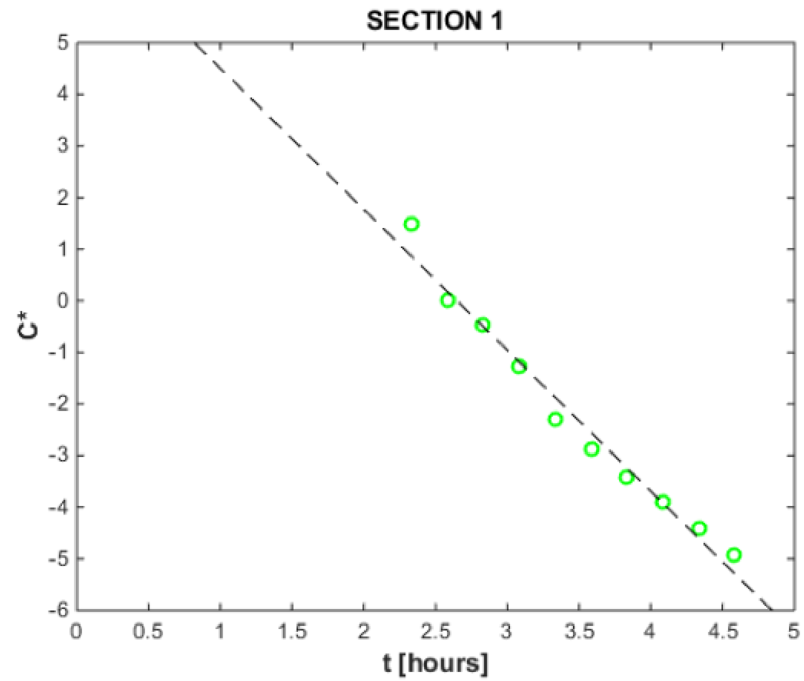
$$C_{max} = \frac{M}{A\sqrt{4\pi K_x t_{max}}} e^{-\cancelto{1}{\frac{(x-Ut_{max})^2}{4K_x t_{max}}}} \longrightarrow C_{max} t_{max} = \frac{M}{A\sqrt{4\pi K_x}} = R$$

And finally:

$$C^* = -\frac{U}{2\sqrt{K_x}} t + \frac{x}{2\sqrt{K_x}}$$

with:

$$\begin{cases} C^* = \sqrt{t \cdot ln \frac{C_{max}\sqrt{t_{max}}}{C\sqrt{t}}} & t \leq t_{max} \\ C^* = -\sqrt{t \cdot ln \frac{C_{max}\sqrt{t_{max}}}{C\sqrt{t}}} & t > t_{max} \end{cases}$$




*$K_x$ and $U$ are calculated by the slope and the intercept of the dashed line*

When the process of dispersion occurs in the Gaussian zone, the variance of the cloud increases linearly, i.e.:

$$\frac{\mathrm{d}{\sigma_x}^2}{\mathrm{d}t} = 2K_x$$

By applying the discretization method, it means:

$$K_x = \frac{1}{2}\frac{{\sigma_x}^2(t_2) - {\sigma_x}^2(t_1)}{t_2 - t_1}$$

Being:

$${\sigma_x}^2(t_i) = \frac{\int_{-\infty}^{+\infty} [x - \mu_x(t_i)]^2 C(x, t_i)\mathrm{d}t}{\int_{-\infty}^{+\infty} C(x, t_i)\mathrm{d}t}$$

→ Statistical moment of order II

$$\mu_x(t_i) = \frac{\int_{-\infty}^{+\infty} xC(x, t_i)\mathrm{d}t}{\int_{-\infty}^{+\infty} C(x, t_i)\mathrm{d}t}$$

→ Statistical moment of order I

In the practice, it is easier measuring $C(x_i, t)$ rather than $C(x, t_i)$. Hence we need to use the temporal variance of the concentration in $x_i$, ${\sigma_t}^2(x_i)$.

Fisher in 1966 demonstrated that:

$$K_x = \frac{1}{2} U_0 \frac{{\sigma_t}^2(x_2) - {\sigma_t}^2(x_1)}{\overline{t_2} - \overline{t_1}}$$

where

$$\overline{t_i} = \frac{A}{M} \int_0^{+\infty} tC(x_i, t)\mathrm{d}t$$

→ Statistical moment of order I.
It is the time of the centroid in $x_i$

$$ {\sigma_t}^2(x_i) = \frac{A}{M} \int_0^{+\infty} [t - \overline{t_i}]^2 C(x_i, t)\mathrm{d}t$$

→ Statistical moment of order II

$$U_0 = \frac{x_2 - x_1}{\overline{t_2} - \overline{t_1}}$$

→ Mean velocity of the cloud centroid between $x_1$ and $x_2$

# THE CALIBRATION METHOD

The Calibration method is one of the most reliable methods to determine the mean velocity $U$ and the dispersion coefficient $K_x$.

The Calibration method assumes the Taylor solution being valid, i.e. for lumped insertion:

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

Generally, the distribution depends on the initial distribution of $C$, then we can consider:

$$\frac{\mathrm{d}M}{A} = C(\xi, t_1)\mathrm{d}\xi$$

*Amount of mass per unit area due to the concentration $C$ in the section $\xi$ at time $t_1$.*

By the fundalmental solution:

$$\mathrm{d}C = \frac{C(\xi, t_1)\mathrm{d}\xi}{\sqrt{4\pi K_x (t-t_1)}}\, e^{-\frac{\left(x-\xi-U(t-t_1)\right)^2}{4K_x(t-t_1)}}$$

*New reference system*

*New reference time*

*Distribution of $C$ due to the contribution $C(\xi, t_1)\mathrm{d}\xi$*

By integrating along $x$ all the contributions of the generic distribution $C(\xi, t_1)$, we find:

$$C(x,t) = \int_{-\infty}^{+\infty} \frac{C(\xi, t_1)}{\sqrt{4\pi K_x (t - t_1)}} \, e^{-\frac{\left(x-\xi-U(t-t_1)\right)^2}{4K_x(t-t_1)}} \, \mathrm{d}\xi$$

It is worth noting that if we know $C(x, t_1)$, i.e. $C(\xi, t_1)$, we can evaluate $C(x, t)$ and thus $C(x, t_2)$, where $t_1$ is the initial condition time and $t_2$ a time of interest of the problem!

The calibration method uses this property, but it is focused on the temporal distribution of $C$, instead of its spatial distribution, i.e.:

$$C(x, t_1) \rightarrow C(x, t_2) \qquad\qquad \boxed{C(x_1, t) \rightarrow C(x_2, t)}$$

This operation is not trivial and it needs of some assumptions. There are two main solutions:

i. <u>Approximation of the Frozen Cloud</u>

ii. <u>Hayami Method</u>

Let's see the approximation of the Frozen Cloud

It is worth noting that given $C(x,t)$:

- Spatial distribution ($t = t_n$). The peak of concetration has the following characteristics:

$$\left.\begin{aligned} x_{max} &= x_g = Ut_n \\ C_{max} &= \frac{M}{A\sqrt{4\pi K_x t_n}} = \frac{M}{A\sqrt{4\pi K_x\, x_{max}/U}} \end{aligned}\right\}$$

$C_{max}$ is in $x_g$!

- Temporal distribution ($x = x_n$).

$$t_{max} \rightarrow \frac{\mathrm{d}C}{\mathrm{d}t} = 0 \longrightarrow t_{max} = \sqrt{\frac{{K_x}^2}{U^4} + \frac{{x_n}^2}{U^2}} - \frac{K_x}{U^2}$$

*Time of the peak of concentration in $x_n$*

---

$$C = \frac{M}{A\sqrt{4\pi K_x t}} \cdot e^{-\frac{(x_n - Ut)^2}{4K_x t}} = f \cdot g \longrightarrow \frac{\mathrm{d}C}{\mathrm{d}t} = fg' + f'g = 0$$

$$f = \frac{M}{A\sqrt{4\pi K_x t}} \longrightarrow f' = -\frac{1}{2}\frac{M 4\pi K_x}{A\sqrt{4\pi K_x t}}\frac{1}{4\pi K_x t} = -\frac{1}{2t}\frac{M}{A\sqrt{4\pi K_x t}} = -\frac{1}{2t} f$$

$$g = e^{-\frac{(x_n - Ut)^2}{4K_x t}} \longrightarrow g' = -\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{(x_n - Ut)^2}{4K_x t}\right] e^{-\frac{(x_n - Ut)^2}{4K_x t}} = -\left[\frac{-2(x_n - Ut)Ut - (x_n - Ut)^2}{4K_x t^2}\right] g = -\frac{U^2t^2 - {x_n}^2}{4K_x t^2} g$$

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -\left(\frac{U^2t^2 - {x_n}^2}{4K_x t^2} + \frac{1}{2t}\right)\underbrace{\cancel{fg}}_{C} = 0 \longrightarrow \frac{U^2t^2 - {x_n}^2 + 2K_x t}{\cancel{4K_x t^2}} = 0 \longrightarrow t_{max} = \frac{-2K_x + \sqrt{4{K_x}^2 + 4U^2{x_n}^2}}{2U^2}$$

# FROZEN CLOUD APPROXIMATION



$$t_g = \bar{t} = \frac{\int_0^\infty tC(x_n,t)\mathrm{d}t}{\int_0^\infty C(x_n,t)\mathrm{d}t} = \frac{x_n}{U} + 2\frac{K_x}{U^2}$$

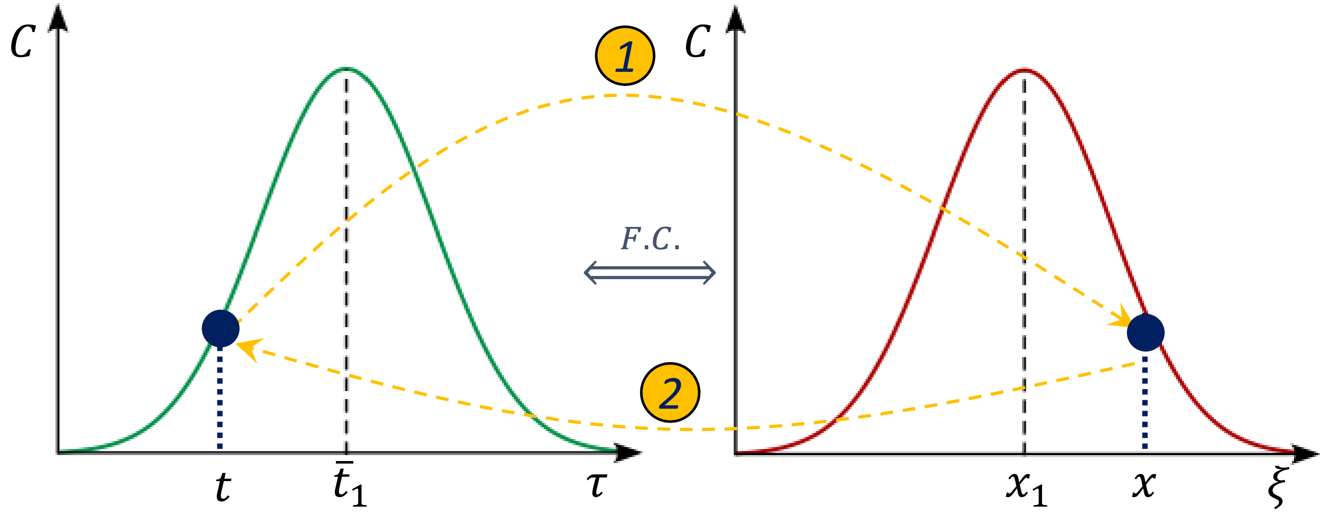
*Time of the centroid in $x_n$*

The peak of concetration time and the centroid time are different: $t_{max} \neq \bar{t}$

The Frozen Cloud (F.C.) approximation assumes that the advection is much greater than dispersion, i.e. $Pe \gg 1$. It implies that:

$$\frac{K_x}{U^2} \ll \frac{x_n}{U} \longrightarrow \bar{t} \cong t_{max} = \frac{x_n}{U}$$

Under this assumption, we can link temporal $C$ distribution in a given section $x_1$ and spatial $C$ distribution in a given time $\bar{t}_1$ as following:



# FROZEN CLOUD APPROXIMATION



Let's analyze the concentration which is highlighted by blue circle in the two planes.

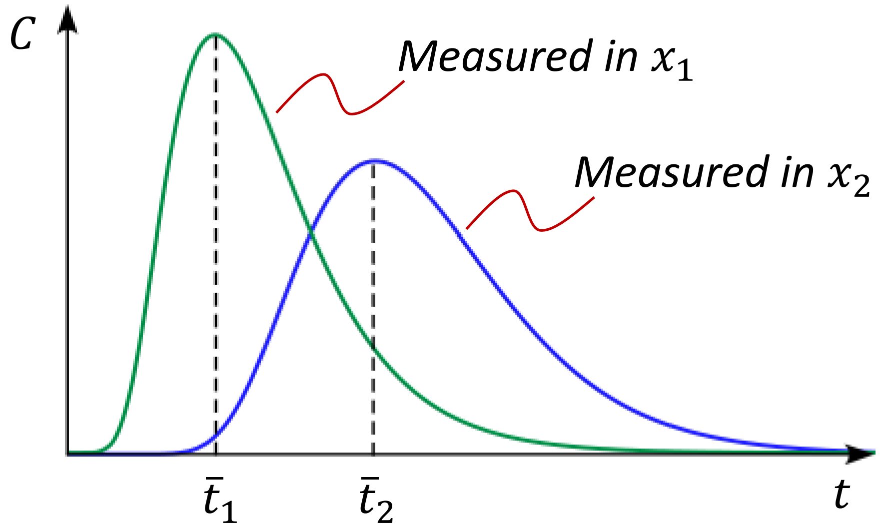
1 $C(x_1, t) \longrightarrow C(x, \bar{t}_1)$ *The position $x$ is reached travelling with $U$ for $\Delta t = \bar{t}_1 - t$*

$C(x_1 + U(\bar{t}_1 - t), \bar{t}_1)$ *The spatial distribution is expressed in $t$*

2 $C(x, \bar{t}_1) \longrightarrow C(x_1, t)$

$C\left(x_1, \bar{t}_1 - \dfrac{x - x_1}{U}\right)$ *The temporal distribution is expressed in $x$*

The variables transformation is then given by: $x = x_1 + U(\bar{t}_1 - t)$

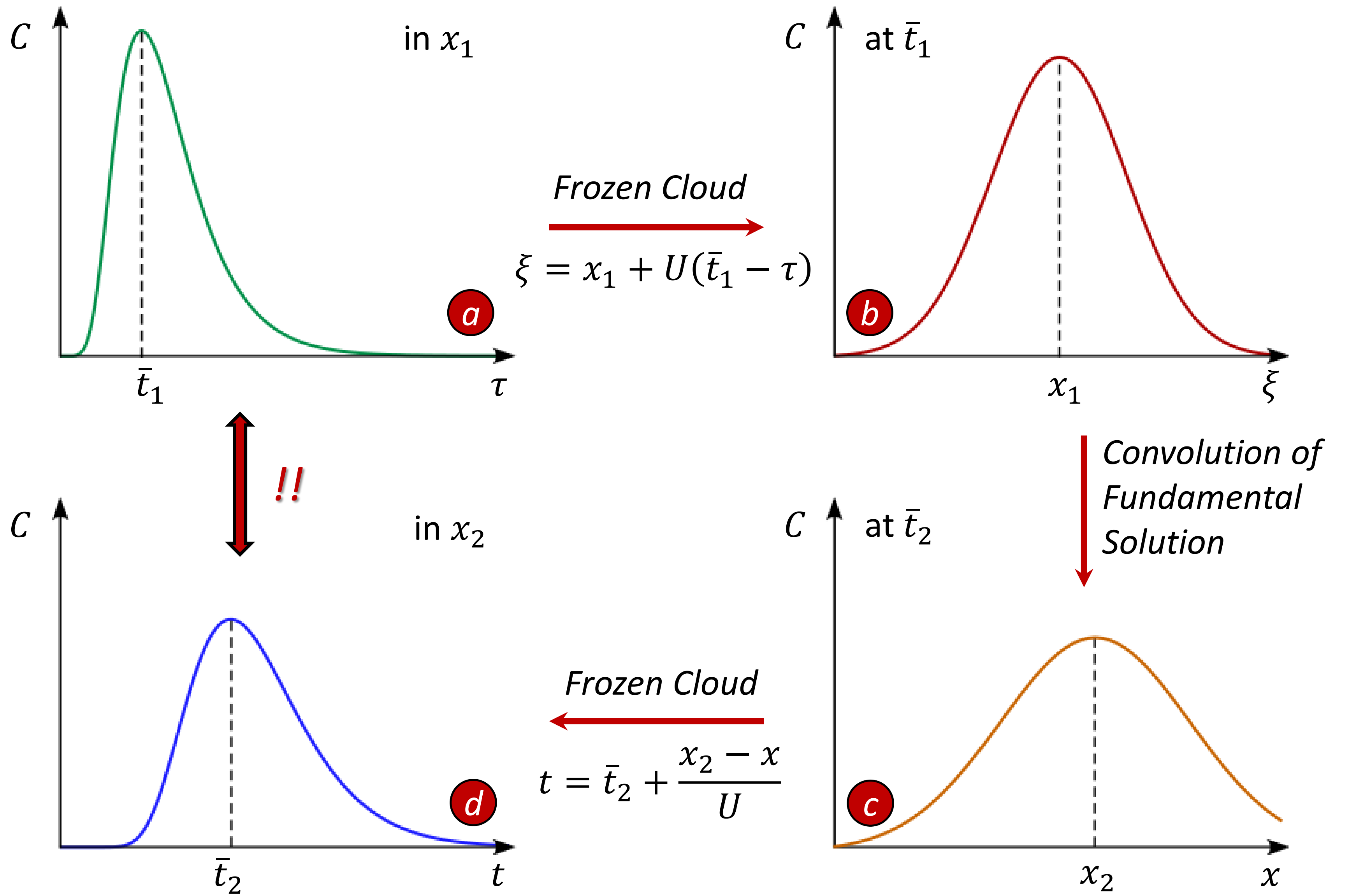



In the practice:

$$C(x_1, t) \overset{?}{\Longleftrightarrow} C(x_2, t)$$

The solution of the problem provides $K_x$ and $U$

# FROZEN CLOUD APPROXIMATION



a → b $C(x_1,\tau) \rightarrow C(\xi,\bar{t}_1)$ *It is the initial condition of the dispersion equation*

b → c

$$C(x,t) = \int_{-\infty}^{+\infty} \frac{C(\xi,\bar{t}_1)}{\sqrt{4\pi K_x(t-\bar{t}_1)}}\, e^{-\frac{\left(x-\xi-U(t-\bar{t}_1)\right)^2}{4K_x(t-\bar{t}_1)}}\, \mathrm{d}\xi$$

$$\Big\downarrow\ t = \bar{t}_2$$

$$C(x,\bar{t}_2) = \int_{-\infty}^{+\infty} \frac{C(\xi,\bar{t}_1)}{\sqrt{4\pi K_x(\bar{t}_2-\bar{t}_1)}}\, e^{-\frac{\left(x-\xi-U(\bar{t}_2-\bar{t}_1)\right)^2}{4K_x(\bar{t}_2-\bar{t}_1)}}\, \mathrm{d}\xi \qquad (*)$$

c → d $C(x,\bar{t}_2) \rightarrow C(x_2,t)$

The distribution in (d) as fuction of the distribution in (a) can be estimated by replacing in $(*)$ the variables transformations due to the Frozen Cloud, that are:

$$\begin{cases} \xi = x_1 + U(\bar{t}_1 - \tau) \\ x = x_2 + U(\bar{t}_2 - t) \end{cases}$$

In the latter the centroid position $x_2$ depends on the centroid position $x_1$ as following:

$$x_2 = x_1 + U(\bar{t}_2 - \bar{t}_1)$$

Then: $$x = x_2 + U(\bar{t}_2 - t) = x_1 + U(\bar{t}_2 - \bar{t}_1) + U(\bar{t}_2 - t)$$

$$x = x_1 + U(2\bar{t}_2 - \bar{t}_1 - t)$$

We can express the difference $x - \xi$ as:

$$x - \xi = x_1 + U(2\bar{t}_2 - \bar{t}_1 - t) - x_1 - U(\bar{t}_1 - \tau)$$

$$\longrightarrow \quad x - \xi = U(2\bar{t}_2 - 2\bar{t}_1 - t + \tau) \qquad (**)$$

The $(**)$ into $(*)$ yields:

$$C(x_2, t) = \int_{-\infty}^{+\infty} \frac{C(\xi, \bar{t}_1)}{\sqrt{4\pi K_x(\bar{t}_2 - \bar{t}_1)}}\, e^{-\frac{\left(U(2\bar{t}_2 - 2\bar{t}_1 - t + \tau) - U(\bar{t}_2 - \bar{t}_1)\right)^2}{4K_x(\bar{t}_2 - \bar{t}_1)}}\, \mathrm{d}\xi$$

$$C(x_2, t) = \int_{-\infty}^{+\infty} \frac{C(\xi, \bar{t}_1)}{\sqrt{4\pi K_x(\bar{t}_2 - \bar{t}_1)}}\, e^{-\frac{U^2(\bar{t}_2 - \bar{t}_1 - t + \tau)^2}{4K_x(\bar{t}_2 - \bar{t}_1)}}\, \mathrm{d}\xi$$

To conclude the demonstration, we need of expressing the initial concentration distribution in terms of temporal concentration distribution. It is useful noting that:

$$\frac{\mathrm{d}M}{A} = C(\xi, \bar{t}_1)\mathrm{d}\xi = C(x_1, \tau)U\mathrm{d}\tau$$

And finally:

$$\longrightarrow \quad C(x_2, t) = \int_{-\infty}^{+\infty} \frac{C(x_1, \tau)U}{\sqrt{4\pi K_x(\bar{t}_2 - \bar{t}_1)}} e^{-\frac{U^2(\bar{t}_2 - \bar{t}_1 - t + \tau)^2}{4K_x(\bar{t}_2 - \bar{t}_1)}} \mathrm{d}\tau$$

The first attempt for $U$ can be:

- $U = \dfrac{x_2 - x_1}{\bar{t}_2 - \bar{t}_1}$
- $U \cong \dfrac{2}{3} U_M$

*Flow velocity which is measured on the free surface*

Another method to determine the pair $(K_x, U)$ was proposed by Hayami.
For Hayami the concentration distribution $C_H$ considering the insertion point in $x_1$ is:

$$C_H(x,t) = C(x,t)\,\frac{x - x_1}{Ut}$$

*Taylor solution*

$$C_H(x,t) = \frac{M(x - x_1)}{AUt\sqrt{4\pi K_x t}}\, e^{-\frac{(x-Ut)^2}{4K_x t}}$$

The solution in the section of interest $x_2$ is the sum of the contribute $C(x_1,\tau)U\mathrm{d}\tau$ inserting in $x_1$ during the time $\tau$:

$$C(x_2,t) = \int_{-\infty}^{+\infty} \frac{C(x_1,\tau)(x_2 - x_1)}{(t-\tau)\sqrt{4\pi K_x(t-\tau)}}\, e^{-\frac{[x_2 - x_1 - U(t-\tau)]^2}{4K_x(t-\tau)}} \mathrm{d}\tau$$

Being $C = \dfrac{M}{A}$

# ABOUT SOLUTE…

The methods described above are effective only when the solute and insertion mode have some characteristics

<u>Solute</u>:

- Negligible bio-chimics reactions
- Negligible adsorption by sediments
- Negligible toxicity
- High solubility
- Neutrally buoyant, i.e. $\gamma_s \cong \gamma_w$
- Easy to chimically analyze
- Dye
- Cheap

→

<u>Sodium Chloride</u>

<u>Magnesium Sulfate</u>

<u>Sodium Nitrate</u>

<u>Sodium Dichromate</u>

<u>Rhodamine</u>

*Most common*

# ABOUT SOLUTE…



The modality of solute insertion depends on the variables of interest that one wants to estimate.

| Variables | Modality |
|---|---|
| $U$ (between two sections) | • Lumped insertion<br>• Step insertion |
| $k_z$<br>$k_y$ | • Continuos insertion |
| $k_x$<br>$K_x$ | • Lumped insertion |