Dispersion in random velocity fields

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We have seen that, even at large Peclet numbers, diffusive processes cannot be ignored because of the existence of boundary layers that ultimately control temperature or concentration gradients and, hence, the heat or mass fluxes. Here we consider two situations where the flow field cannot be described exactly but rather in a statistical manner: flows within a porous medium and turbulent flows.

Flows in porous media are almost always low Reynolds number flows, without temporal fluctuations, but the geometry of the medium can only be described by averaged values, essentially the permeability and the porosity. As a result transport properties can only be calculated in a statistical manner.

On the other hand, turbulence creates an intricate structure of fluctuating vortices with a range of length scales and time scales which is wider and wider as the Reynolds number increases.

1 Transport in porous media

In many situations of industrial interest or in Nature, transport of mass or heat occurs within a confined flow in or a porous medium. In the limit of very large Peclet numbers, there is a dispersion, with a paradoxical effective diffusivity, which is due to the velocity gradients within the flow.

Two examples of transport in a porous medium are the distribution of concentration in a chromatography column or in an underground aquifer. The basic question is the following: if a solute is injected very locally in the flow, how does it spread in the direction of the mean flow and in the transverse direction ? This phenomenon can be observed in detail, either experimentally using micromodels or numerically. Fig. 1 shows the result of a simulation done in a very simple geometry with a few circular obstacles within a channel, at Peclet numbers varying from 10 to 10^4. At the largest value of Pe, the simulation shows clearly the dispersion due to the heterogeneity of the velocity field within the assembly of disks.

Conversely at $Pe = 10$, the assembly of disks has a small influence on the longitudinal dispersion which is essentially due to molecular diffusion. There is no solute remaining for

a long time on the wall of the cylinders. Molecular diffusion is efficient enough to transport the solute across the streamlines and release it from the stagnation regions.

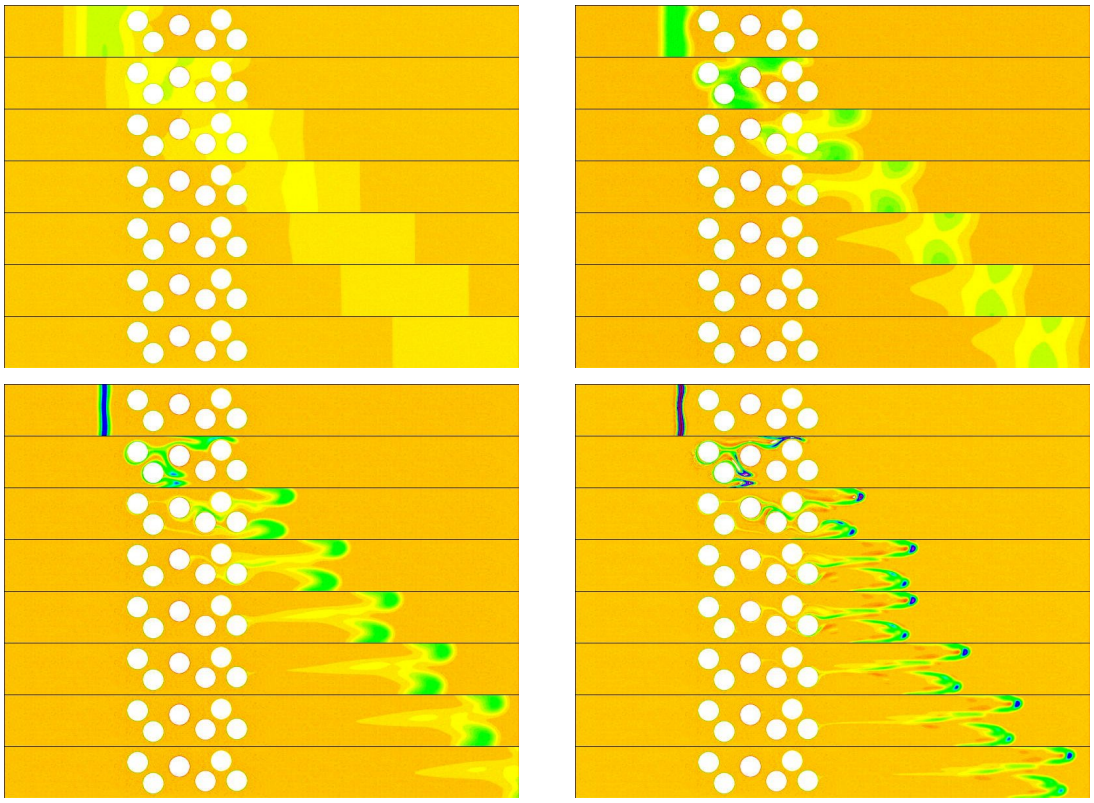

Figure 1: Evolution in time of the concentration of a solute through a series of disks at different Peclet numbers. The fluid flows from left to right at a very small Reynolds number. Upper left, : $Pe = 10$, upper right :$Pe = 10^2$, lower left : $Pe = 10^3$, lower right : $Pe = 10^4$.

These observations at the scale of a pore provide an insight on the local mechanisms but do not give a quantitative information at a scale much larger than the pore size. The *hydrodynamic dispersion* in an homogeneous porous medium (for example a stack of spherical beads of uniform size a) can be measured exprimentally:

- by varying suddenly the concentration of solute at the inlet and monitoring the outlet concentration as a function of time, for example by adding salt to an aqueous solution and by measuring conductivity at the outlet. If the concentration follows a diffusion law with an effective diffusion coefficient $D_{\|}$, the concentration step at the inlet leads to an error function profile at the outlet with a transition width w which scales as

$\sqrt{D_\parallel t}$ where t is the elution time :

$$\frac{C(L,t)}{C_0} = 1 - \mathrm{erf}\left(\frac{L-Ut}{2\sqrt{D_\parallel t}}\right) \tag{1}$$

where L is the thickness of the porous meium, U the average velocity given by Darcy's law and C_0 the step in concentration imposed at the inlet.

- by injecting during a short amount of time a small quantity of solute (as in chromatography). In this case, if hydrodynamic dispersion is a diffusive process, we expect at the outlet a peak of concentration witha gaussian profile of width scaling as $\sqrt{D_\parallel t}$.

The mean flow introduces an anisotropy in the dispersion process and the dispersion in the crossstream direction is *a priori* different from the dispersion along the direction parallel to the flow. The transverse dispersion can be measured by injecting into the porous medium two parallel fluxes of solute at different concentrations.

Systematic data on the dispersion within porous media were obtained by Fried & Combarnous (fig. 2). They show that effective diffusion coefficients in the longitudinal and transverse directions increase linearly with Peclet number as soon as $Pe > 1$. The longitudinal diffusion coefficient is significantly larger than the transverse coefficient. At small Peclet number, the effective diffusion coefficient is equal to the molecular diffusivity.

The asymptotic behavior at large Peclet number can be understood by considering the motion of solute through the porous medium as a random walk. At each pore, the solute can take several equivalent paths. The length of each step is comparable to d, the pore size. The time required to complete each step is on the order of $\tau = d/U$. After a large number N of steps, the dispersion is on the order of $\delta = d\sqrt{N}$. The number of steps is $N = t/\tau = Ut/d$, t being the time necessary to complete the N steps. We get :

$$\delta = d\sqrt{Ut/d} = \sqrt{U\ d\ t}. \tag{2}$$

In this random walk model, the diffusion coefficient is Ud and its ratio to the molecular diffusivity is precisely the Peclet number.

To get analytical results beyond this very simple model, it is necessary to idealize porous media as assembly of tubes (when the porosity is small) or as assembly of particles (when the porosity is large). Saffman performed the calculation in the first case [1]. His analysis leads to an effective dispersion coefficient scaling as $Pe \ln Pe$. The $\ln Pe$ term comes from the zero velocity condition on the solid walls. It is necessary to take into account the long residence time of the solute in the low velocity regions.

[1] P.G. Saffman, A theory of dispersion in porous media, J. Fluid Mech. 6, 321, 1959

Koch & Brady [2] did the analysis in the second model, considering the porous medium as an assembly of spheres occupying a fraction ϕ of the volume (the porosity is 1-ϕ). At large Peclet number, they find $D_{\|}/D = 1 + 3/4Pe + \alpha\phi Pe \ln Pe$ where α is a numerical coefficient. The $\ln Pe$ term appears for the same reason as in the tube model, because of the low velocity regions near the solid surfaces. Except when Pe is extremely large, it is very difficult to see the influence of the logarithmic term on experimental data. Even if the analysis of Koch & Brady is done for low values of ϕ, it describes well the data on porous media where $\phi \approx 0,6$ (fig. 2).

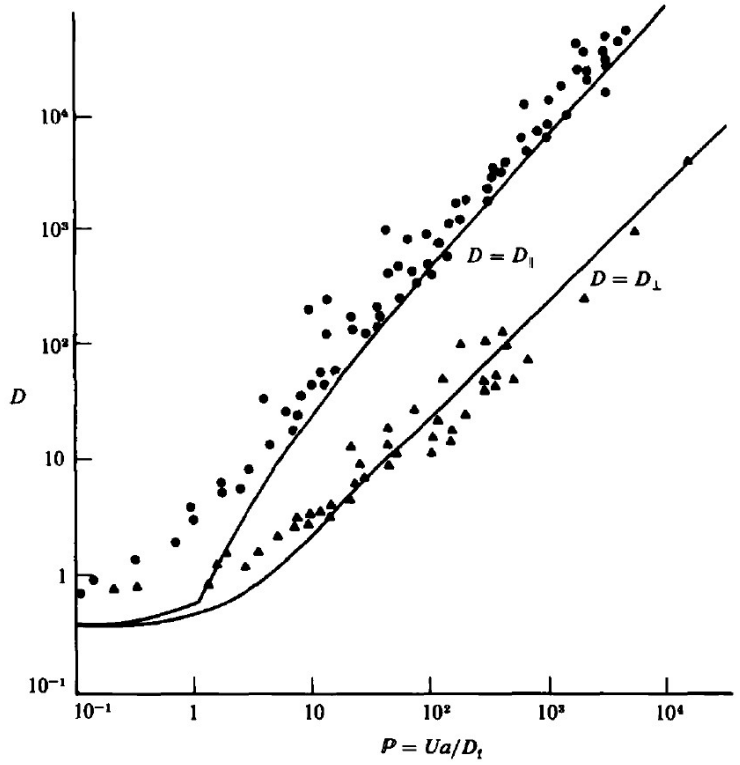

Figure 2: Effective diffusion coefficients D_{eff} (in directions parallel and perpendicular to the flow) in a porous medium as a function of the Peclet number. D_{eff} is normalized by the molecular diffusion coeffiicent D. Symbols : experimental data from Fried & Combarnous. Lines : theory from Koch & Brady (1985). Figure from Koch & Brady, J. Fluid Mech. 154, 399.

[2]Dispersion in fixed beds, J. Fluid Mech. 154, 399 (1985)

2 Turbulent dispersion

Mixing a small amount of syrup into a glass of water with a spoon demonstrates readily that turbulence is very efficient to disperse mass. Beyond this kitchen observation, turbulent dispersion can be quantified in laboratory experiments such as the one shown on fig.3. This efficiency of mixing stems from the creation of a wide distribution in space and time of velocity fluctuations. In order to understand dispersion, it is necessary to do a statistical analysis of the velocity fluctuations.

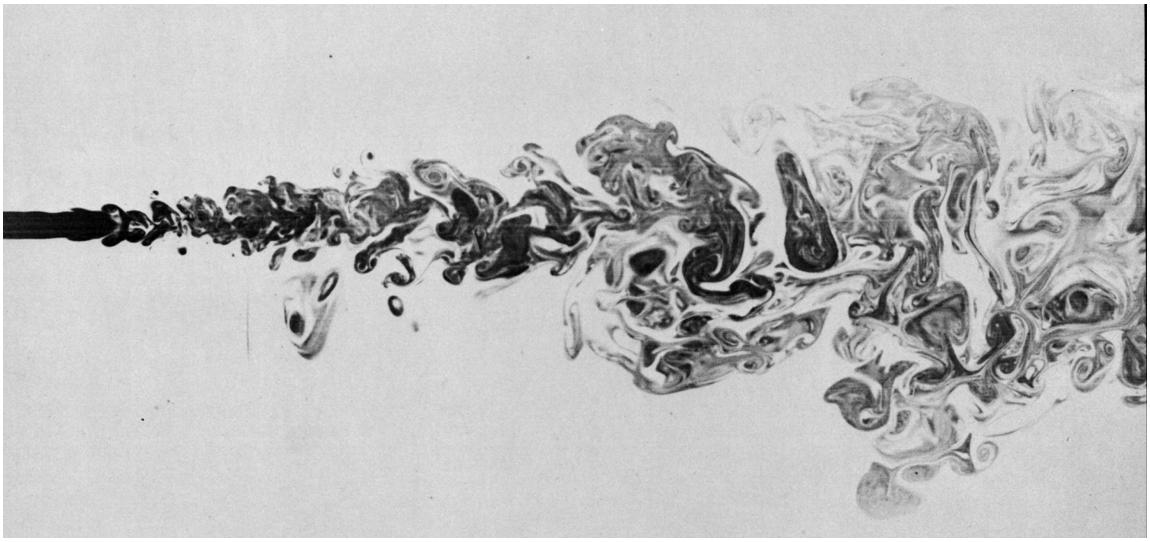

Figure 3: Turbulent jet ($Re = 2000$) visualized by laser-induced fluorescence. Image by P. Dimotakis (Caltech) reproduced from M. Van Dyke, "An Album of Fluid Motion"

2.1 Turbulence: an elementary statistical description

2.1.1 Reynolds decomposition

In a turbulent flow, the transport equation for mass or heat is the same as in a laminar flow. But, since the velocity field has a random character, it is necessary to write evolution equations for quantities that are averaged in time. To write these equations, we use *Reynolds' decomposition* which consists in separating the velocity field $\mathbf{u}$ and the temperature field T into a mean value, averaged over time, and a fluctuating part with zero mean value $\mathbf{u} = \mathbf{U} + \mathbf{v}$, with $\mathbf{U} = \bar{\mathbf{u}}$ and $\bar{\mathbf{v}} = 0$ and $T = \Theta + \theta$ with $\Theta = \bar{T}$ and $\bar{\theta} = 0$. Using this decomposition in the Navier-Stokes and in the transport equation, averaging over time we get the following equations for the velocity component i and the temperature:

$$\rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \eta \Delta U_i - \rho \frac{\partial \overline{v_i\ v_j}}{\partial x_j} \tag{3}$$

$$\rho C_p U_j \frac{\partial \Theta}{\partial x_j} = \lambda \Delta \Theta - \rho C_p \frac{\partial \overline{\theta\ v_j}}{\partial x_j} \tag{4}$$

In these two equations there is an additional term compared to the Navier-Stokes and transport equations. This term involves the *fluctuation correlations*, on one hand between the velocity field components, on the other hand between the temperature and the velocity.

In the momentum equation, the additional term is the divergence of the turbulent *Reynolds stresses* $\tau_{ij} = -\rho\overline{v_i\ v_j}$. For example, in a turbulent boundary layer this term is dominated by the correlation of the velocity fluctuations along and normal to the wall. It is possible to determine the Reynolds stresses experimentally from time resolved velocity fields, but it is in general very difficult to predict them from the structure of the time averaged velocity field. Any attempt to determine the evolution of Reynolds stresses leads to equations involving correlations of higher order. Several types of hypotheses have been used for this *closure* problem. The simplest one is the definition of an empirical turbulent viscosity ν_T relating the fluctuation correlations with the mean velocity gradient:

$$-\overline{v_i\ v_j} = \nu_T \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \bar{k} \delta_{ij} \tag{5}$$

where $\bar{k}$ is the mean turbulent kinetic energy $1/2\overline{v_i v_i}$.

2.1.2 Correlations velocity-temperature

For the temperature field, there is an additional heat flux $-\rho C_p \overline{\theta\ v_i}$, proportional to the correlation between the temperature and the velocity fluctuations.

Consider a particular, but very common situation, of a boundary layer, that is to say a shear flow in which the mean velocity has a single component U_x which varies essentially with the cross-stream coordinate y and varies much more slowly along x, the streamwise coordinate. The mean temperature field Θ varies also quickly with y and much more slowly with x. The heat flux, related to fluctuations, in the cross-stream direction is : $J_y = -\rho C_p \overline{\theta\ v_y}$. Similarly to the turbulent viscosity, it is possible to define a *turbulent heat diffusivity* κ_T relating the heat flux to the mean temperature gradient:

$$J_y = -\rho C_p \kappa_T \frac{\partial \Theta}{\partial y} \tag{6}$$

It is simply a definition since κ_T incorporates the effect of turbulent fluctuations.

The experiment shows that κ_T have ν_T the same order of magnitude, that is to say that momentum and heat are transported similarly by turbulent fluctuations.In this situation,

called Reynolds analogy, where the turbulent Prandtl number $P_T = \nu_T/\kappa_T$ is of order 1, the transverse heat flux is given by:

$$J_y = -C_p \tau_{xy} \frac{\partial \Theta/\partial y}{\partial U_x/\partial y}. \tag{7}$$

where $\tau_{xy} = \rho \overline{u_x u_y}$.

The influence of turbulence is clearly visible when measuring, for example, the transverse heat flux for the flow in a tube (fig. 4). The transition from laminar to turbulent flow corresponds to a sudden increase of the Nusselt number (dimensionless heat flux). When the turbulent flow is fully established, the Nusselt grows faster ($\propto Re^{0,8}$) than in laminar flow ($\propto Re^{1/3}$, the 1/3 exponent being related to the parabolic velocity profile).

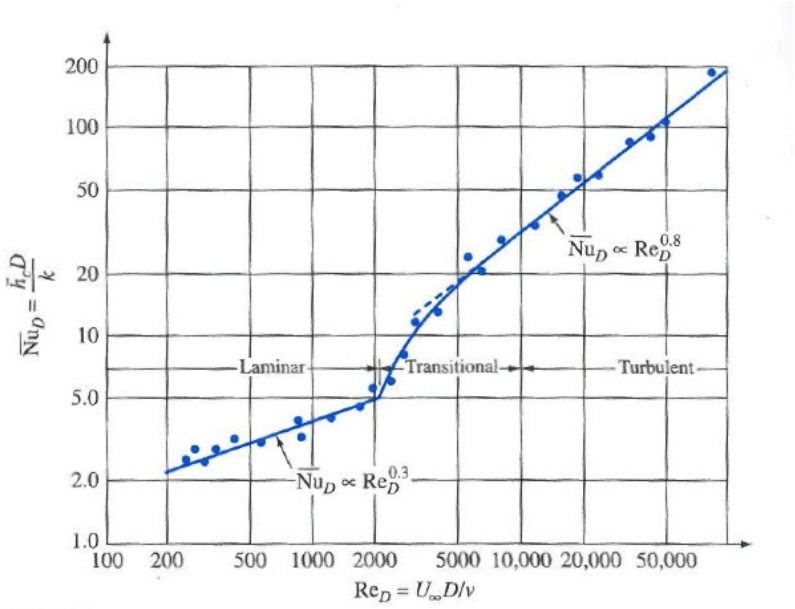

Figure 4: Nusselt number (heat flux normalized by diffusion flux) as a function of Reynolds number. Figure from Kreith et al., Principles of heat transfer.

2.2 Dispersion in fully developed turbulence

2.2.1 Spectral distribution of velocity fluctuations and Kolmogorov's scaling law

The russian mathematician Kolomogorov has suggested that, in a flow at very large Reynolds number, there is a domain of lengthscales with universal characteristics. For

these lengthscales, the properties of the fluctuations do not depend on the mean flow at large scale which the source of the turbulence and they do not depend either on the particular lengthscale considered, they are invariant upon a scale change. In this theoretical framework, Kolmogorov considers only the flows in which the fluctuations are isotropic (there is no preferred direction) and homogeneous (they do not depend on the particular location in the flow). These are conditions which are very difficult to achieve in a real flow, except in special cases such as the turbulence generated behind a grid in a wind tunnel. Otherwise, the fluctuations remain in general anisotropic because they retain some characteristics of the large scale flow, for example in a turbulent boundary layer. Nevertheless, some observations in very large number flows, either in wind tunnels or in geophysical flows are compatible with Kolmogorov's description.

In this framework, turbulent kinetic energy is injected at the largest spatial scales in the flow and is transferred towards smaller and smaller scales until viscous dissipation stops this *energy cascade*. The strong hypothesis made by Kolmogorov is that the rate of kinetic energy transfer ϵ is independent of the spatial scale considered, in the *inertial domain* i.e. for length scales large enough for viscous dissipation to be negligible.

In this scaling law analysis, a velocity scale characteristic of the fluctuations $u(\ell)$ is defined for each length scale ℓ. The fluctuation kinetic energy per unit mass of fluid is proportional to $u(\ell)^2$. A fixed proportion of this kinetic is transferred towards smaller scales during a characteristic time $\tau(\ell)$. This time should be proportional to $\ell/u(\ell)$. Hence the rate of energy transfer per unit mass is such that: $\epsilon \propto u(\ell)^2/\tau(\ell) \propto u(\ell)^3/\ell$. Assuming that ϵ is constant and independent of the lengthscale ℓ leads to Kolomogorov's scaling law for the velocity fluctuations:

$$u(\ell) \propto \epsilon^{1/3}\ell^{1/3}. \tag{8}$$

This equation shows that the intensity of fluctuations increases with the length scale considered, as a power law with an exponent 1/3.

The kinetic energy per unit mass is $u^2(\ell)$. If we consider the distribution of this kinetic energy in Fourier space, i.e. considering wavevectors k instead of lengthscales ℓ, we get the spectral density of energy, the amount of energy between wavevectors k and $k + dk$:

$$E(k) = E_0\epsilon^{2/3}k^{-5/3}. \tag{9}$$

This is Kolmogorov's -5/3 scaling law which is effectively observed in flows at very high Reynolds numbers, either in natural flows, in large wind tunnels or in direct numerical simulations of the Navier-Stokes equation (fig. 5).

The inertial range is limited at small length scales (large wavevectors) by viscous dissipation. The scale at which dissipation becomes dominant is such that the Reynolds number $Re(l) = lu(l)/\nu = \epsilon^{1/3}l^{4/3}/\nu$ is of order 1. This defines *Kolmogorov's microscale* l_D such that : $\epsilon^{1/3}l_D^{4/3} \approx \nu$. Hence:

$$l_D \approx \nu^{3/4}\epsilon^{-1/4}. \tag{10}$$

The Reynolds number of the global flow is computed with the largest scale L where the kinetic energy is injected: $Re_L = \epsilon^{1/3} L^{4/3}/\nu$. Kolmogorov's microscale is related to the integral scale L by: $l_D = L Re_L^{-3/4}$. The range of spatial scales between L and l_D thus increases with Reynolds number. This wide range of scales poses a fundamental problem for the numerical simulation of turbulent flows since, if one wants to resolve all scales, the number of simulation cells should scale as $Re^{9/4}$ in three dimensions. For example, if we consider the flow of air around a car body, $L \approx 1$m, $U \approx 20$m/s and $Re_L \approx 1,5 \times 10^6$ so that $l_D \approx L/30000$; the number of cells for a 3D direct numerical simulation would be 9×10^{12} !

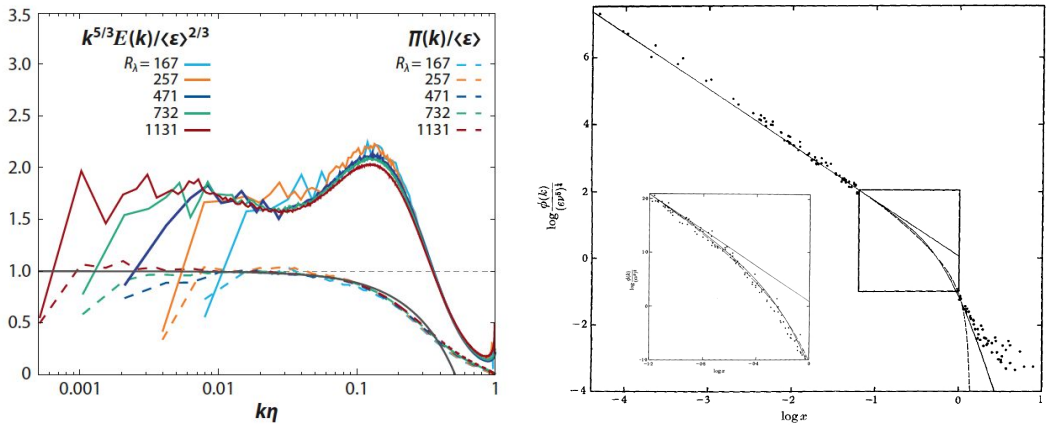

Figure 5: Experimental and numerical checks of Kolmogorov's scaling laws. On the left, results of direct numerical simulations at different Reynolds numbers R_λ: spectrum of turbulent kinetic energy $E(k)$ normalized by $k^{-5/3}$ and rate of energy transfer $\Pi(k)$ as a function of $k\eta$, the wavevector normalized by Kolmogorov's microscale η. (figure reproduced from Ishihara et al., Annual Rev. Fluid Mech. 41,165 (2009)). On the right, experimental results on the fluctuations within a tidal stream (Discovery strait in British Columbia) at $Re \approx 3 \times 10^8$ (figure reproduced from Grant et al., J. Fluid Mech. 12, 241 (1962)).

As a side remark, turbulent flows are better characterized by a Reynolds number R_λ different from the classical Reynolds number defined on the average velocity and lengthscale L. R_λ is defined on the root mean square of the velocity fluctuations and on a length scale λ related to energy dissipation : $R_\lambda = \langle u^2 \rangle^{1/2} \lambda/\nu$. In a flow, the power dissipated per unit mass is $\epsilon = nu(\nabla \mathbf{u})^2$; λ, characteristic of the velocity gradient is defined by: $\epsilon = 15\nu\langle u^2 \rangle/\lambda^2$. R_λ gives a good representation of the fluctuations within the flow. Its value is typically smaller than Re_L by one of two orders of magnitude.

2.2.2 Dispersion in developed turbulence. Richardson's 4/3 law.

The understanding of turbulent diffusion made a major stride with a pioneering work of Lewis Richardson in the 1920s. In a paper titled "Atmospheric diffusion shown on a distance-neighbour graph", Richardson introduces the notion of the probability $q(s, s_0)$ for two tracers transported by the flow to be at distance s, knowing that these two tracers started at an initial distance s_0. When the process of dispersion is solely due to diffusive transport obeying Fick's law, the temporal evolution of $q(s)$ is given by a diffusion equation:

$$\frac{\partial q}{\partial t} = 2K \frac{\partial^2 q}{\partial s^2}$$

where K is the diffusion coefficient for a single tracer.

More generally, it is possible to write the evolution equation for $q(s)$ as follows:

$$\frac{\partial q}{\partial t} = \frac{\partial}{\partial s}\left(F(s)\frac{\partial q}{\partial s}\right) \tag{11}$$

where $F(s)$ is a diffusion coefficient depending on the separation s of the tracers, but not of their absolute position in space, assuming the flow to be statistically homogeneous in space. By looking at different experimental results, including his own investigations, Richardson constructed the diagram on fig. 6 showing that $F(s)$ increases with separation s as a power law with an exponent 4/3. This exponent was determined purely in an empirical manner, since there was, at that time, no statistical theory of turbulence able to predict such a result.

Richardson performed other experiments later, in particular with Stommel [3] in which they threw slices of parsnip into the waters of Loch Long in Scotland and tracked the paths of these white floating tracers. Their data are shown in fig. 6 as the mean square distance r^2 between two tracers (after a fixed dispersion time) as a function of the initial separation r_0. Fitting these data with a power law yields $r^2 \propto r_0^{1,5}$ with an exponent close to 4/3.

The experimental data show that dispersion in a turbulent flow can be seen as an *hyperdiffusive* phenomenon with an effective diffusion coefficient varying with the 4/3 power of the spatial scale. This experimental finding is in agreement with Kolomogorov's theory on developed turbulence.

Indeed the dispersion of tracers separated by a distance s is essentially governed by fluctuations at the s s.

Vortices at larger scales transport the two particles together and do not affect their separation. Smaller vortices change the separation by a quantity much smaller than s. If we assume that vortices are not correlated in time, transport at scale s can be viewed as a random walk with steps of length s and a number of steps by unit length of order $u(s)$. The effective diffusion coefficient is then: $F(s) \propto u(s)s = \epsilon^{1/3}s^{4/3}$ with an exponent agreeing with Richardson's observations. This is true only if we consider length scales in

[3] L. Richardson & H. Stommel, J. Meteorol. 5, 238 (1948)

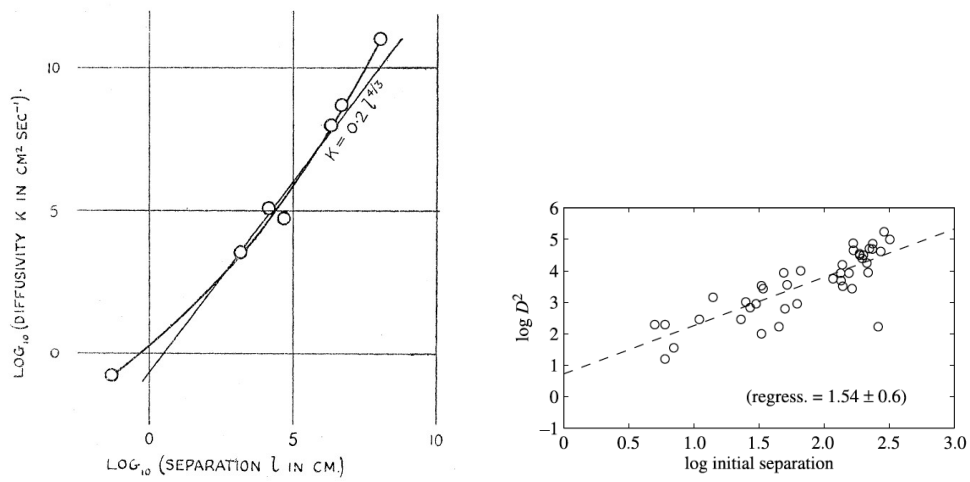

Figure 6: Data on turbulent dispersion from L.F. Richardson. Left, effective diffusion coefficient as a function of the initial separation of tracers. From L.F. Richardson, Proc. Roy. Soc. A 110, 709 (1926). Right, reinterpretation of Richardson and Stommel's experiment. Mean square spacing of tracers dispersed in an estuary as a function of their initial separation. From D.M. Summers, Proc. Roy. Soc. A 461, 1811 (2005)

the so-called *inertial domain* of turbulence, i.e. between Kolmogorov's microscale and the integral scale of the flow L.

The equation for the probability density q is then:

$$\frac{\partial q}{\partial t} = k_0 \epsilon^{1/3} \frac{\partial}{\partial s}\left(s^{4/3} \frac{\partial q}{\partial s} \right) \tag{12}$$

A dimensional analysis of this equation yields: $1/t \propto k_0 \epsilon^{1/3} s^{-2/3}$, that is: $s \propto k_0^{3/2} \epsilon^{1/2} t^{3/2}$. This suggests to introduce a rescaled variable $x = s k_0^{-3/2} \epsilon^{-1/2} t^{-3/2}$ and that the mean square separation $\langle r^2 \rangle = \int_0^\infty s^2 q(s) ds$ scales as t^3.

With the rescaled variable x the self-similar solutions of the equation are:

$$q(s,t) = A \langle r(t)^2 \rangle^{-3/2} \exp\left[- \left(B \frac{s^2}{\langle r(t)^2 \rangle} \right)^{1/3} \right] \tag{13}$$

with a time dependence of the mean square separation:

$$\langle r(t)^2 \rangle \propto \epsilon t^3. \tag{14}$$

This shows indeed the hyperdiffusive nature of turbulent dispersion. In a standard diffusive process, the mean square displacement grows linearly with time. Here it varies much more quickly with the cube of time, because the effective diffusivity increases with the separation.

The law $\langle r(t)^2 \rangle \propto t^3$ relies on strong hypotheses, among which the absence of time correlation of fluctuations which is not true experimentally at short time scales. Nevertheless, hyperdiffusive behaviors are observed in the oceans (fig. 7) and in direct numerical simulations (fig. 8) ; in this last case, the scaling law is observed only for a very limited range of scales.

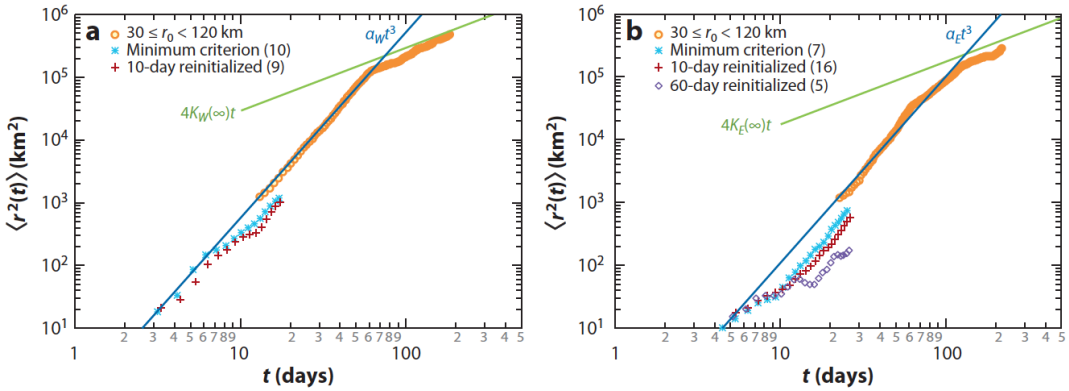

Figure 7: Results of the TOPOGULF experiment. Mean square spacing of floaters drifting in the northern Atlantic, as a function of time. Left (a) in the western part of the ocean, right (b) in the eastern part. The blue lines shows the hyperdiffusive behavior $r^2(t) \propto t^3$. Figure from Salazar and Collins, Ann. Rev. Fluid Mech. 41, 405 (2009)

3 Summary

- At large Peclet numbers, in a random velocity field, dispersion can be considered as a random walk
- In a flow within porous media, with a pore size d and an average velocity U the effective diffusivity scales as $U\ d$. Longitudinal dispersion is significantly larger than transverse dispersion.
- In a flow at very large Reynolds numbers, velocity fluctuations obey Kolmogorov's scaling law, i.e. velocity at scale s varies as $s^{1/3}$. Dispersion in a turbulent flow can be considered as a random walk due to fluctuating eddies resulting in an effective dispersion coefficient scaling as $s^{4/3}$ (Richardson's law).

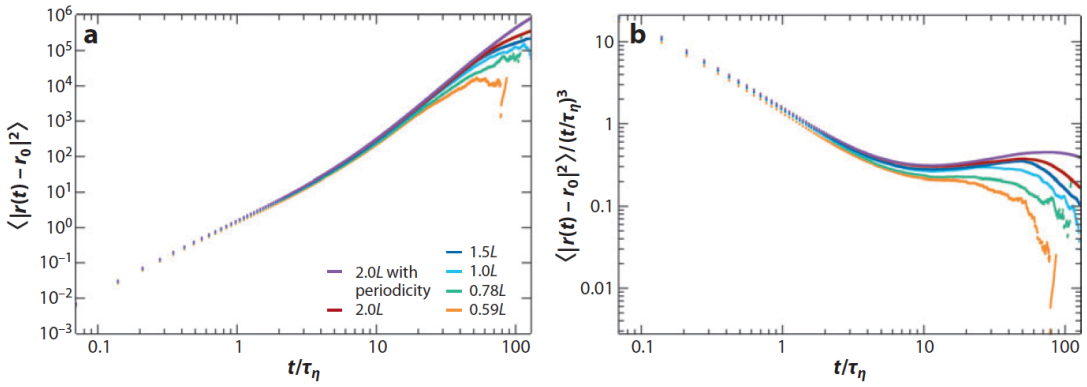

Figure 8: Mean square spacing of tracers as a function of time in a direct numerical simulation of turbulent flow (spatial resolution 1024^3 at R_λ=284). Time is normalized by the characteristic time of Kolmogorov's microscale τ_D. On the right, data normalized by $(t/\tau_D)^3$ pour mettre en vidence la loi de Richardson. The different curves correspond to statistics obtained on trajectories of different lengths from 0.59 L to 1.5 L where L is the size of the simulation domain. The scaling $(r(t) - r_0)^2 \propto t^{1/3}$ is more apparent for long trajectories. Figure from Salazar and Collins, Ann. Rev. Fluid Mech. 41, 405 (2009)