LESSON 7: SOLUTE CLOUD DYNAMICS

DYNAMICS OF SOLUTE CLOUD

Assumptions on the turbulent diffusion of solute:

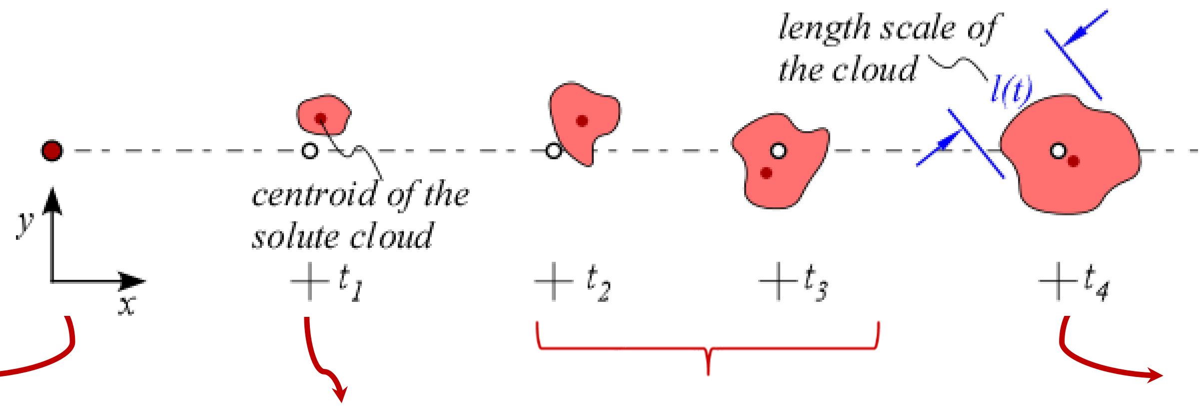
i. Turbulence is homogeneous and stationary (ergodic process)

ii. Flow is 1D and uniform, i.e. $\boldsymbol{u} = (u_0,\ 0,\ 0\ )$

It means that Taylor's hypothesis is valid

iii. The process is 2D (actually it is 3D!)

The solute evolution after the injection at the time t_0 is shown in figure.



Case j=1

The reference system moves along x with velocity u_0.

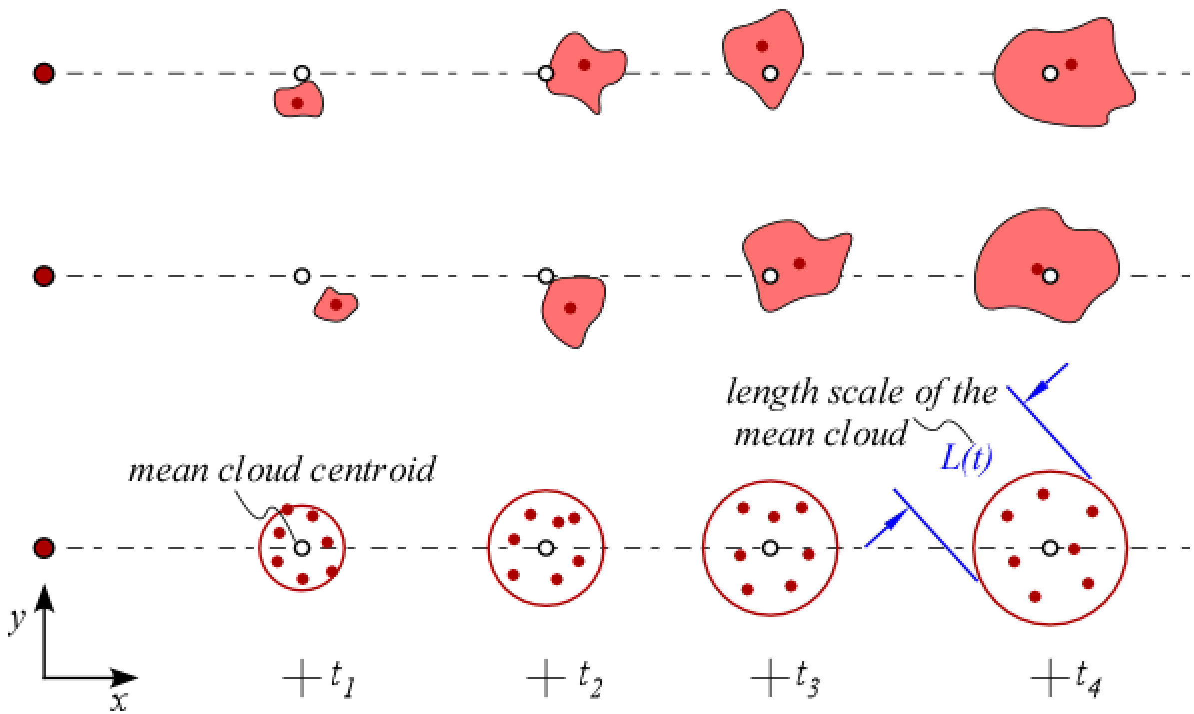
t_1 ≪. Microvortexes determine the cloud deformation

Cloud transport is due to macrovortexes (t is small but not negligible)

t_4 ≫. The cloud is larger than macrovortexes. Diffusivity is constant!

DYNAMICS OF SOLUTE CLOUD

If we consider the process being repeated *N* times (*N* is large):



Case j=2

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.

.

Case j=N

<u>Mean Cloud</u> (it is determined by the *N* centroids)

→ The origin of the reference system corresponds to the mean cloud centroid

CLOUD STATISTICAL MOMENTS

The problem must be investigated though probabilistic approach.

In each realization (*j*=1…*N*) the concentration of the solute is: $c = c(\boldsymbol{x}, t)$

Therefore the concentration mean cloud is:

$$C(\boldsymbol{x}, t) = < c(\boldsymbol{x}, t) > = \int_{-\infty}^{+\infty} c\, p(c|\boldsymbol{x}, t)\, \mathrm{d}c$$

The average of the realization equal to the temporal mean of c*. It is due to ergodicity!*

Statistical moments:

Cloud

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

$$x_{gi} = \frac{1}{M}\int_{-\infty}^{+\infty} x_i\, c(\boldsymbol{x}, t)\, \mathrm{d}x_i$$

$${\sigma_i}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} \left(x_i - x_{gi}\right)^2 c(\boldsymbol{x}, t)\, \mathrm{d}x_i$$

Mean cloud

$$C(\boldsymbol{x}, t) = \int_{-\infty}^{+\infty} c\, p(c|\boldsymbol{x}, t)\, \mathrm{d}c$$

$$X_{gi} = \frac{1}{M}\int_{-\infty}^{+\infty} x_i\, C(\boldsymbol{x}, t)\, \mathrm{d}x_i$$

$${\Sigma_i}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} \left(x_i - X_{gi}\right)^2 C(\boldsymbol{x}, t)\, \mathrm{d}x_i$$

Let's compare the variance of generic cloud and the mean cloud.

For the generic cloud, the variance can be write as:

$$\sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty}\left(x_i{}^2 - 2x_i x_{gi} + x_{gi}{}^2\right) c(\boldsymbol{x},t)\,\mathrm{d}x_i$$

$$\sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} x_i{}^2 c(\boldsymbol{x},t)\mathrm{d}x_i - \frac{2x_{gi}}{M}\int_{-\infty}^{+\infty} x_i c(\boldsymbol{x},t)\mathrm{d}x_i + \frac{x_{gi}{}^2}{M}\int_{-\infty}^{+\infty} c(\boldsymbol{x},t)\mathrm{d}x_i$$

$$\sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} x_i{}^2 c(\boldsymbol{x},t)\mathrm{d}x_i - \frac{2x_{gi}}{M} M x_{gi} + \frac{x_{gi}{}^2}{M} M$$

$$\sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} x_i{}^2 c(\boldsymbol{x},t)\mathrm{d}x_i - x_{gi}{}^2$$

And then the average variance considering the *N* realization is

$$< \sigma_i{}^2 > = \frac{1}{M}\int_{-\infty}^{+\infty} x_i{}^2 C(\boldsymbol{x},t)\mathrm{d}x_i - < x_{gi}{}^2 >$$

The variance of the mean cloud is:

$$\Sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} \left(x_i{}^2 - 2x_i X_{gi} + X_{gi}{}^2\right) C(\boldsymbol{x},t)\,\mathrm{d}x_i$$

$$\Sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} x_i{}^2 C(\boldsymbol{x},t)\mathrm{d}x_i - \frac{2X_{gi}}{M}\int_{-\infty}^{+\infty} x_i C(\boldsymbol{x},t)\mathrm{d}x_i + \frac{X_{gi}{}^2}{M}\int_{-\infty}^{+\infty} C(\boldsymbol{x},t)\mathrm{d}x_i$$

$$\Sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} x_i{}^2 C(\boldsymbol{x},t)\mathrm{d}x_i - \frac{2X_{gi}}{M} M X_{gi} + \frac{X_{gi}{}^2}{M} M$$

$$\Sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty} x_i{}^2 C(\boldsymbol{x},t)\mathrm{d}x_i - X_{gi}{}^2$$

By replacing the latter into the mean variance of the clouds, we find:

$$<\sigma_i{}^2> = \Sigma_i{}^2 + X_{gi}{}^2 - <x_{gi}{}^2>$$

This relationship can be rearranged as following:

$$\longrightarrow \quad \Sigma_i{}^2 = <\sigma_i{}^2> + <\left(x_{gi} - X_{gi}\right)^2> \quad \rightarrow \quad \Sigma_i{}^2 > <\sigma_i{}^2>$$

The length scale of the cloud and of the the mean cloud are then defined as:

Cloud

$$l(t) = \sqrt{\frac{\sigma_x{}^2 + \sigma_y{}^2 + \sigma_z{}^2}{3}}$$

Mean cloud

$$L(t) = \sqrt{\frac{\Sigma_x{}^2 + \Sigma_y{}^2 + \Sigma_z{}^2}{3}}$$

By replacing the definitions of variances, we find:

$$L(t)^2 = \frac{<\sigma_x{}^2 + \sigma_y{}^2 + \sigma_z{}^2>}{3} + \frac{<\left(x_{gx} - X_{gx}\right)^2 + \left(x_{gy} - X_{gy}\right)^2 + \left(x_{gz} - X_{gz}\right)^2>}{3}$$

$$x'_{gi} = X_{gi} - x_{gi}$$

$$\longrightarrow \quad L(t)^2 = <l(t)^2> + \frac{<x_{gx}{}'^2 + x_{gy}{}'^2 + x_{gz}{}'^2>}{3} \quad \rightarrow \quad L(t) > <l(t)>$$

N.B. The mean square difference among the centroid of the cloud and the mean cloud is defined as following:

$$<\left(x_{gi} - X_{gi}\right)^2> = <x_{gi}{}^2 - 2x_{gi}X_{gi} + X_{gi}{}^2>$$

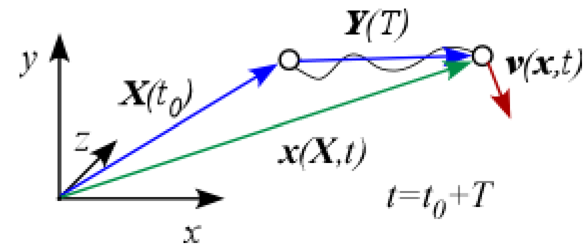
$$<\left(x_{gi} - X_{gi}\right)^2> = <x_{gi}{}^2> - 2<x_{gi}>X_{gi} + X_{gi}{}^2 \quad \longrightarrow \quad <\left(x_{gi} - X_{gi}\right)^2> = <x_{gi}{}^2> - X_{gi}{}^2$$

EVOLUTION OF MEAN CLOUD LENGTH

It is useful to study the problem through Lagrangian approach. In this condition particles are describe by:

- Initial position: $\boldsymbol{X}$
- Lagrangian velocity: $\boldsymbol{v}$
- Particle trajectory: $\boldsymbol{x} = \boldsymbol{X} + \boldsymbol{Y}(\boldsymbol{X}, t)$

Particle motion



By these definition the particle trajectory can be rewritten as:

$$\boldsymbol{x} = \boldsymbol{X} + \int_{t_0}^{t_0+T} \boldsymbol{v}(\boldsymbol{x}, t)\,\mathrm{d}t \longrightarrow \boldsymbol{Y}(T) = \int_{t_0}^{t_0+T} \boldsymbol{v}(\boldsymbol{x}, t)\,\mathrm{d}t$$

By the Lagrangian point of view, the probability that particle in $\boldsymbol{X}$ at t_0 is located in $\boldsymbol{x} + \mathrm{d}\boldsymbol{x}$ at t is defined as:

Conditional probability

$$p(\boldsymbol{Y}|\boldsymbol{X}, t)$$

$\boldsymbol{Y}$ represents the displacement, i.e. $\boldsymbol{x}$

Being the flow turbulent, we can also decompose the velocity and the motion of the particle:

$$\left.\begin{aligned} \boldsymbol{Y}' &= \boldsymbol{Y} - <\boldsymbol{Y}> \\ \boldsymbol{v}' &= \boldsymbol{v} - <\boldsymbol{v}> \end{aligned}\right\}$$

Fluctuation of particle velocity and motion

EVOLUTION OF MEAN CLOUD LENGTH

The single particle has mass m. Being the cloud of *n* particles, the total mass of the cloud is $M = m \cdot n$. Then the <u>mean concentration</u> of the cloud is:

$$C(\boldsymbol{x}, t) = n \cdot m \, p(\boldsymbol{Y}|\boldsymbol{X}, t) = M \, p(\boldsymbol{Y}|\boldsymbol{X}, t)$$

Mean concentration in according to the Lagrangian point of view.

The <u>centroid of the mean cloud</u> is given by:

$$X_{gi} = \frac{1}{M}\int_{-\infty}^{+\infty} x_i \, C(\boldsymbol{x}, t) \, \mathrm{d}x_i$$

$$X_{gi} = \frac{1}{M}\int_{-\infty}^{+\infty} x_i M \, p(\boldsymbol{Y}|\boldsymbol{X}, t) \mathrm{d}x_i = \int_{-\infty}^{+\infty} x_i \, p(\boldsymbol{Y}|\boldsymbol{X}, t) \mathrm{d}x_i$$

$$X_{gi} = \int_{-\infty}^{+\infty} (X_i + Y_i) \, p(\boldsymbol{Y}|\boldsymbol{X}, t) \mathrm{d}Y_i = X_i \int_{-\infty}^{+\infty} \cancelto{1}{p(\boldsymbol{Y}|\boldsymbol{X}, t) \mathrm{d}Y_i} + \int_{-\infty}^{+\infty} Y_i \, p(\boldsymbol{Y}|\boldsymbol{X}, t) \mathrm{d}Y_i$$

$$\longrightarrow \quad X_{gi} = X_i + \langle Y_i \rangle$$

EVOLUTION OF MEAN CLOUD LENGTH

Similarly, the variance of the mean cloud is:

$$\Sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty}\left(x_i - X_{gi}\right)^2 C(\boldsymbol{x},t)\,\mathrm{d}x_i$$

$$\Sigma_i{}^2 = \frac{1}{M}\int_{-\infty}^{+\infty}(Y_i - < Y_i >)^2 M\, p(\boldsymbol{Y}|\boldsymbol{X},t)\mathrm{d}Y_i = \frac{1}{M}\int_{-\infty}^{+\infty} Y_i'^2 M\, p(\boldsymbol{Y}|\boldsymbol{X},t)\mathrm{d}Y_i \qquad \sigma^2 =< Y'_i{}^2 >$$

$$\longrightarrow \quad \Sigma_i{}^2 =< Y'_i{}^2 >$$

The Length of the mean cloud is finally:

$$L(t)^2 = \frac{\Sigma_x{}^2 + \Sigma_y{}^2 + \Sigma_z{}^2}{3} = \frac{< Y'_x{}^2 + Y'_y{}^2 + Y'_z{}^2 >}{3}$$

Injection point

$$L(t)^2 = L(0)^2 + \frac{< Y'_x{}^2 + Y'_y{}^2 + Y'_z{}^2 >}{3}$$

Injection of volume $\forall_0$ and concentration $< c >_0$

It is trivial demonstrating that:

$$x_i = X_i + Y_i$$
$$X_{gi} = X_i + < Y_i >$$
$$\longrightarrow \quad x_i - X_{gi} = X_i + Y_i - X_i - < Y_i > \quad \longrightarrow \quad Y_i - < Y_i > = Y_i'$$

EVOLUTION OF MEAN CLOUD LENGTH

The Length of the mean cloud can be rewritten as:

$$L(t)^2 = L(0)^2 + \frac{D_{xx} + D_{yy} + D_{zz}}{3}$$

Where D_{ij} is the cross-correlation function of the fluctuation of particle displacement, which is defined as:

$$D_{ij} =< Y'_i(t) Y'_j(t) >$$

It is worth noting that D_{ij} depends on time t, being: $\boldsymbol{v}' = \frac{\mathrm{d}\boldsymbol{Y}'}{\mathrm{d}t}$

Hence, D_{ij} is fuction of t and it can be expressed in terms of v'!

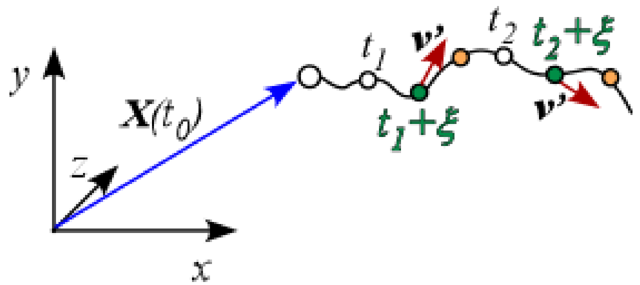
To describe the evolution of the mean cloud with time variying, it is then useful considering the Lagrangian function of temporal cross-correlation, that is defined as:

$$Q_{ij}^L(t_1, t_2) =< v'_i(\boldsymbol{X}, t_0, t_1) v'_j(\boldsymbol{X}, t_0, t_2) >$$

Since the process is ergodic, i.e. the hypotheses of homogeneity and stationarity are valid, we can rearrange Q_{ij}^L considering only the variable $\tau = t_2 - t_1$:

EVOLUTION OF MEAN CLOUD LENGTH

$$Q_{ij}^{L}(\tau) = \lim_{\tau\to\infty} \frac{1}{T}\int_0^T v'_i(\boldsymbol{X}, t_0, t_1 + \xi)v'_j(\boldsymbol{X}, t_0, t_2 + \xi)\,\mathrm{d}\xi$$



N.B. *When the process is ergodic, we need of <u>one realization</u> to obtain the time averaged information*

Moreover, stationarity implies that: $< \boldsymbol{v}(\boldsymbol{X}, t_0, t) > = < \boldsymbol{u}(\boldsymbol{x}, t) >$

Averaged velocity in Lagrangian system

Averaged velocity in Eulerian system

In this condition, we have $D_{ij} \propto Q_{ij}^{L}$, but they depend on time intervals. We need of a <u>Time scale</u> that helps us to describe the cloud diffusion.
To define the time scale we normalize the Lagrangian cross-correlation function:

$$R_{ij}^{L}(\tau) = \frac{Q_{ij}^{L}(\tau)}{\sigma_{ui}(t_1)\sigma_{uj}(t_2)}$$ <u>Lagrangian cross-correlation coefficient</u>

σ_u is Eularian, being $\boldsymbol{u}(\boldsymbol{x}, t)$

LAGRANGIAN TEMPORAL MACROSCALE

Finally, the time scale of the mean cloud diffusion is defined by:

$$T_L = \max\left(\int_0^{\infty} R_{ii}^L(\boldsymbol{x},\tau)\,\mathrm{d}\tau\right)$$

Lagrangian Temporal Macroscale

we use this parameter to distinguish three type of diffusion (as described at the beginning of the lecture):

i. $t \ll T_L$

ii. $t \cong T_L$

iii. $t \gg T_L$

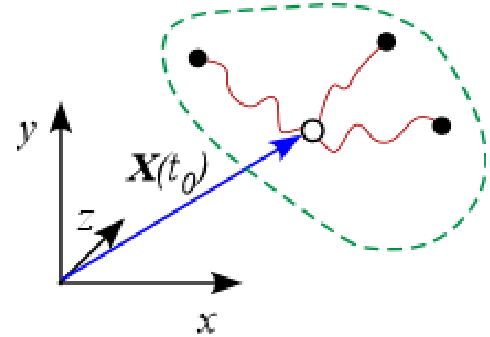
The behavior of the cloud changes in each intervals!

DIFFUSION COEFFICIENT FOR t<<T$_L$

In the short time interval after the insertion, the solute stays aroud the insertion point $(\boldsymbol{X}, t_0)$. In this condition we can assume:

i. Eulerian velocity is the same within the interval, i.e. $\boldsymbol{u}(\boldsymbol{X}, t) \cong \boldsymbol{u}(\boldsymbol{X}, t_0)$

ii. Lagrangian and Eulerian velocities are similar, i.e. $\boldsymbol{u} = \boldsymbol{v}$



Under these assumptions: $\boldsymbol{v} = \frac{\mathrm{d}\boldsymbol{Y}}{\mathrm{d}t} \overset{\int}{\Longrightarrow} \boldsymbol{Y} = \boldsymbol{v}\, t \cong \boldsymbol{u}\, t$

Considerig t_0 the initial time of the process and $t = t_0 + \tau$ a generic time of the process, we find:

$$\boldsymbol{Y} = \int_{t_0}^{t} \boldsymbol{v}(\boldsymbol{x}, \tau)\, \mathrm{d}\tau \cong \boldsymbol{u}\, \tau$$

It follows that: $\boldsymbol{Y}' = \boldsymbol{Y} - <\boldsymbol{Y}> = (\boldsymbol{u} - <\boldsymbol{u}>)\tau = \boldsymbol{u}'\, \tau$

By replacing the latter into the cross-correlation function, it reads:

$$D_{ii} =< {Y'}_i^2(\tau) >=< {u'}_i^2 > \tau^2$$

DIFFUSION COEFFICIENT FOR t<<T$_L$

When $t \ll T_L$ the mean cloud length scale is then:

$$L(t)^2 = L(0)^2 + \frac{< {u'_x}^2 > + < {u'_y}^2 > + < {u'_z}^2 >}{3} \tau^2$$

The cloud spreads quickly in the interval of time after the insertion!

We do not demonstrate it, but the turbulent diffusion is expressed as:

$$\longrightarrow \quad e_{ij} = \frac{1}{2}\frac{\mathrm{d}D_{ij}}{\mathrm{d}t}$$

In this case:

$$\longrightarrow \quad e_{ij} = < u'_i u'_j > \tau = Q_{ij}\,\tau$$

Eulerian cross-correlation function

N.B. Turbulent diffusion coefficient e_{ij} increases linearly with time increasing, and it is proportional to the turbulent fluctuations of velocity.

DIFFUSION COEFFICIENT FOR $t \gg T_L$

It is the most useful case in the practice. I observe the cloud always downstream of the insertion point.

To find the diffusion coefficient, we start from the definition of the cross-correlation function:

$$D_{ij} = \langle Y'_i(t_1) Y'_j(t_2) \rangle$$

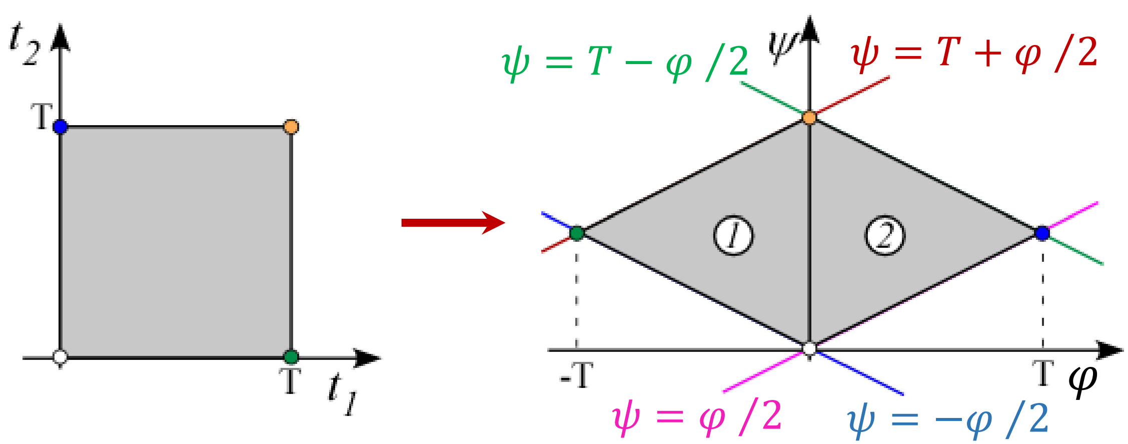
$$D_{ij} = \int_0^T \int_0^T \langle v'_i(t_1) v'_j(t_2) \rangle \, \mathrm{d}t_1 \, \mathrm{d}t_2 = \int_0^T \int_0^T Q_{ij}^L(t_2 - t_1) \mathrm{d}t_1 \, \mathrm{d}t_2$$

To solve the integral it is necessary to change the integration variables, as following:

$$\begin{cases} t_1 \\ t_2 \end{cases} \rightarrow \begin{cases} \psi = \dfrac{t_1 + t_2}{2} \\ \varphi = t_2 - t_1 \end{cases}$$

It means: $\mathrm{d}t_1 \mathrm{d}t_2 = J \mathrm{d}\varphi \mathrm{d}\psi$

$$J = \begin{vmatrix} \dfrac{\partial \psi}{\partial t_1} & \dfrac{\partial \varphi}{\partial t_1} \\ \dfrac{\partial \psi}{\partial t_2} & \dfrac{\partial \varphi}{\partial t_2} \end{vmatrix} = \begin{vmatrix} \dfrac{1}{2} & -1 \\ \dfrac{1}{2} & 1 \end{vmatrix} = 1$$



In the new system the limits of integration becomes:

$$\begin{cases} t_1 : [0, T] \\ t_2 : [0, T] \end{cases} \rightarrow \begin{cases} \varphi : [-T, T] \\ \psi : [0, T] \end{cases}$$

The integrals into two triangles composing the rhombus are then:

1 $$\int_{-T}^{0} \int_{-\varphi/2}^{T+\varphi/2} Q_{ij}^{L}(\varphi) \mathrm{d}\varphi \, \mathrm{d}\psi$$

2 $$\int_{0}^{T} \int_{\varphi/2}^{T-\varphi/2} Q_{ij}^{L}(\varphi) \mathrm{d}\varphi \, \mathrm{d}\psi$$

$$\longrightarrow \quad D_{ij} = \int_{-T}^{0} \int_{-\varphi/2}^{T+\varphi/2} Q_{ij}^{L}(\varphi) \mathrm{d}\varphi \, \mathrm{d}\psi + \int_{0}^{T} \int_{\varphi/2}^{T-\varphi/2} Q_{ij}^{L}(\varphi) \mathrm{d}\varphi \, \mathrm{d}\psi$$

DIFFUSION COEFFICIENT FOR t>>T$_L$

Since $Q_{ij}^L(\varphi) = Q_{ij}^L(-\varphi)$, the D_{ij} can be simplified as:

$$D_{ij} = 2\int_0^T \int_{\varphi/2}^{T-\varphi/2} Q_{ij}^L(\varphi)\mathrm{d}\varphi\,\mathrm{d}\psi = 2\int_0^T (T-\varphi)Q_{ij}^L(\varphi)\mathrm{d}\varphi$$

To evaluate $L(t)$, we have to study the case $i = j$ (and replace T with t):

$$D_{ii} = 2\int_0^T (T-\varphi)Q_{ii}^L(\varphi)\mathrm{d}\varphi = 2t\int_0^t Q_{ii}^L(\varphi)\mathrm{d}\varphi - 2\int_0^t \varphi\, Q_{ii}^L(\varphi)\mathrm{d}\varphi$$

It is worth noting that:

$$t \gg T_L \Longrightarrow Q_{ii}^L \to 0 \Longrightarrow \int_0^t R_{ii}^L(\varphi)\mathrm{d}\varphi \cong T_L$$

$$R_{ii}^L = \frac{Q_{ii}^L}{{\sigma_{ui}}^2}$$

and:

$$\int_0^t \varphi\, Q_{ii}^L(\varphi)\mathrm{d}\varphi = {\sigma_{ui}}^2 \int_0^t \varphi\, R_{ii}^L(\varphi)\mathrm{d}\varphi \cong {\sigma_{ui}}^2 R_i$$

It is a finite value

DIFFUSION COEFFICIENT FOR t>>T$_L$

the approximations into D_{ii} yield:

$$\longrightarrow \quad D_{ii} = 2{\sigma_{ui}}^2(tT_{Li} - R_i) \cong 2{\sigma_{ui}}^2 T_{Li} t$$

When t is large enough!

It means that:

$$L(t)^2 = L(0)^2 + \left[\sum_{i=1}^{3} \frac{2}{3}({\sigma_{ui}}^2 T_{Li})\right] t$$

The cloud area increases linearly with time increasing

The cloud size exceeds the size of macrovortex length scale, i.e. the solute particles lost memory of their initial condition.

Finally, the turbulent diffusion coefficient is:

$$\longrightarrow \quad e_{ii} = \frac{1}{2}\frac{\mathrm{d}D_{ii}}{\mathrm{d}t} \cong {\sigma_{ui}}^2 T_{Li} \quad \longrightarrow \quad e_{ii} \cong < {u'_i}^2 > T_{Li}$$

It is constant! I can use the analogy with molecular diffusivity!

In the turbulent diffusion we can distinguish three phases:

i. $t \ll T_L$. The cloud spreads quickly being its length scale as much as the microvortexes scale. The Diffusion coefficient increases lineraly with time increasing.

$$\longrightarrow \quad e_i = < {u'_i}^2 > t$$

ii. $t \cong T_L$. Solute particles have lost memory of initial condition, but the cloud is still smaller than the macrovortexes. In this case:

$$\longrightarrow \quad e_i = f\left(< {u'_i}^2 > T_{Li}\right) \propto {L_{Li}}^{4/3}$$

<u>Lagrangian Macroscale Length</u> of the cloud

$$L_{Li} = \sqrt{< {u'_i}^2 > T_{Li}}$$

iii. $t \gg T_L$. Solute particles have lost memory of initial condition and the cloud is larger than the macrovortexes. The coefficient of diffusion does not depend on t anymore.

$$\longrightarrow \quad e_i = < {u'_i}^2 > T_{Li} = \sqrt{< {u'_i}^2 >}\, L_{Li}$$