SMS-618, Particle Dynamics, Fall 2009
Conservation equations in fluids

Concepts we need:

Tensor (Stress), Vectors (e.g. position, velocity) and scalars (e.g. T, S, CO_2). Provide means to describe conservation laws with compact notation
We need to define a coordinate system (x,y,z), with unit normal vector $(\hat{i}, \hat{j}, \hat{k})$, and an (infinitesimal) element of volume δV=δxδyδz.

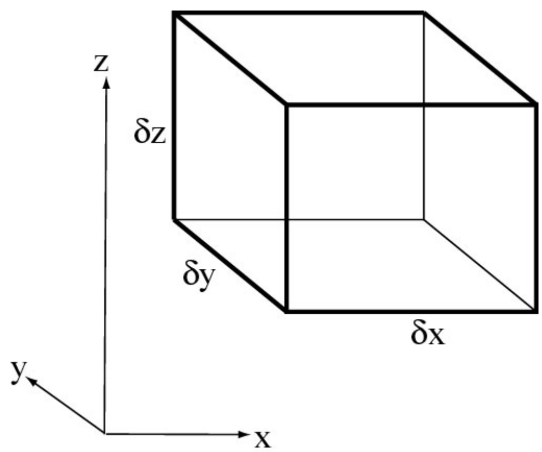

Figure 1: coordinate system and infinitesimal volume.

The Lagrangian framework is the framework in which the laws of classical mechanics are often stated. Assume a particle initially at position **x**(t=0)=$\mathbf{x_0}$**.** The coordinates **x**=**x**(t) describe the trajectory of this particles. The density may change along the trajectory ρ=ρ(**x**(t),t). The change of density (or other scalar) along the trajectory is derived using the chain rule (in vector notation):

$$\frac{d\rho}{dt} = \frac{d\vec{x}}{dt}\left(\frac{\partial\rho}{\partial\vec{x}}\right)_{t=const} + \left(\frac{\partial\rho}{\partial t}\right)_{\vec{x}=const} = \vec{u}\cdot\nabla\rho + \frac{\partial\rho}{\partial t}$$

$$\rightarrow \frac{d\rho(\vec{x}(t),t)}{dt} = \left(\frac{\partial}{\partial t} + \vec{u}\cdot\nabla\right)\rho(\vec{x},t) \equiv \frac{D\rho}{Dt}$$

The rate of change along the trajectory (Lagrangian frame) equals the local rate of change plus the advection of gradients (Eulerian frame). The Lagrangian derivative (D/Dt) need not be zero, e.g. if there is a source or sink.

Example:
Let's assume that we are in a river that feeds on glacial melt. Let's assume that the water warms at a constant rate that is a function of distance from the source (x), i.e. there is a source of heat (the air). If we drift down river (A la 'Huckleberry Fin'), the temperature increases with time (DT/Dt>0). At one point along the river, however, we see no change

in temperature with time (∂T/∂t=0), as the water arriving there is always at the same temperature. The heat flux is *advective*, ($u\partial T/\partial x>0$).

Mass conservation

a. Eulerian, differential approach:

Accounting for the change in mass ($M=\rho V$) inside a fixed, constant-volume volume:

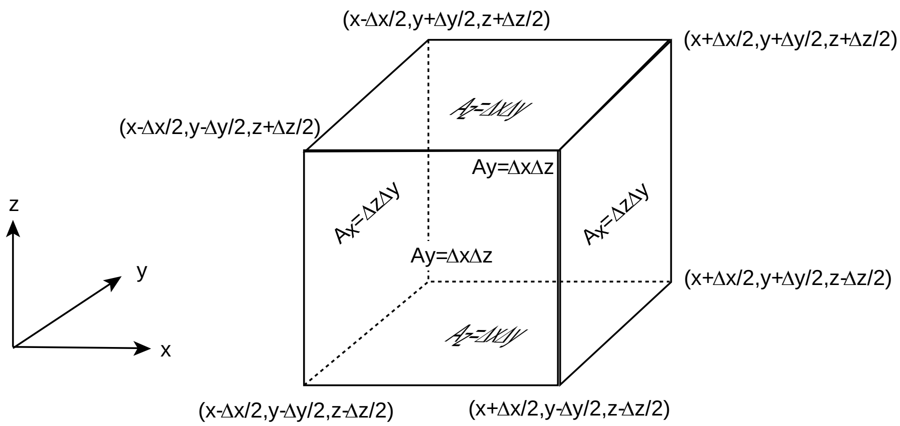

Figure 2. A fixed volume.

Change of mass within the volume are due to differences of fluxes between what comes in and what goes out:

$$\frac{\partial(\rho V)}{\partial t} = -A_x\left(\rho u|_{+\Delta x/2} - \rho u|_{-\Delta x/2}\right) - A_y\left(\rho v|_{+\Delta y/2} - \rho v|_{-\Delta y/2}\right) - A_z\left(\rho w|_{+\Delta z/2} - \rho w|_{-\Delta z/2}\right)$$

Substituting for the areas and deviding by V= ΔxΔyΔz:

$$\frac{\partial \rho}{\partial t} = -\frac{1}{\Delta x}\left(\rho u|_{+\Delta x/2} - \rho u|_{-\Delta x/2}\right) - \frac{1}{\Delta y}\left(\rho v|_{+\Delta y/2} - \rho v|_{-\Delta y/2}\right) - \frac{1}{\Delta z}\left(\rho w|_{+\Delta z/2} - \rho w|_{-\Delta z/2}\right)$$

Taking the limits Δx, Δy, Δz → 0, and in vector notation form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial y}(\rho w) = \frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{u}) = 0$$

b. Eulerian, integral approach:

Accounting for the change in mass inside a fixed, constant-volume volume (V_0), using the divergence theorem (∂V_0 denotes the surface area enclosing the volume):

$$\frac{d}{dt}\int_{V_0} \rho dV = -\int_{\partial V_0} \rho\vec{u}\cdot\vec{n}dS \rightarrow \int_{V_0} \frac{\partial}{\partial t}\rho dV = -\int_{V_0} \nabla\cdot\rho\vec{u}dV \rightarrow \frac{\partial}{\partial t}\rho + \nabla\cdot\rho\vec{u} = 0$$

c. Comparison of Lagrangian and Eulerian:

The Lagrangian mass conservation is simply:

$$\frac{D}{Dt}\int_{V}\rho dV = 0$$

Where the volume allowed to change along the trajectory V=V(t).
The Eulerian mass conservation is:

$$\frac{d}{dt}\int_{V_0}\rho dV = -\int_{V_0}\nabla\cdot(\rho\vec{u})dV$$

d. Continuity equation and non-divergence:
The mass conservation can be written as:

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{u})=0$$

Which is equivalent to:

$$\frac{1D\rho}{\rho Dt}+\nabla\cdot\vec{u}=0$$

The second term is the divergence of the flow (rate of outflow of volume per unit volume). In the absence of forcing, this can be nonzero only for compressible fluids. It is the rate of loss of density due to expansion.

For both water and air we can assume that $\nabla\cdot\vec{u}=0$ in terms of their dynamics. For some processes (e.g. sound propagation) compressibility cannot be neglected.

Conservation of mass of a scalar:
The mass of a scalar is CρV, where C denotes the concentration (e.g. in mol or mg per Kg fluid). Adding the possibility for a diffusive flux (Fick's law), and subtracting CD(ρV)/Dt=0:

$$\int_{V_0}\frac{\partial C}{\partial t}dV = -\int_{\partial V_0}(C\vec{u}-K\nabla C)\cdot\vec{n}dS$$

Using the divergence theorem:

$$\int_{V_0}\left[\frac{\partial C}{\partial t}+\nabla\cdot(C\vec{u}-K\nabla C)\right]dV=0$$

And since the volume is arbitrary,

$$\frac{\partial C}{\partial t}+\nabla\cdot(C\vec{u})=\nabla\cdot(K\nabla C)$$

Momentum balance (the Navier-Stokes equations):
Newton's 2nd law of motion states that the time rate of change of momentum of a particle is equal to the force acting on it. This law is Lagrangian, the "time rate of change" is with respect to a reference system following the particle. Thus:

$$\frac{d}{dt}\int_{V(t)} \rho \vec{u}\, dV = \int_{V(t)} \rho \vec{g}\, dV + \int_{\partial V(t)} \vec{T}\, dS$$

Where **g** is the body force per unit mass (e.g. gravity) and **T** is the surface force per unit surface area bounding V. If the volume is small enough that the integrands can be taken out of the integral:

$$\frac{d}{dt}\int_{V(t)} \rho \vec{u}\, dV = \frac{d}{dt}\left(\rho \vec{u} \int_{V(t)} dV\right) = \frac{d}{dt}\left(\rho \vec{u}\, \delta V\right) = \rho \delta V \frac{d\vec{u}}{dt} + \vec{u}\,\frac{d(\rho \delta V)}{dt} = \rho \delta V \frac{d\vec{u}}{dt}$$

where conservation of mass along the path eliminated a term.
The body force is similarly treated:

$$\int_{V(t)} \rho \vec{g}\, dV = \rho \vec{g}\, \delta V$$

Defining a stress tensor: $\vec{T} = \mathrm{T} \cdot \vec{n}$ and applying the divergence theorem:

$$\int_{\partial V(t)} \vec{T}\, dS = \int_{V(t)} \nabla \cdot \mathrm{T}\, dV = \nabla \cdot \mathrm{T}\, \delta V$$

We get:

$$\rightarrow \rho \frac{D\vec{u}}{Dt} = \rho \vec{g} + \nabla \cdot \mathrm{T}$$

Surface forces (stresses): For an inviscid fluid, the surface force exerted by the surrounding fluid is normal to the surface, i.e. **T**=-p**n**, and p is called the pressure force. In general, viscous stress force **σ** is also present, so for viscous fluids: **T**=-p**n**+**σ**.
By definition **T**=*T*·**n,** and we now have *T*=-pI+Σ, where **σ** =Σ·**n** and I is the identity tensor. Note that the pressure is isotropic at any given point.

For Newtonian incompressible fluids (see below),

$$\nabla \cdot \Sigma = \mu \nabla^2 \vec{u}$$

And the resultant Navier-Stokes equations are (see below):

$$\rho \frac{D\vec{u}}{Dt} = \rho \vec{g} - \nabla p + \mu \nabla^2 \vec{u}$$

Some characteristics of the stress tensor, T:

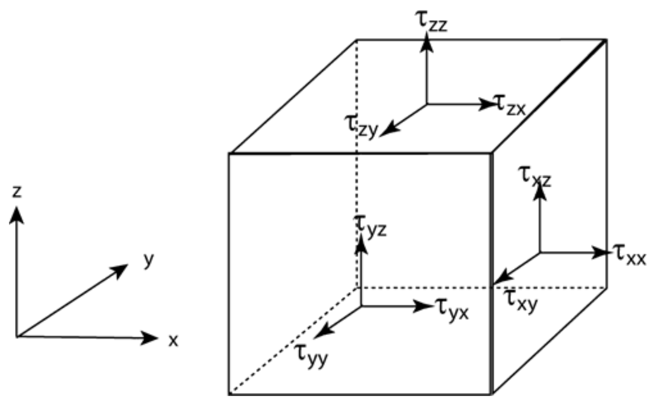

Figure 3: The direction and notation of the element of the stress tensor.

The stress tensor is symmetric:

$$T = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix} = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \tau_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{pmatrix}$$

Pressure is related to the diagonal elements of the stress tensor:

$$-p \equiv \frac{1}{3}\left(\tau_{xx} + \tau_{yy} + \tau_{zz}\right)$$

In Newtonian fluids the stress is linearly related to the shear and the proportionality constant is the dynamic viscosity μ.

$$T = \begin{pmatrix} -p + 2\mu\frac{\partial u}{\partial x} & \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\ \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & -p + 2\mu\frac{\partial v}{\partial y} & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) \\ \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) & -p + 2\mu\frac{\partial w}{\partial z} \end{pmatrix} = -p\delta_{ij} + \mu\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)$$

Stokes, 1845:
1. Σij linear function of velocity gradients.
2. Σij should vanish if there is no deformation of fluid elements.
3. Relationship between stress and shear should be isotropic.

Deriving the RHS of the Navier-Stokes equation:

$$\hat{i}\cdot\left(\nabla\cdot T\right) = \frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{yx}}{\partial y} + \frac{\partial T_{zx}}{\partial z} = -\frac{\partial p}{\partial x} + 2\mu\frac{\partial^2 u}{\partial x^2} + \mu\frac{\partial^2 u}{\partial y^2} + \mu\frac{\partial^2 v}{\partial y\partial x}$$

$$+\mu\frac{\partial^2 u}{\partial z^2} + \mu\frac{\partial^2 w}{\partial z\partial x} = -\frac{\partial p}{\partial x} + \mu\nabla^2 u + \frac{\partial\left(\nabla\cdot\vec{u}\right)}{\partial x} = -\frac{\partial p}{\partial x} + \mu\nabla^2 u$$

The Navier-Stokes equation (vector and non-vector notation):

$$\frac{D\vec{u}}{Dt} = -\frac{\nabla p}{\rho} + \frac{\mu}{\rho}\nabla^2\vec{u} + \vec{g},\ \nabla \cdot \vec{\mathrm{u}} = 0$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{\mu}{\rho}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \frac{\mu}{\rho}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right)$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \frac{\mu}{\rho}\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) + g$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

The Boussinesq approximation:
Separate balance of fluid at rest (denoted by zero) from moving fluid (denoted by prime).

$$p = p_0 + p'$$
$$\rho = \rho_0 + \rho'$$

The primary balance is the hydrostatic balance:

$$0 = -\frac{1}{\rho_0}\frac{\partial p_0}{\partial z} + g$$

The next order balance is the modified (Boussinesq) N-S equations:

$$\rho_0 \frac{D\vec{u}}{Dt} = -\nabla p' + \mu\nabla^2\vec{u} + g\rho',\ \nabla \cdot \vec{\mathrm{u}} = 0$$

Reynolds decomposition of the N-S equations:
Assume a perturbed (e.g. turbulent) flow. At any given point in space we separate the mean flow (mean can be in time, space, or ensemble) and deviation from the mean such that:

$$p = \overline{p} + p', u = \overline{u} + u', u = \overline{v} + v', u = \overline{w} + w'$$
$$\langle p \rangle = \overline{p}, \langle p' \rangle = 0, etc'$$

Substituting into the continuity equation (linear):

$$\frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{v}}{\partial y} + \frac{\partial \overline{w}}{\partial z} = 0; \frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial w'}{\partial z} = 0$$

Substituting into x-momentum Navier-Stokes equation:

$$\frac{\partial \overline{u}}{\partial t} + \overline{u}\frac{\partial \overline{u}}{\partial x} + \overline{v}\frac{\partial \overline{u}}{\partial y} + \overline{w}\frac{\partial \overline{u}}{\partial z} = -\frac{1}{\rho_0}\frac{\partial \overline{p}}{\partial x} + \frac{\mu}{\rho_0}\left(\frac{\partial^2 \overline{u}}{\partial x^2} + \frac{\partial^2 \overline{u}}{\partial y^2} + \frac{\partial^2 \overline{u}}{\partial z^2}\right)$$
$$-\left(\frac{\overline{\partial(u'u')}}{\partial x} + \frac{\overline{\partial(v'u')}}{\partial y} + \frac{\overline{\partial(w'u')}}{\partial z}\right)$$

The evolution of the mean is forced by correlations of fluctuating properties.
The correlation terms time the density are the “Reynolds stresses”. These terms dominate over the molecular stresses. The new stress tensor is:

$$T = \begin{pmatrix} -\overline{p} + 2\mu\frac{\partial u}{\partial x} - \rho_0\overline{u'u'} & \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) - \rho_0\overline{v'u'} & \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) - \rho_0\overline{w'u'} \\ \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) - \rho_0\overline{v'u'} & -\overline{p} + 2\mu\frac{\partial v}{\partial y} - \rho_0\overline{v'v'} & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) - \rho_0\overline{w'v'} \\ \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) - \rho_0\overline{w'u'} & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) - \rho_0\overline{w'v'} & -\overline{p} + 2\mu\frac{\partial w}{\partial z} - \rho_0\overline{w'w'} \end{pmatrix}$$

Substituting into a scalar conservation equation:

$$\frac{\partial \overline{C}}{\partial t} + \overline{u}\frac{\partial \overline{C}}{\partial x} + \overline{v}\frac{\partial \overline{C}}{\partial y} + \overline{w}\frac{\partial \overline{C}}{\partial z} = \frac{K}{\rho}\left(\frac{\partial^2 \overline{C}}{\partial x^2} + \frac{\partial^2 \overline{C}}{\partial y^2} + \frac{\partial^2 \overline{C}}{\partial z^2}\right)$$
$$-\left(\frac{\overline{\partial(u'C')}}{\partial x} + \frac{\overline{\partial(v'C')}}{\partial y} + \frac{\overline{\partial(w'C')}}{\partial z}\right)$$

The closure problem: to develop equations for the evolution of the Reynolds stresses themselves, higher order correlation are needed (e.g. w'u'u') and so on. For this reason theories have been devised to describe *T* in terms of the mean flow.

One solution to the closure problem is to link the Reynolds' stress to mean-flow Quantities. For example:

$$K_{eddy,z} \equiv -\rho_0 \overline{w'C'} \Big/ \left\{ \partial \overline{C} / \partial z \right\}, \qquad \mu_{eddy,z} \equiv -\rho_0 \overline{w'u'} \Big/ \left\{ \partial \overline{u} / \partial z \right\}$$

This type of formulation is appealing because it:

a. Provide for down-gradient flux.
b. Is reminiscent of molecular diffusion and viscosity.
c. Provide closure to the equations of the mean fields.

This type of formulation is problematic because:

a. K_{eddy} is a property of the flow and not the fluid.
b. K_{eddy} is likely to vary with direction (e.g. vertical eddy diffusivity is smaller than horizontal eddy diffusivity, due to gravity), unlike molecular processes.

How is K_{eddy} related to the turbulence?
Assume a gradient in a mean property (momentum, heat, solute, etc'. Remember: no mean gradient→no flux). Assume a fluctuating velocity field:

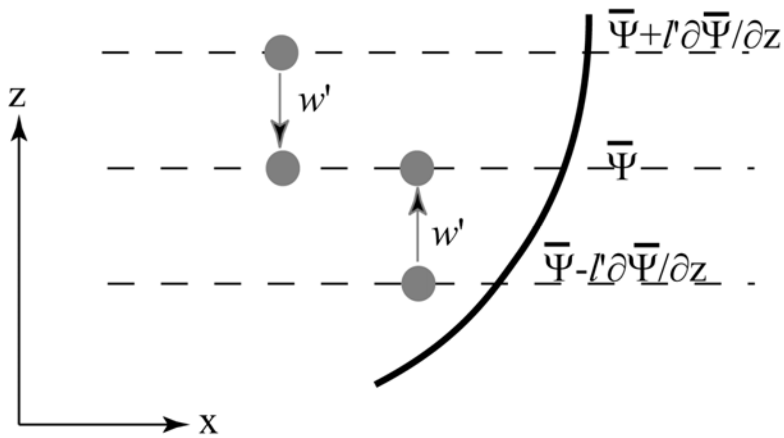

Figure 4: change of position of fluid parcels in the presence of a mean gradient in a scalar Ψ results in a flux of properties.

l' is the distance a parcel travels before it loses its identity. The rate of upward vertical turbulent transfer of <Ψ> is down the mean gradient:

$$\overline{w'\left(\overline{\psi} + l'\frac{\partial \overline{\psi}}{\partial z}\right)} = \overline{w'l'}\frac{\partial \overline{\psi}}{\partial z} = -K_{eddy}\frac{\partial \overline{\psi}}{\partial z}$$

How is K_{eddy} related to the turbulence?

$$K_{eddy,z} \equiv -\rho_0 \overline{w'C'} \Big/ \left\{ \partial \overline{C} / \partial z \right\}, \qquad \mu_{eddy,z} \equiv -\rho_0 \overline{w'u'} \Big/ \left\{ \partial \overline{u} / \partial z \right\}$$

Tennekes and Lumley (1972) approach this problem from dimensional analysis based on assuming a single length scale-*l* and a single velocity scale $\omega = \langle w'w' \rangle^{1/2}$.

$$-\rho_0 \overline{w'u'} = -\rho_0 \frac{\overline{w'u'} \sqrt{\overline{w'^2}} \sqrt{\overline{u'^2}}}{\sqrt{\overline{w'^2}} \sqrt{\overline{u'^2}}} = c\rho_0 \omega^2; \; c \sim O(1)$$

The eddies involved in momentum transfer have vorticities, ω/l; this vorticity is maintained by the mean shear (l is the length scales of the eddies, e.g. the decorrelation scale).

$$\omega / l = c \frac{\partial U}{\partial z}; \; c \sim O(1)$$

It follows that:

$$\mu_{eddy} \sim l\omega \sim l^2 \left| \frac{\partial U}{\partial z} \right|$$

In analogy with momentum flux, for a solute we have:

$$-\rho_0 \overline{w'C'} = K_{eddy} \frac{\partial C}{\partial z}$$

It is most commonly assumed, and verified that $K_{eddy} = \mu_{eddy}$.

Eddy-diffusion: perspective from a dye patch (figures from lecture notes by Bill Young, UCSD):

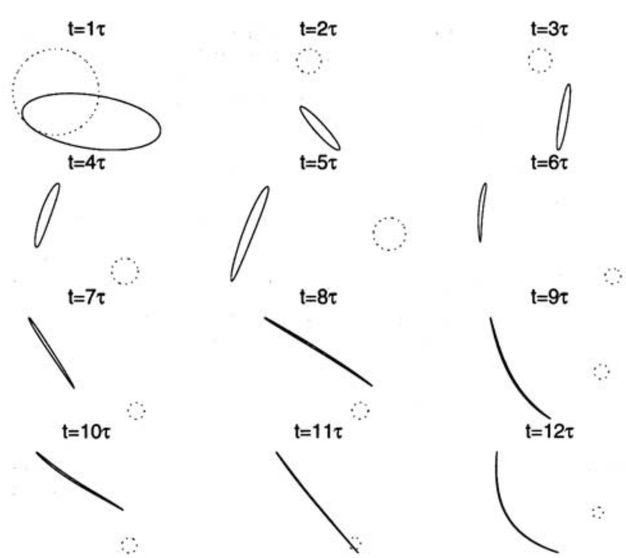

Figure 5a: Dye patch << dominant scale of eddies. Dashed circle denotes initial position and size of tracer patch.

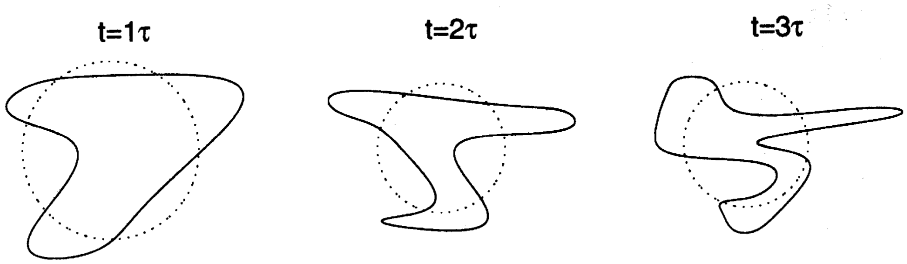

Figure 5b: Dye patch ~ dominant scale of eddies. Dashed circle denotes initial position and size of tracer patch.

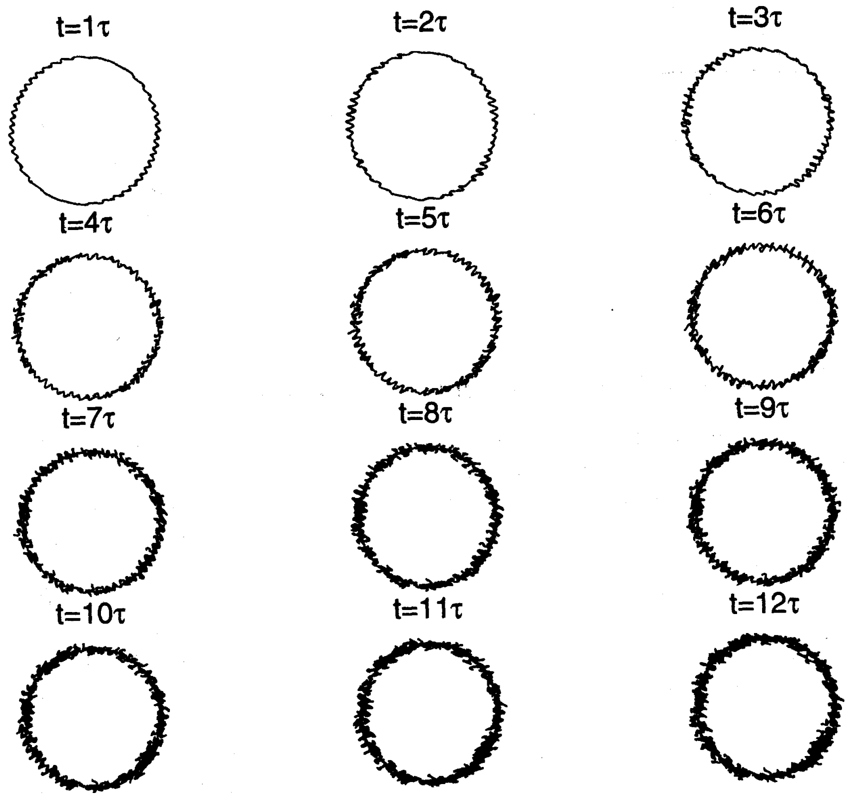

Figure 5c: Dye patch >> dominant scale of eddies.

Useful references:

Acheson, D. J., 1990, Elementary fluid dynamics., Oxford U. press.
Tennekes, H., and J. L. Lumley, 1972, A first Course in Turbulence, MIT press.
Wilkes, J. O., 1999, Fluid Mechanics for Chemical Engineers. Prentice Hall.

Appendix:
Convective derivative:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z} = \frac{\partial}{\partial t} + \vec{u}\cdot\nabla$$

Gradient of a scalar (is a vector):

$$\nabla\phi = \hat{i}\,\frac{\partial\phi}{\partial x} + \hat{j}\,\frac{\partial\phi}{\partial y} + \hat{k}\,\frac{\partial\phi}{\partial z}$$

Divergence of a vector (is a scalar):

$$\nabla\cdot\vec{\varphi} = \frac{\partial\varphi_x}{\partial x} + \frac{\partial\varphi_y}{\partial y} + \frac{\partial\varphi_z}{\partial z}$$

Divergence of a tensor (is a vector):

$$\nabla\cdot T = \hat{i}\left(\frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{yx}}{\partial y} + \frac{\partial T_{zx}}{\partial z}\right) + \hat{j}\left(\frac{\partial T_{xy}}{\partial x} + \frac{\partial T_{yy}}{\partial y} + \frac{\partial T_{zy}}{\partial z}\right) +$$
$$\hat{k}\left(\frac{\partial T_{xz}}{\partial x} + \frac{\partial T_{yz}}{\partial y} + \frac{\partial T_{zz}}{\partial z}\right)$$

Laplacian of a vector (is a vector):

$$\nabla^2\vec{\varphi} = \nabla\cdot\left(\nabla\cdot\vec{\varphi}\right) = \hat{i}\left(\frac{\partial^2\varphi_x}{\partial x^2} + \frac{\partial^2\varphi_x}{\partial y^2} + \frac{\partial^2\varphi_x}{\partial z^2}\right) +$$
$$\hat{j}\left(\frac{\partial^2\varphi_y}{\partial x^2} + \frac{\partial^2\varphi_y}{\partial y^2} + \frac{\partial^2\varphi_y}{\partial z^2}\right) + \hat{k}\left(\frac{\partial^2\varphi_z}{\partial x^2} + \frac{\partial^2\varphi_z}{\partial y^2} + \frac{\partial^2\varphi_z}{\partial z^2}\right)$$