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TRANSPORT OF MARINE POLLUTANTS

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A brief review of marine pollutant transport processes is given, with the objective of introducing the basic concepts required for studying these processes. The subject is obviously one of great extent and detail, and a continuously developing area of research that is motivated by many practical interests. Marine pollutant transport processes are of great importance in many aspects of marine science, including engineering services related to marine waste disposal, the assessment of adverse effects of shipping and industrial sites, and the conservation of water quality in coastal and inland seas.

While most of the steps in the derivations are given for the benefit of the student, a more complete discussion and detailed derivations of the equations can be found in a number of basic books on fluid dynamics (Batchelor, 1967), and transport processes (Csanady, 1973; Fischer *et al.*, 1979; Kullenberg, 1982). Some of the fundamental theorems utilized in the following can be found in books on university level calculus (Hildebrand, 1965).

The basics of hydromechanic theory is briefly summarized in Section 1. Simple solutions to the turbulent transport equations are reviewed in Section 2. The basics of shear flow dispersion are then provided in Section 3. Applications to transport of suspended sediments are considered in Section 4. Estuarine transport processes are reviewed in Section 5.

1. FLUID MOTION AND DIFFUSION IN FLUIDS

The governing equations for fluid motion and diffusion will be briefly reviewed. The equations will be derived from basic hydromechanical concepts.

1.1 CONTINUITY (MASS CONSERVATION) EQUATION

Consider a *material volume* (a volume made of fluid particles or *material points*) V bounded by a *material surface* S. If mass is neither created nor destroyed within this volume, we can express its conservation by

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$$\frac{d}{dt} \int_V \rho dV = 0 \tag{1.1}$$

where ρ is the density of the fluid, and **d/dt** represents a *total* or *material* derivative. Let $\vec{u}$ be the fluid velocity (also valid on S) and $\hat{n}$ be the normal to this surface. The above expression can be expanded employing Leibnitz' rule

$$\int_V \frac{\partial \rho}{\partial t} dV + \int_S \rho \vec{u}\bullet\hat{n} \, dS \quad . \tag{1.2}$$

This integral form expresses the fact that the local rate of change of mass within the volume is balanced by matter exported or imported through the bounding surface. Through the divergence theorem, this is equivalent to

$$\int_V \left(\frac{\partial \rho}{\partial t} + \nabla\bullet\rho\vec{u} \right) dV = 0 \tag{1.3}$$

Since V is arbitrary, the integrand must vanish for any and all such volumes. The equation given by the vanishing integrand is the *continuity equation*. Alternatively we can write (1.3) as

$$\frac{D\rho}{Dt} + \rho \nabla\bullet\vec{u} = 0 \tag{1.4}$$

by making use of the definition of the *material derivative*

$$\frac{DX}{Dt} = \frac{\partial X}{\partial t} + \vec{u}\bullet\nabla X \quad . \tag{1.5}$$

[Note the different notations used for material derivatives of an integral quantity in (1.1) and that of a field property in (1.4), following Batchelor (1967)]. An *incompressible fluid* is defined as one in which the density of material elements of the fluid does not change, i.e.

$$\nabla\bullet\vec{u} = 0 \quad . \tag{1.6}$$

1.2 MOMENTUM (MOMENTUM CONSERVATION) EQUATION

Newton's Second Law of Motion states that the rate of change of momentum $\vec{P}$ of a material element of fluid should be balanced by the total force $\vec{F}_T$ applied on the fluid:

$$\frac{d\vec{P}}{dt} = \vec{F}_T \quad . \tag{1.7}$$

The momentum of the fluid is

$$\vec{P} = \int_V \rho\vec{u}\, dV \tag{1.8}$$

and the total applied force is due to body (volume) and surface forces ($\vec{F}$ and $\vec{\Sigma}$ respectively)

$$\vec{F}_T = \int_V \rho\vec{F}\, dV + \int_S \vec{\Sigma}\, dS \tag{1.9}$$

Making use of Leibnitz' rule and after recombinations of the resulting terms, the left hand side of equation (1.7) can be shown to be

$$\begin{aligned}\frac{d\vec{P}}{dt} &= \int_V \frac{d}{dt}(\rho\vec{u})\, dV + \int_S \rho\vec{u}\, \vec{u}\bullet\hat{n}\, dS \\ &= \int_V \rho\frac{D\vec{u}}{Dt}\, dV + \int_V \vec{u}\left(\frac{\partial\rho}{\partial t} + \nabla\bullet\rho\vec{u}\right) dV \,.\end{aligned} \tag{1.10}$$

Here the second term vanishes by virtue of the continuity equation (1.3). The first term of (1.9) represents the body forces, which in this case is the gravity **g** (force per unit mass)

$$\rho\vec{F} = \rho\vec{g}\,, \tag{1.11}$$

whereas the second term in (1.9) is the surface stresses (force per unit area) integrated over the material surface enclosing the fluid.

It can be shown that (Batchelor, 1967) the surface stresses can be expressed as the normal components of a stress tensor $\underline{\sigma} = \sigma_{ij}$ with respect to the outward normal $\hat{n}$ to the surface, so that through divergence theorem

$$\int_S \vec{\Sigma}\, dS = \int_S \underline{\sigma}\bullet\hat{n}\, dS = \int_V \nabla\bullet\underline{\sigma}\, dV \tag{1.12}$$

By assembling (1.10), (1.11) and (1.12), we can again obtain a volume integrated equation which has to vanish for an arbitrary volume, so that the integrand yields

$$\rho\frac{D\vec{u}}{Dt} = \rho\vec{g} + \nabla\bullet\underline{\sigma}\,. \tag{1.13}$$

The stress tensor $\underline{\sigma}$ includes both normal and shear stresses. Part of the normal stresses is the fluid pressure p. The remaining normal and shear stresses are generated as a result of the motion of a viscous fluid, and are therefore essentially related to the motion. The stress tensor can thus be decomposed into two parts

$$\underset{\sim}{\sigma} = -p\mathrm{I} + \underset{\sim}{d}$$

or

$$\sigma_{ij} = -p\delta_{ij} + d_{ij} \tag{1.14}$$

where p is the pressure and d_{ij} is the deviatoric stress tensor, the latter being due to the motion of the fluid (Batchelor,1967). For a simple fluid in the laminar regime, the stress tensor d_{ij} can therefore be related to the rate of strain and the well-known Navier-Stokes equation can be obtained. The details of these derivations are to be found in Batchelor (1967).

For an incompressible fluid, the Navier-Stokes equation is

$$\frac{D\vec{u}}{Dt} = \vec{g} - \frac{1}{\rho}\nabla p + \nu\nabla^2\vec{u} \; . \tag{1.15}$$

Here ν is the kinematic viscosity with dimensions of L^2T^{-1} and the last term on the right hand side represents the frictional (viscous) forces (per unit mass), alternatively representing the diffusion of momentum. The above *equation of motion* expresses the fact that fluid accelerations are generated in response to gravity, pressure gradients or viscous friction..

The momentum equation is modified considerably on a moving frame of reference. Consider the earth's motion with respect to a fixed (inertial) frame of reference. After transforming the equations from the inertial to the moving frame of reference, fictitious terms arise in the momentum conservation equation, being related to the angular velocity $\vec{\Omega}$ of the earth, and as a result of the redefinition of the material derivative with respect to the moving coordinates (Batchelor, 1967):

$$\frac{D\vec{u}}{Dt} + 2\vec{\Omega}\times\vec{u} + \vec{\Omega}\times\vec{\Omega}\times\vec{x} = \vec{g} - \frac{1}{\rho}\nabla p + \nu\nabla^2\vec{u} \; . \tag{1.16}$$

The second term on the left hand side is known as the *Coriolis acceleration* (or Coriolis force per unit mass of the fluid if carried over on the right hand side). This term represents an acceleration that is normal to both the motion (the velocity vector) and the angular velocity vector, and therefore the motion is deflected *sideways* (with respect to the velocity that would occur on an inertial frame), depending on the position on the earth. The third term on the left hand side represents *centrifugal acceleration* resulting from the rotation and can simply be expressed as a force $|\Omega|^2 r$ acting outwards from the rotation axis (x being the position with respect to the earth's center and r being the position measured perpendicular from the rotation axis).

Due to the conservative nature of the gravitational and centrifugal accelerations, these forces can be embedded (if the fluid is homogeneous) in the modified pressure P:

$$-\frac{1}{\rho}\nabla p + g - \vec{\Omega}\times\vec{\Omega}\times\vec{x} = -\frac{1}{\rho}\nabla\left(p - \rho\vec{g}\cdot\vec{x} + \frac{\rho}{2}\Omega^2 r^2\right)$$

$$= -\frac{1}{\rho}\nabla P \qquad (1.17)$$

so that, in effect, equation (1.16) simplifies to

$$\frac{D\vec{u}}{Dt} + 2\vec{\Omega}\times\vec{u} = -\frac{1}{\rho}\nabla P + \nu\nabla^2\vec{u} . \qquad (1.18)$$

1.3 THERMODYNAMIC (ENERGY CONSERVATION) EQUATION

The *First Law of Thermodynamics* expresses the energy conservation

$$\frac{dE_T}{dt} = \frac{dH}{dt} + \frac{dW}{dt} , \qquad (1.19)$$

namely that the rate of change of the total energy (E_T) is balanced by the rate at which heat (H) is supplied to the fluid and the rate at which work (W) is done on the fluid by the surroundings. The total energy for a material volume of fluid is defined as

$$E_T = \int_V \rho\epsilon \, dV \qquad (1.20)$$

where

$$\epsilon = e + \frac{1}{2}\vec{u}\cdot\vec{u} - \vec{g}\cdot\vec{x} \qquad (1.21)$$

is the total energy per unit mass, including the internal energy (or specific entropy) e, the kinetic energy (second term), and the potential energy (third term) components. Here $\vec{x}$ is a position vector with respect to an arbitrary datum ($\vec{x}$ increasing in the opposite sense of the gravity vector $\vec{g}$ leads to positive values of the potential energy).

The first term in (1.19) can be expressed as follows, consecutively using the Leibnitz' rule, the divergence theorem, and the continuity equation. (1.4)

$$\frac{dE_T}{dt} = \frac{d}{dt}\int_V \rho\epsilon \, dV = \int_V \frac{\partial\rho\epsilon}{\partial t} + \int_S \rho\epsilon \, \vec{u}\cdot\hat{n} \, dS$$

$$= \int_V \left(\frac{\partial\rho\epsilon}{\partial t} + \nabla\cdot(\rho\epsilon\vec{u}) \right) dV$$

$$= \int_V \rho \frac{D\epsilon}{Dt}\, dV \qquad (1.22)$$

On the other hand, we define

$$\frac{dH}{dt} = \int_V \rho Q\, dV - \int_S \vec{q}\cdot\hat{n}\, dS$$

$$= \int_V (\rho Q \quad \nabla\cdot\vec{q})\, dV \qquad (1.23)$$

where Q is the rate of internal heating (per unit mass) and $(-\vec{q})$ the heat flux (per unit surface area) entering the fluid volume through the enclosing surface.

The rate of work done by the surrounding on the fluid is due to the stresses $\vec{\Sigma}$ applied on the enclosing surface which is deformed with velocity **u**, so that (using 1.12)

$$\frac{dW}{dt} = \int_S \vec{\Sigma}\cdot\vec{u}\, dS = \int_S (\underline{\sigma}\cdot\hat{n})\cdot\vec{u}\, dS$$

$$= \int_S (\vec{u}\cdot\underline{\sigma})\cdot\hat{n}\, dS$$

$$= \int_V \nabla\cdot(\vec{u}\cdot\underline{\sigma})\, dV \qquad (1.24)$$

Combining (1.22), (1.23) and (1.24) yields (for arbitrary volume element V)

$$\rho \frac{D\epsilon}{Dt} = - \nabla\cdot\vec{q} + \rho Q + \nabla\cdot(\vec{u}\cdot\underline{\sigma}) \ . \qquad (1.25)$$

The last term on the right hand side can be expanded making use of the momentum equation (1.3)

$$\nabla\cdot(\vec{u}\cdot\underline{\sigma}) = \vec{u}\cdot(\nabla\cdot\underline{\sigma}) + (\underline{\sigma}\cdot\nabla)\cdot\vec{u}$$

$$= \vec{u}\cdot(\rho\frac{D\vec{u}}{Dt} - \rho\vec{g}) + (\underline{\sigma}\cdot\nabla)\cdot\vec{u}$$

$$= \rho\vec{u}\cdot\frac{D\vec{u}}{Dt} - \rho\vec{u}\cdot\nabla(\vec{g}\cdot\vec{x}) + (\underline{\sigma}\cdot\nabla)\cdot\vec{u}$$

$$= \rho\frac{D}{Dt}\,(\frac{1}{2}\vec{u}\cdot\vec{u} - \vec{g}\cdot\vec{x}) + (\underline{\sigma}\cdot\nabla)\cdot\vec{u} \ . \qquad (1.26)$$

The above equation expresses the *conservation of mechanical energy*. Substituting (1.26) in (1.25) and making use of

(1.21), the energy equation is reduced to a form that accounts solely for the *conservation of thermal energy* (i.e. the *thermodynamic equation*):

$$\rho\frac{De}{Dt} = -\nabla\cdot\vec{q} + \rho Q + (\underline{\sigma}\cdot\nabla)\cdot\vec{u} \ . \tag{1.27}$$

The last term, representing the working of the surface stresses in deforming the fluid, can be written alternatively (using (1.14) and the continuity equation (1.4)) as

$$\begin{aligned}(\underline{\sigma}\cdot\nabla)\cdot\vec{u} &= -p\nabla\cdot\vec{u} + (\underline{d}\cdot\nabla)\cdot\vec{u} \\ &= \frac{p}{\rho}\frac{D\rho}{Dt} + \rho\Phi\end{aligned} \tag{1.28}$$

where Φ represents the heat generated (mechanical energy dissipated) by viscous friction.

The diffusive (conductive) heat flux is formulated through *Fourier's Law* which linearly relates the flux to the local temperature gradient (in an isotropic medium, cf. Batchelor, 1967) as

$$\vec{q} = -\kappa\nabla T \tag{1.29}$$

so that the heat flows from regions of high temperature to those of low temperature. The proportionality constant κ is the *thermal conductivity*.

Substituting (1.28) and (1.29), equation (1.27) takes the form

$$\frac{De}{Dt} - \frac{p}{\rho^2}\frac{D\rho}{Dt} = \frac{1}{\rho}\nabla\cdot\kappa\nabla T + (Q+\Phi) \ . \tag{1.30}$$

The thermodynamic laws describing the state of the fluid must be used to transform the thermodynamic equation to its final form. The *Second Law of Thermodynamics* states that

$$\begin{aligned}T\frac{Ds}{Dt} &= \frac{De}{Dt} + p\frac{D\upsilon}{Dt} \\ &= \frac{De}{Dt} - \frac{p}{\rho^2}\frac{D\rho}{Dt}\end{aligned} \tag{1.31}$$

which is equal to the left hand side of (1.30). Here s is the *specific entropy* and $\upsilon=1/\rho$ is the specific volume.

The thermodynamic state of a fluid of fixed composition (fixed mixing ratios of its constituents) is fully described by a unique relation of three of its thermodynamic variables. This relation is therefore called the *equation of state*. For seawater, the equation of state is an empirical nonlinear equation relating for instance, pressure, density and temperature as well as salinity (since the composition of seawater changes with salinity). The equation of state can be linearized about local (subscripted) reference values, and neglecting pressure effects we can write

$$\rho = \rho_o \, [1 - \alpha_T(T-T_o) + \alpha_S(S-S_o)] \; . \tag{1.32}$$

Since specific entropy s in equation (1.31) is also a state variable, it can be related to other state variables, say temperature and pressure, so that

$$T \frac{Ds}{Dt} = T\left(\frac{\partial s}{\partial T}\right)_p \frac{DT}{Dt} + T\left(\frac{\partial s}{\partial p}\right)_T \frac{Dp}{Dt} \; . \tag{1.33}$$

where subscripted parantheses denote differentiation for constant values of the subscripts. The rate of change of the heat content Tds with respect to temperature is called the *specific heat*. The specific heat at constant pressure is thus a constant

$$T \left(\frac{\partial s}{\partial T}\right)_p = c_p \tag{1.34}$$

The second term of (1.33) can be expressed through the *Maxwell relation*

$$\left(\frac{\partial s}{\partial p}\right)_T = -\left(\frac{\partial \upsilon}{\partial T}\right)_p = \frac{1}{\rho^2}\left(\frac{\partial \rho}{\partial T}\right)_p \tag{1.35}$$

whereas using (1.32) we make the approximation

$$\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \approx \frac{1}{\rho_o}\left(\frac{\partial \rho}{\partial T}\right)_p \approx -\alpha_T \; . \tag{1.36}$$

Substituting (1.31),(1.33),(1.34),(1.35) and (1.36) into (1.30) yields

$$\frac{DT}{Dt} - \frac{\alpha_T}{c_p} \frac{T}{\rho} \frac{Dp}{Dt} = \nabla \cdot K \nabla T + \frac{1}{c_p}(Q+\Phi) \tag{1.37}$$

where $K=\kappa/(\rho c_p)$ is the *thermal diffusivity coefficient*.

The above equation is valid for a general (compressible, inhomogeneous) moving fluid. The second term on the left hand side is often small and in fact vanishes for a fluid that is at rest. Seawater can be assumed to be incompressible and, its contribution being small, this term can again be neglected. If we also neglect the heating due to any internally distributed sources (e.g. solar radiation) and the frictional generation of heat, we can set $Q=\Phi=0$. Under these assumptions, we then simplify (1.37) to have the heat equation

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T = \nabla\cdot k\nabla T \qquad (1.38)$$

1.4 DIFFUSION EQUATION (CONSERVATION OF MASS FOR DISSOLVED CONSTITUENTS IN A FLUID)

In this Section we will derive the conservation equations governing the diffusion of dissolved substances that may be present in a fluid. Before considering the case of a weak solute, consider a *binary system* consisting of a mixture of two different fluids. The density ρ_A of the first constituent represents its mass per unit volume of the mixture, and likewise ρ_B represents the density of the second constituent per unit volume of the mixture. The density of the fluid mixture is then

$$\rho = \rho_A + \rho_B \, . \qquad (1.39)$$

We can define the *concentration* of each constituent in the fluid as the mass of each constituent per unit mass of the mixture, i.e.

$$c_A = \frac{\rho_A}{\rho}, \qquad c_B = \frac{\rho_B}{\rho} \qquad (1.40)$$

so that

$$c_A + c_B = 1 \qquad (1.41)$$

by virtue of (1.39).

In a moving fluid mixture, we define the fluxes (passing through a fixed surface) of each constituent as

$$\begin{aligned} \vec{N}_A &= \rho_A\vec{u}_A \\ \vec{N}_B &= \rho_B\vec{u}_B \end{aligned} \qquad (1.42.a,b)$$

where $\vec{u}_A$ and $\vec{u}_B$ are "velocities" assigned to each constituent. These are not real (particle) velocities, but rather hypothetical velocities that an infinitesimal group (or cloud) of particles would have on the average. It can be verified that these fluxes represent the momenta of each constituent per unit volume of the mixture. The total momentum (or total flux) of the mixture is

$$\rho\vec{u} = \rho_A\vec{u}_A + \rho_B\vec{u}_B$$

or $\qquad (1.43.a,b)$

$$\vec{u} = c_A\vec{u}_A + c_B\vec{u}_B \, .$$

We thus define the hydrodynamic velocity $\vec{u}$ of the mixture by (1.43.b).

The fluxes defined in (1.42.a,b) are with respect to a fixed observer and involve both diffusion and bodily transport (convection) with the fluid velocity. For example, we can write (1.43.a) as

$$\vec{N}_A = \rho_A \vec{u}_A$$
$$= \rho_A(\vec{u}_A - \vec{u}) + \rho_A \vec{u} \qquad (1.44)$$

so that the first term represents the transport relative to an observer moving with the fluid (i.e. diffusive transport) and the second term represents the convective (advective) transport.

The diffusive flux is commonly modelled by *Fick's Law* (an analogue of Fourier's Law in heat conduction) which relates this flux to the local gradients of the density of each constituent. In the general non-isotropic case, the flux vector can be expressed as the product of a tensor coefficient with the gradient vector. If the medium is assumed to be isotropic, the constant of proportionality is a scalar and we can write

$$\rho_A(\vec{u}_A - \vec{u}) = - D_{AB} \nabla \rho_A \qquad (1.45)$$

for constituent A and similarly for constituent B. Here, the diffusion coefficient D_{AB} characterizes the diffusivity of constituent A in medium B, and likewise the diffusivity of constituent B in A is represented by D_{BA}.

We consider a *fixed* control volume V enclosed by a surface S, and write a statement of the conservation of mass for each constituent. For constituent A we have

$$\frac{\partial}{\partial t} \int_V \rho_A dV = - \int_S \vec{N}_A \cdot \hat{n} dS + \int_V r_A dV, \qquad (1.46)$$

i.e. the rate of change of the mass in volume V is increased by the flux of mass entering through the fixed surface S (with outward normal $\hat{n}$) and by any sources of material in the volume. Here r_A is the rate of production of the mass of constituent A per unit time per unit volume of the mixture. These local sources of mass in a binary system can be important as a result of the chemical interactions between the two constituents. Since the total mass of the mixture should be conserved,

$$r_A + r_B = 0, \qquad (1.47)$$

i.e. the rate of production of either constituent must be at the expense of the destruction of the other.

Using the divergence theorem, the first term on the right hand side of (1.46) can be converted to a volume integral for which the volume V is arbitrary. Then, the conservation laws become

$$\begin{aligned}&\frac{\partial \rho_A}{\partial t} + \nabla\cdot\vec{N}_A = r_A\\ \text{and}\\ &\frac{\partial \rho_B}{\partial t} + \nabla\cdot\vec{N}_B = r_B \,.\end{aligned}\tag{1.48.a,b}$$

By adding together (1.48.a,b) and utilizing the definitions (1.39), (1.42.a,b), (1.43.a) and (1.47) we arrive at

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{u}) = 0, \tag{1.49}$$

i.e. the continuity equation (1.3) being re-derived, proving that the total mass of the mixture is conserved.

Substituting (1.44) and (1.45) in (1.48.a) and utilizing (1.40.a) yields

$$\frac{\partial(\rho c_A)}{\partial t} + \nabla\cdot(\rho c_A\vec{u}) = \nabla\cdot D_{AB}\nabla\rho c_A + r_A \tag{1.50}$$

or

$$\rho\left(\frac{\partial c_A}{\partial t} + \vec{u}\cdot\nabla c_A\right) = \nabla\cdot D_{AB}\nabla\rho c_A + r_A \,, \tag{1.51}$$

obtained by expanding terms and making use of (1.49). A similar equation is obtained for c_B. If the mixture is relatively homogeneous we can assume **$\rho\approx$constant**. The diffusivities D_{AB} and D_{BA} can also be assumed constant. Then the conservation equations are

$$\begin{aligned}&\frac{Dc_A}{Dt} = D_{AB}\nabla^2 c_A + \frac{r_A}{\rho}\\ \text{and}\\ &\frac{Dc_B}{Dt} = D_{BA}\nabla^2 c_B + \frac{r_B}{\rho} \,.\end{aligned}\tag{1.52.a,b}$$

If the presence of each constituent influences the density, so that ρ is not constant, it can be verified that the equations are coupled through density, which then means that the diffusion equation (1.51) (and its counterpart for c_B) must be solved together with the continuity (1.4), the momentum (1.18) equations, and an equation of state incorporating the effects of the constituents on density such as

$$\rho = \rho(p,\ c_A,\ c_B) \,. \tag{1.53}$$

Likewise, in the case of sea water, having temperature and salinity variations that influence the density in addition to the above, an equation of state in the form

$$\rho = \rho(p, T, S, c_A, c_B) \tag{1.54}$$

must be added to the above equations, and furthermore the energy equation (1.37), a diffusion equation (similar to (1.51)) for salinity (a third constituent) must also complement the above equations in order to be able to solve the system. In the above cases, note that the equations are coupled to each other through variable density, which requires their simultaneous solution.

It is quite common that the mixture of interest is a weak (dilute) solution of one of the constituents (say $c_A << c_B$). Then by virtue of (1.41)

$$\begin{aligned} & c_B \approx 1, \\ c \equiv\ & c_A << 1, \\ & \rho \approx \text{constant}, \end{aligned} \tag{1.55.a-c}$$

so that the second equation (1.52.b) becomes irrelevant and the conservation of mass for the dilute solution is expressed by the single equation

$$\frac{\partial c}{\partial t} + \vec{u}\cdot\nabla c = D\nabla^2 c + R \tag{1.56}$$

where R and D have replaced r_A/R and D_{AB} respectively. In this case, the convective diffusion equation (1.56) is decoupled from the remaining equations, so that the velocity field $\vec{u} = \vec{u}(x,t)$ is a known function obtained by solving the remaining equations.

Likewise, the influence of temperature and salinity on the density of seawater can often be neglected when the gradients of both properties are sufficiently small. To a good degree of approximation, the ocean can be assumed incompressible and homogeneous, as a result of which the energy and salt diffusion equations are decoupled from the continuity and momentum equations. Therefore, in principle, we first solve the hydrodynamics from (1.4) and (1.18) to determine the velocity field $\vec{u}(x,t)$. Consequently, for given velocity field, we seek solutions to equation (1.56).

1.5 TURBULENT MOTIONS

The equations derived in the preceeding sections are generally for laminar (orderly) flows of fluids. Most fluids become turbulent (by the generation of chaotic motions) due to various reasons. Turbulence in fluids may be generated as a result of instabilities with respect to fluctuations deriving their energy from the mean motion, wind stirring or mechanical stirring at the boundaries, etc. The motions in the upper ocean are therefore commonly turbulent. The result is the random motion of fluid "particles" consisting of lumps (eddies) of various sizes, superposed on the mean motion (which exists at a larger scale than the typical maximum eddy size). It is possible to derive the governing equations in the turbulent state of the fluid corresponding to the previously described conservation laws, through an averaging procedure. However, since the motions are random and chaotic, a full description of turbulent flows is in the realm of statistics, which on the other hand is strongly dependent on the structure and generating mechanisms of the turbulence activity. In order to overcome the difficulties posed by the often incomplete knowledge and the poorly determined nature of the turbulence statistics; the statistical quantities are estimated through simple empirical parameterizations (closure).

In order to derive the turbulence equations, we proceed by separating the flow variables into slowly varying and fluctuating parts with respect to a time scale T, which is assumed to be the upper limit of the turbulence time scales. For the variables $\vec{u}$ and **c** in equation (1.56) we can write

$$\vec{u} = \bar{\vec{u}}(x,\ T^{-1}t) + \vec{u}\,'(x,\ t)$$

and (1.57.a,b)

$$c = \bar{c}(x,\ T^{-1}t) + c'(x,\ t)$$

where the quantities with overbars denote the long term (with respect to T) averages, for example in the case of the concentration

$$\bar{c} = \frac{1}{T}\int_{0}^{T} c\ dt \qquad (1.58)$$

and the primed quantities denote the components with fluctuations that are typically more rapid than the turbulence time scale T. It can be verified that (by definition)

$$\overline{c'} = \overline{c - \bar{c}} = 0. \qquad (1.59)$$

The turbulence equations are then obtained by averaging the respective equations over a time period T. Since the conservation equations given in the earlier sections, namely the continuity (1.4), momentum (1.18), energy (1.37) and diffusion (1.56) equations are basically the same types (i.e. have the similar time derivative, convective, and diffusive terms), the averaging procedure results in similar terms. It will therefore suffice to average one of these equations, that case being the diffusion equation.

It is obvious that, after averaging, the linear terms in the equations will preserve their form in that they will be the same differential terms operating on the mean quantities (since the averages of the fluctuating parts vanish). On the other hand, the nonlinear terms give rise to additional terms arising due to the averaging of the products of fluctuating variables, which in general do not vanish since the individual fluctuations of the variables can be correlated (arising due to the common cause of turbulence). These turbulent products mainly originate from the nonlinear convective fluxes and represent the turbulent fluxes, of buoyancy in the case of the continuity equation (1.4) [although for homogeneous, incompressible fluids, the linear equation (1.5) does not yield such fluxes], of momentum (Reynolds' stresses) in the case of the momentum equation (1.18), and of heat or concentration in the cases of the convective-diffusion equation (1.38 and 1.56).

Proceeding with the turbulent averaging of the diffusion equation (1.56), we first put it in the flux form (i.e. a form compatible with (1.50), making use of the continuity equation), substitute (1.57.a,b), and take averages:

$$\frac{\partial}{\partial t}\overline{(\bar{c}+c')} + \nabla\bullet\overline{(\bar{c}+c')(\vec{\bar{u}}+u')} = D\nabla^2\overline{(\bar{c}+c')} + \overline{\bar{R}+R'} \qquad (1.60)$$

By making use of the definitions (1.58) and (1.59), this equation immediately reduces to

$$\frac{\partial\bar{c}}{\partial t} + \nabla\bullet\bar{c}\vec{\bar{u}} + \nabla\bullet\overline{c'\vec{u}'} = D\nabla^2\bar{c} + \bar{R} \qquad (1.61)$$

i.e. the same as equation (1.56) with the exception of the term $\nabla\bullet\overline{c'\vec{u}'}$ arising due to the averaging of the nonlinear convective terms in the preceeding equation.

As we have noted above, the product $\overline{c'\vec{u}'}$ describes the statistical correlation of the fluctuating components of concentration and velocity, which are expected to be strongly correlated in a turbulent field. Because of the practical problems discussed above, these terms are often parameterized, using empirical formulations. The form of this term in (1.61) actually suggests that it may represent the divergence of a flux in much the same way that the molecular flux divergence appears in (1.48.a). We can therefore define

$$\vec{N}_T = \rho\overline{c'\vec{u}'} \qquad (1.62)$$

as the *turbulent flux* of the matter represented by the concentration $\bar{c}$.

One way to parameterize this flux is to make an analogy to Fick's Law, and adopt it for turbulent flows (Further discussion of the *mixing length theory* on which the present approximation is based can be found in Schlichting (1968), and Tennekes and Lumley (1972)). With this analogy, we relate the turbulent fluxes to the local gradients of the mean properties (in this case the mean concentration). For a turbulent fluid, the statistical properties of which we can not fully prescribe, it is imperative that we use a anisotropic version of the analogy, i.e.

$$\overline{c'u'_i} = E_{ij} \frac{\partial \bar{c}}{\partial x_j} \qquad (1.63)$$

where i=1,2,3 are indices denoting the directions in three dimensional coordinates x_i, and E_{ij} the *turbulent diffusivity tensor*.

In the sea, the smallness of the vertical motions as compared to the horizontal motions and the fact that the depth of the ocean is quite often smaller than the horizontal scales of interest (i.e. the shallow water approximation) results in the common situation that the vertical stratification is far greater than that occurs in the horizontal. Therefore, it is reasonable to expect that the vertical coordinate coincides with one of the *principal axes*, and the horizontal axes can (by choice) be aligned with the remaining principal coord nates of the diffusivity tensor E_{ij}, which then reduces (1.63) to the special form

$$N_i = \rho\overline{c'u'_i} = - \rho E_i \frac{\partial \bar{c}}{\partial x_i} \qquad (1.64.a)$$

where $E_i = E_{ii}$ are the principal components of the diffusivity tensor. Writing in vector form this becomes

$$\begin{aligned} N_T &= \rho\overline{c'\vec{u}'} = - \rho(E \bullet \nabla)\bar{c} \\ &= - \rho(E_x \frac{\partial \bar{c}}{\partial x} \hat{i} + E_y \frac{\partial \bar{c}}{\partial y} \hat{j} + E_z \frac{\partial \bar{c}}{\partial z} \hat{k}) \end{aligned} \qquad (1.64.b)$$

where E_x, E_y and E_z are the turbulent diffusivities in the principal coordinates **(x,y,z)**, for which the unit vectors are $(\hat{i}, \hat{j}, \hat{k})$.

The vertical stratification in the sea (e.g. near the thermocline) has an inhibiting influence on vertical motion (including the vertical components of turbulent fluctuation velocities **w'**), hence on the vertical turbulent flux $\rho c'w'$, so that typically we expect $E_x, E_y >> E_z$. On the other hand, in the surface mixed layer, vertical mixing is very efficient due to wind stirring and therefore it can be assumed reasonably that $E_z >> E_x, E_y$. In open sea conditions it is natural to approximate $E_x = E_y = E_H$, i.e. horizontally isotropic turbulent diffusion. It has been remarked earlier that the x and y coordinates are assumed to coincide with the principal axes since the horizontal axes can be rotated to align with these axes without loss of generality. Near a coastal boundary it is often found that the offshore component of diffusivity is more important than the alongshore component $E_x >> E_y$ (with y axis aligned with the coast). In the general case when the referenced coordinates do not coincide with the principal axes, the general non-isotropic form (1.63) must be used.

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(1.68) may not often be appropriate. This is a consequence of the probabilty distribution of different length and time scales embodied in the turbulence field. At initial stages of the spreading, the material will be redistributed mainly by small scale eddies, and therefore diffuse at a relatively slower rate. On the other hand, as the patch size grows, larger eddies will begin to influence it, and distribute the material in a more efficient way. It is therefore reasonable to expect that the diffusivity increases with time or proportionally with the size of the cloud.

In addition, due to the random nature of the process, each realization of the ensemble will appear in an irregular form and will be different from other possible realizations as shown in Fig.s 1.1.a,b. The irregularities are only smoothed out if take the ensemble average of the process with respect to fixed coordinates and at the same time intervals after the release; then the constant concentration surfaces will be circular as shown in Fig. 1.1.c (i.e. if the medium is isotropic). On the other hand, the center of mass of the diffusing cloud of each realization may be shifted randomly with respect to the ensemble mean center of mass, due to the influence of eddies that are larger than the cloud size (*meandering*) as shown in the first two figures. If the ensemble averages were to be taken by shifting the origin to the instantaneous center of mass of each realization, then the average cloud would look smaller than that in fixed coordinates as shown in Fig.1.1.d, for then we extract the influence of meandering (Fischer *et al.*, 1979). Note that in fact, during the initial stages of development, diffusion by small scale eddies, and advection by large scale eddies are inseparable, making the definition of turbulent diffusion somewhat arbitrary.

FIGURE 1.1 Turbulent diffusion from a small source. (a,b) Random spread of two identical clouds, (c) Spread of the ensemble mean, (d) Spred of the ensemble mean obtained by shifting the origin to the centeroid of each realization. (After Fischer *et al.*,1979).

The *apparent diffusion* is that corresponding to Fig. 1.1.c, and we should in principle use the apparent turbulent diffusivity in the turbulent diffusion equation. On the other hand, it is more convenient to obtain the *relative diffusivity* through experiments, i.e. that corresponding to Fig. 1.1.d, since individual clouds can be averaged irrespective of their relative positions.

A good measure of the spreading of a cloud can be obtained by calculating its variance (i.e. the normalized second moment of the concentration distribution), defined as

$$\sigma_s{}^2 = \frac{\int_{-\infty}^{+\infty} cs^2 \, ds}{\int_{-\infty}^{+\infty} c \, ds} \tag{1.69}$$

where c is the ensemble mean concentration and s stands for any of the coordinates (x,y,z) measured from the centroid of the cloud, and therefore σ_x, σ_y, σ_z are in essence the lenth scales (standard deviations) of the diffusing cloud. It can be verified, through multiplication of equation (1.65) with x^2, y^2, z^2 respectively and through integration by parts that

$$E_s = - \frac{d\sigma_s{}^2}{dt} \tag{1.70}$$

for each of the coordinates s = x,y,z, i.e. the turbulent diffusivities are proportional to the rate of spreading.

The transformation between the ensemble mean values in fixed coordinates and those obtained by coinciding the centroids of different realizations is then obtained from (Csanady, 1973)

$$\sigma_s{}^2 = \sigma_{\hat{s}}{}^2 + m_s{}^2 \tag{1.71}$$

where $\hat{s}$ refers to the coordinates with respect to the centroid in each relization and $m_s{}^2$ represents the variance due to the meandering.

For sufficiently long time after the injection (i.e. after the scale of diffusion becomes larger than the largest eddy sizes) $m_s{}^2$ becomes constant, so that it does not contribute to the diffusivities in (1.70). The time required for this to happen is typically the *Lagrangian time scale* (Fischer *et al.*, 1979).

For time larger than the Lagrangian time scale, the diffusivities are constant (i.e. the variance increases linearly with time in 1.70), and the solution of (1.65) with constant coefficients is appropriate in this case. On the other hand, for initial time after the release of a small patch, this approach is not valid as demonstrated above, for then the diffusion is proportional to eddy sizes. Fischer *et al.* (1979) show that in this case the Fickian diffusion equation (1.65) is valid with respect to relative coordinates.

shifted to the instantaneous center of mass of the cloud, provided that the diffusivities are prescribed as

$$E = \frac{1}{2}\frac{d\sigma^2}{dt} = \alpha\ \sigma^{4/3} \ . \qquad (1.72)$$

This *"4/3 Law"* has experimentally been shown (Okubo, 1974) to apply to a wide range of diffusion problems (see Fig. 1.2); it simply states that the diffusivity increases as a power of the cloud size.

Variations to the thoery arising due to the consideration of eddy sizes, their stochastic bases and relation to statistical theory are discussed and interpreted with considerably more latitude in Csanady (1973) and Fischer *et al.* (1979), which are some of the best references among the various literature on the subject.

In the following sections, we will mainly consider the cases in which the diffusivities are assumed to be constant. The corresponding solutions, considering eddy diffusivity variations at initial stages of diffusion have also been investigated by a number of authors and can be found in various expedient books on the subject.

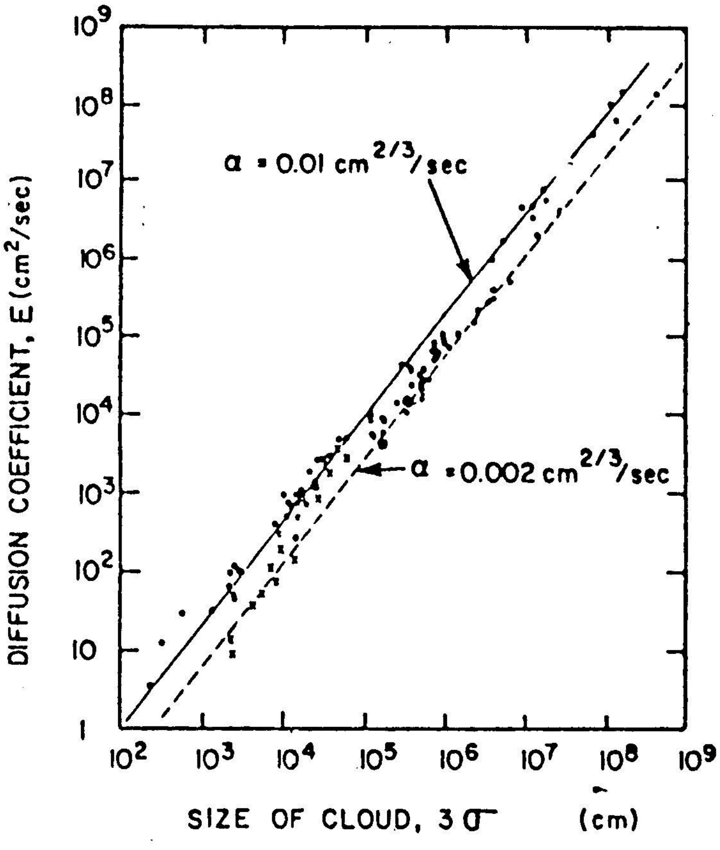

FIGURE 1.2 The turbulent diffusion coefficient as a function of patch size (After Okubo, 1974).

2. SIMPLE MODELS OF TURBULENT DIFFUSION AND TRANSPORT

In this Section, the convective diffusion equation developed above will be solved under different initial and boundary conditions corresponding to typical simple situations that may be encountered in the environment. Although the real processes in the ocean can be more complex mainly due to the physical prescription of the yet undetermined turbulent diffusivity coefficients, these simple solutions will serve to illustrate the basic mechanics of diffusion. These classical solutions can be found in a number of basic references, including Csanady (1973) and Harleman (1970). They have also been developed in conjunction with the familiar heat diffusion problems.

Even with the Fickian flux and other approximations involved in the derivations, equation (1.68) is in general not very easy to solve under general flow situations, often due to the variable coefficients introduced by the velocity field **u**. For a given flow situation, the velocity field **u(x,t)** is obtained by solving the equations of motion governing the hydrodynamics, and then a solution to (1.68) is seeked by substituting these variable coefficients in the turbulent diffusion equation. An alternative approach is to lump the variability of the velocity field into the turbulent diffusivity coefficients which already involve a number of simplifications in parameterizing the turbulence. As to be shown later (Section 3), this is the essence of *dispersion* formulations (as opposed to diffusion), which are based on such an incorporation of the velocity gradients into the modified diffusive terms.

When the fluid is at rest, the convective diffusion equation reduces to the form representing diffusion in a solid such as that occurs for heat conduction in solids. In this case, the form of the equation remains the same irrespective of the magnitude of the diffusivities; and the equation for molecular diffusion (1.56) can in fact be recovered by letting $E_x=E_y=E_z=D$ in equation (1.68).

We set out to investigate a simple class of problems in which the velocity field is uniform (constant) with speed **U** arbitrarily selected to be aligned with the x-axis. This case is equivalent to the diffusion in a solid (except that the diffusivities can now be linked to turbulence) with the implication that the whole process is viewed by an observer fixed with respect to the uniform bodily motion of the fluid (as will be shown briefly, this difference can in fact be accounted for with a suitable transformation of coordinates). In addition, we will assume homogeneous, non-isotropic turbulence and a non-conservative constituent which decays linearly. Namely, we consider the equation

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = E_x\frac{\partial^2 c}{\partial x^2} + E_y\frac{\partial^2 c}{\partial y^2} + E_z\frac{\partial^2 c}{\partial z^2} - kc \; . \qquad (2.1)$$

This equation can be put in a much simpler form by appropriate transformations. We define the coordinate transformations

$$X = \left(\frac{E}{E_x}\right)^{1/2}(x-Ut), \quad Y = \left(\frac{E}{E_y}\right)^{1/2}y, \quad Z = \left(\frac{E}{E_z}\right)^{1/2}z,$$

$$T = t, \qquad (2.2.a\ d)$$

so that the total advective rate of change (left hand side of 2.1) becomes

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = \left(\frac{\partial X}{\partial t}\frac{\partial c}{\partial X} + \frac{\partial T}{\partial t}\frac{\partial c}{\partial T}\right) + U\left(\frac{\partial X}{\partial t}\frac{\partial c}{\partial X} + \frac{\partial T}{\partial t}\frac{\partial c}{\partial T}\right)$$

$$= \left(-\left(\frac{E}{E_x}\right)^{1/2}U\frac{\partial c}{\partial X} + \frac{\partial c}{\partial T}\right) + U\left(\left(\frac{E}{E_x}\right)^{1/2}\frac{\partial c}{\partial X}\right)$$

$$= \frac{\partial c}{\partial T}, \qquad (2.3)$$

and the terms on the right hand side are transformed in a similar way as given for the first term below

$$E_x\frac{\partial^2 c}{\partial x^2} = E_x\frac{\partial X}{\partial x}\frac{\partial}{\partial X}\left(\frac{\partial X}{\partial x}\frac{\partial c}{\partial X}\right) = E_x\left(\frac{\partial X}{\partial x}\right)^2\frac{\partial^2 c}{\partial X^2}$$

$$= E\frac{\partial^2 c}{\partial X^2}\ . \qquad (2.4)$$

In equations (2.2.a-c) E was an unknown constant, which we now set equal to

$$E^3 = E_x\ E_y\ E_z \qquad (2.5)$$

i.e. one of the *invariants* of the anisotropic diffusivity tensor. With these transformations we then write equation (2.1) in the following form:

$$\frac{\partial c}{\partial t} = E\left(\frac{\partial^2 c}{\partial X^2} + \frac{\partial^2 c}{\partial Y^2} + \frac{\partial^2 c}{\partial Z^2}\right) - Kc\ . \qquad (2.6)$$

We further make the transformation

$$c = \Phi\ e^{-KT} \qquad (2.7)$$

upon which (2.6) is replaced by

$$\frac{\partial \Phi}{\partial T} = E\left(\frac{\partial^2 \Phi}{\partial X^2} + \frac{\partial^2 \Phi}{\partial Y^2} + \frac{\partial^2 \Phi}{\partial Z^2}\right)\ . \qquad (2.8)$$

This form of the equation in transformed variables is equivalent to the diffusion equation for a conservative substance in an isotropic field at rest. On the other hand, this equation is the familiar heat equation equivalently modelling heat conduction in an isotropic solid, for which the classical theory provides various solutions (e.g. Carslaw and Jaeger, 1959). We can in principle develop these classical solutions for (2.8), and back transform them by substituting (2.2.a-d), (2.5) and (2.7) to obtain solutions for (2.1).

We next consider the basic solution to the diffusion equation for a point source initial condition, and show how other solutions are developed from this basic solution.

2.1 THE BASIC SOLUTION TO DIFFUSION EQUATION (INSTANTANEOUS POINT SOURCE)

Consider the simple diffusion equation (isotropic conservative diffusion, stationary fluid)

$$\frac{\partial c}{\partial t} = E\, \nabla^2 c \; . \qquad (2.9)$$

We want to investigate the simple symmetric diffusion pattern in the case of an instantaneous point source, i.e. of some material injected at the point $\mathbf{x} = \mathbf{x}' = (x',y',z')$ released at some initial instant $t = 0$. We seek the solution to (2.9) with the initial condition

$$\begin{aligned} c(\mathbf{x},0) &= \frac{M}{\rho}\, \delta(x-x')\; \delta(y-y')\; \delta(z-z') \\ &= \frac{M}{\rho}\, \delta(\mathbf{x}-\mathbf{x}') \end{aligned} \qquad (2.10)$$

where M is the total mass of the substance introduced and ρ is the density of the mixture, which for all practical purposes can be taken as the density of the receiving fluid. Here $\delta(\mathbf{x}-\mathbf{x}')$ is the *Dirac delta "function"* with the important properties of

$$\begin{aligned} &\int_{-\infty}^{+\infty} \delta(x)\, dx = 1 \\ &\int_{-\infty}^{+\infty} F(x')\delta(x-x')dx = F(x) \\ &\int_{-\infty}^{+\infty} e^{iKx}\, dK = 2\pi\, \delta(x) \; . \end{aligned} \qquad (2.11.a\text{-}c)$$

The delta function was introduced by the well known physicist Dirac in 1926, but it was later shown by Schwartz in 1950 not to be a "function", but rather a *generalized function* or *functional*, i.e. a set of functions which in some limiting case approach zero everywhere except at the relative origin

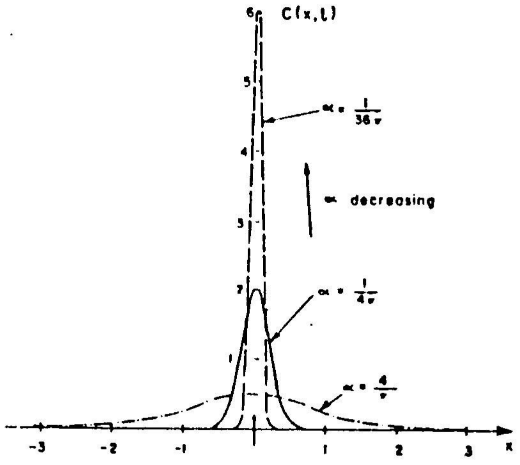

FIGURE 2.1 $f_\alpha(x)=(\alpha\pi)^{-1/2}\exp[-(x)^2/\alpha]$, the set of functions which reduce to the delta function as $\alpha \to 0$.

$x=x'$, where its value becomes infinite. We can visualize a set of functions which monotonously decay away from the relative origin, such as in the case of the set constructed from $f_\alpha(x) = (\alpha\pi)^{-1/2}\exp[-(x-x')^2/\alpha]$ with varying values of α, as shown in Fig. 2.1. As $\alpha \to 0$, the peak at $x=x'$ becomes narrower and increases in height, approaching $\delta(x-x')$ in the limit.

The first property (2.11.a) of the delta function requires that the area under its curve be unity, the second (2.11.b) requires that its integral product with another function evaluates to the value of that function at the relative origin. The third property (2.11.c) states that it is the Fourier transform of unity.

If we integrate (2.10) in an infinite volume V_∞ enclosing the instantaneous source, we obtain from (2.11.a)

$$\int_{V_\infty} \rho c(x,0)\,dV = M\iiint_{-\infty}^{+\infty}\delta(x-x')\,\delta(y-y')\,\delta(z-z')\,dx\,dy\,dz = M \qquad (2.12)$$

yielding the mass of the substance introduced, in agreement with the definition of concentration (1.40.a).

Since the source is located at an infinitely small point, the solution to (2.9) is expected to be radially symmetric. Writing (2.9) in the spherical coordinates $(r,\ \theta,\ \Phi)$ centered at the relative origin of the source and dropping the azimuthal and zonal terms (due to radial symmetry), the equation is

$$\frac{\partial c}{\partial t} = E\,\frac{1}{r^2}\,\frac{\partial}{\partial r}\,r^2\,\frac{\partial c}{\partial r}\,. \qquad (2.13)$$

where $r^2 = (x-x')^2+(y-y')^2+(z-z')^2$. The solution to (2.13) with the initial condition (2.10) can be obtained through various techniques, including Laplace transforms (Carslaw and Jaeger, 1959), or similarity transforms as will be presented here. We assume the solution is self-similar with the form

$$c = \zeta^{-m} f(\eta) \tag{2.14}$$

in the transformed coordinates

$$\eta = \frac{r^2}{4Et} , \qquad \zeta = 4Et . \tag{2.15}$$

The transformation to the original variables are

$$r = (\eta\zeta)^{1/2} , \quad t = \zeta/(4E) , \tag{2.16.a,b}$$

and the corresponding cross-derivatives are

$$\begin{aligned} \frac{\partial \zeta}{\partial t} &= 4E , \qquad \frac{\partial \nu}{\partial t} = - \frac{r^2}{4Et^2} = - 4E \frac{\eta}{\zeta} , \\ \frac{\partial \zeta}{\partial r} &= 0 , \qquad \frac{\partial \eta}{\partial r} = \frac{2r}{4Et} = 2 \frac{\eta}{r} = 2(\frac{\eta}{\zeta})^{1/2}, . \end{aligned} \tag{2.17.a-d}$$

The individual terms in (1.85) are then calculated as

$$\begin{aligned} \frac{\partial c}{\partial t} &= \frac{\partial c}{\partial \zeta} \frac{\partial \zeta}{\partial t} + \frac{\partial c}{\partial \eta} \frac{\partial \eta}{\partial t} \\ &= - 4E\zeta^{-m-1} (\eta f_\eta + mf) \end{aligned} \tag{2.18}$$

and

$$\begin{aligned} \frac{1}{r^2} \frac{\partial c}{\partial r} (r^2 \frac{\partial c}{\partial r}) &= \eta^{-1}\zeta^{-1} \frac{\partial \eta}{\partial r} \frac{\partial}{\partial \eta} (\eta\zeta \frac{\partial \eta}{\partial r} \frac{\partial c}{\partial \eta}) \\ &= 4 \eta^{-1/2}\zeta^{-3/2} \frac{\partial}{\partial \eta} (\eta^{3/2}\zeta^{1/2}\zeta^{-m} \frac{\partial f}{\partial \eta}) \\ &= 4 \zeta^{-m-1} (\eta f_{\eta\eta} + \frac{3}{2} f_\eta) \end{aligned} \tag{2.19}$$

where subscripts denote differentiation with respect to the transformed variable η.

With these substitutions we transform the partial differential equation (1.85) into the ordinary differential equation

$$\eta (f_{\eta\eta} + f_\eta) + (\frac{3}{2} f_\eta + mf) = 0 \tag{2.20}$$

This equation is of second order, and general solutions can be obtained in series expansions. However, it is obvious that we can only obtain a similarity solution if we select the yet undetermined exponent in (2.14) as $m=3/2$. Then, by letting

$$g = f_\eta + f \qquad (2.21)$$

(1.92) becomes

$$\eta\, g_\eta + \frac{3}{2}\, g = 0\ , \qquad (2.22)$$

which directly integrates to

$$g = A\, \eta^{-3/2} \qquad (2.23)$$

or

$$f_\eta + f = A\, \eta^{-3/2}\ . \qquad (2.24)$$

This last equation can be reintegrated with use of integration factors as follows

$$f = B\, e^{-\eta} + A\, e^{-\eta} \int \eta^{-3/2}\, e^{\eta}\, d\eta, \qquad (2.25)$$

where the first term represents the homogeneous solution and the second term is the particular solution.

Inspecting this solution for small values of $\eta = r^2/(4Et)$ (i.e. as $t \rightarrow \infty$), it can be seen that the particular solution (the second term) is a growing solution with a trend of $\eta^{-3/2}$ or $t^{3/2}$. Since the initial concentration should decay with time through diffusion in the medium, this solution can not be accepted and therefore we set $A = 0$. The remaining solution is

$$c = \frac{B}{(4Et)^{3/2}} \exp\left(-\frac{r^2}{4Et}\right) \qquad (2.26)$$

The constant B can be evaluated from the initial condition (2.10). In spherical coordinates we have

$$\begin{aligned} \frac{M}{\rho} &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} c(r)\, dr\; r\, d\Phi\; r\sin\Phi\, d\theta \\ &= 4\pi \int_0^{\infty} r^2\, c(r)\, dr \\ &= 4\pi \int_0^{\infty} \eta\zeta\, \frac{f(\eta)}{\zeta^{3/2}}\, \frac{1}{2} \left(\frac{\zeta}{\eta}\right)^{1/2} d\eta \\ &= 2\pi \int_0^{\infty} f(\eta)\, \eta^{1/2}\, d\eta \end{aligned} \qquad (2.27)$$

$$= 2\pi B \int_0^\infty \eta^{1/2} e^{-\eta} d\eta$$

$$= \pi^{3/2} B .$$

Therefore the solution of the problem becomes

$$c(r,t) = \frac{(M/\rho)}{(4\pi Et)^{3/2}} \exp(-\frac{r^2}{4Et}) \qquad (2.28)$$

or writing in Cartesian coordinates

$$c(x,y,z,t) = \frac{(M/\rho)}{(4\pi Et)^{3/2}} \exp-(\frac{(x-x')^2+(y-y')^2+(z-z')^2}{4Et}) . \qquad (2.29)$$

The instantareous point source solution (2.28) decays as $t^{-3/2}$ and goes to zero ewerywhere as $t \longrightarrow \infty$. At any fixed time the solution decays away from the relative origin as $\exp(-ar^2)$ (i.e. the spatial distribution is Gaussian). In fact, the behaviour of the solution can be visualized with the help of Fig. 2.1, replacing α = 4Et. The shape of the function with respect to the radia distance measured from the source (instead of x in Fig. 2.1) is the same for any given time, although the time rate of decrease faster (as $t^{-3/2}$) than that would correspond to Fig. 2.1 (this time dependence is a result of the three-dimensionality of the problem). At any time, the constant concentration surfaces (of say $c=c_0$) are spheres, a cross section of which is shown in Fig. 2.2.a. The volume enclosed by $c=c_0$ is

$$V_0 = \frac{4\pi}{3} (4Et)^{3/2} \ln^{3/2} (\frac{c_{max}}{c_0}) \qquad (2.30)$$

where c_{max} is the concentration value at the center of the diffusing cloud.

The solution in the non-isotropic non-conservative, uniform flow case can be obtained by simply making use of (2.2.a-d), (2.5) and (2.7) as

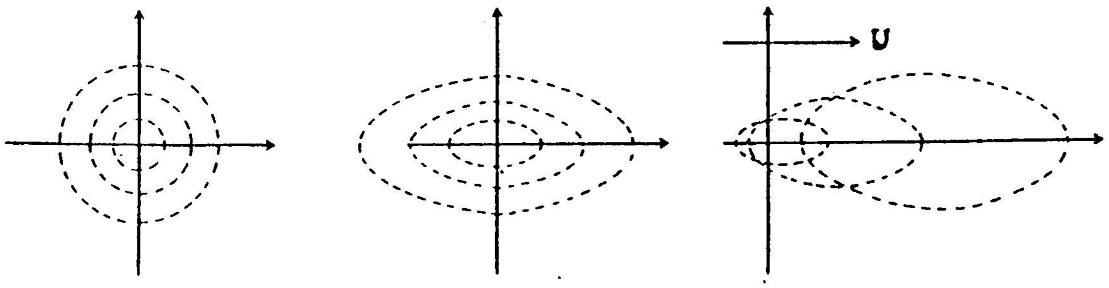

FIGURE 2.2 Diffusion from a point source (a) isotropic, (b) anisotropic cases with respect to relative coordinates, (c) with respect to fixed coordinates.

$$c=\frac{M/\rho}{(4\pi E t)^{3/2}}\exp -\left[\frac{(x-x'-Ut)^2}{4E_x t}+\frac{(y-y')^2}{4E_y t}+\frac{(z-z')^2}{4E_z t}+kt\right] \tag{2.31}$$

where $E^3=E_xE_yE_z$. In this case, the constant concentration surfaces are ellipsoids. With respect to the shifted coordinates the pattern looks like in Fig. 2.2.b, while it is as shown in Fig. 2.2.c seen by a fixed observer.

The variance (cf. equation 1.69) defined with respect to the center of the patch is

$$\sigma_s{}^2=\frac{\int_{-\infty}^{+\infty} c\,\tilde{s}^2\,d\tilde{s}}{\int_{-\infty}^{+\infty} c\,d\tilde{s}} \tag{2.32}$$

where $\tilde{s}$ stands for any of the shifted coordinates $\tilde{x}=x-x'-Ut$ or $\tilde{y}=y-y'$ or $\tilde{z}=z-z'$ in equation (2.31). Noting that

$$\frac{\int_{-\infty}^{+\infty} r^2\exp(-r^2/a)}{\int_{-\infty}^{+\infty}\exp(-r^2/a)}=\frac{(\pi a)^{1/2}\,a/2}{(\pi a)^{1/2}}=a/2 \tag{2.33}$$

(2.32) evaluates to (for each axis)

$$\begin{aligned}\sigma_x &= (2E_x t)^{1/2},\\ \sigma_y &= (2E_y t)^{1/2},\\ \sigma_z &= (2E_z t)^{1/2}\end{aligned} \tag{2.34.a-c}$$

in the case of the instantaneous point source solution (2.31). If the medium is isotropic, the spread is obviously symmetric in all directions with $\sigma=(2Et)^{1/2}$. Note that these results are in agreement with equation (1.70).

2.2 CONSTRUCTION OF ELEMENTARY SOLUTIONS FROM THE BASIC SOLUTION

We can construct other elementary solutions from the basic solution obtained above, through *convolution* operations. For example consider the case of an initial concentration distribution $C(x)$ at $t=0$

$$c(x,0) = C(x) = C(x,y,z) \ . \tag{2.35}$$

Consider the simple diffusion equation (2.9) written as

$$\mathcal{L}(c) = 0 \tag{2.36}$$

where $\mathcal{L}$ represents the diffusion operator

$$\mathcal{L} = \frac{\partial}{\partial t} - E\nabla^2 \ . \tag{2.37}$$

Let $\bar{c}(x',t)$ be the basic solution of (2.33) (or 2.9) for an instantaneous point source $\bar{c}(x,0)=\delta(x-x')\delta(y-y')\delta(z-z')$ disregarding the dimensional coefficient M/ρ in (2.10). The solution to (2.36) with the initial condition (2.35) is constructed as

$$c(x,t) = \iiint_{-\infty}^{+\infty} C(x') \ \bar{c}(x-x',t) \ dx'dy'dz' \tag{2.38}$$

where $\bar{c}$ is (2.29) normalised with M/ρ. The proof is given as follows. Operating on (2.35) yields

$$\mathcal{L}(c) = \iiint_{-\infty}^{+\infty} C(x') \ \mathcal{L}(\bar{c}) \ dx' \ dy' \ dz' = 0 \tag{2.39}$$

since $\mathcal{L}$ operates on x and t only and $\bar{c}$ satisfies (2.36). Evaluating (2.38) at $t=0$, we obtain from (2.10)

$$c(x,0) = \iiint_{-\infty}^{+\infty} C(x') \ \delta(x-x') \ dx' \ dy' \ dz' = C(x) \tag{2.40}$$

by virtue of (2.11.b). The expression in (2.39) is therefore proved to be the solution. The method can be applied to arbitrary initial conditions, examples of which are given below.

2.3 INSTANTANEOUS LINE SOURCE

The concept of using the basic solution to construct other solutions is applied to the diffusion from an *instantaneous line source* with the initial condition

$$c(x,0) = (m'/\rho)\ \delta(x-x'')\ \delta(y-y'') \qquad (2.41)$$

i.e. a point source in two-dimensions, located at $x=(x'',y'')$ with mass m'. Comparing with (2.10), the source strength m' is defined according to

$$m' = M\ \delta(z-z'),$$
$$\int_{-\infty}^{+\infty} m'\ dz = M, \qquad (2.42.a-c)$$
$$m'\ dz = dM,$$

such that m' is distributed along the z-axis, with its total influence conceptually equalling M. Applying (2.38) we obtain

$$c(x,t)=\iiint_{-\infty}^{+\infty} \frac{m'}{\rho(4\pi Et)^{3/2}} \exp-(\frac{\tilde{r}^2}{4Et})\delta(x'-x'')\delta(y'-y'')dx'dy'dz' \qquad (2.43.a)$$

where $\tilde{r}^2 = (x-x')^2+(y-y')^2+(z-z')^2$.
Using (2.11.b) this is reduced to

$$c(x,t) = \int_{-\infty}^{+\infty} \frac{m'}{\rho(4\pi Et)^{3/2}} \exp-(\frac{\hat{r}^2}{4Et})\ dz' \qquad (2.43.b)$$

where $\hat{r}^2 = (x-x'')^2+(y-y'')^2+(z-z')^2$.
Integrating further yields the two-dimensional solution

$$c(x,t) = \frac{m'}{\rho 4\pi Et} \exp-\{\frac{(x-x'')^2+(y-y'')^2}{4Et}\} \qquad (2.44)$$

The solution in the more general case (anisotropic, linear decay and uniform current) is easily obtained through the substitutions (2.2.a-d), (2.5) and (2.7).

An alternative interpretation of the convolution method rests in equations (2.40) and (2.39.b). We are equivalently summing up the influences of a sequence of point sources with strengths dM along the z-axis, to obtain the line souce solution.

Note that the instantaneous line source solution decays as t^{-1} as $t \rightarrow \infty$, at a slower rate compared to the point source solution. At any fixed time the spatial decay of the solution is again Gaussian. At any instant isolines of constant concentration c_0 are circles (ellipses in the anisotropic case) enclosing an area of

$$A_0 = (4\pi Et)\ \ln(c_{max}/c_0) \qquad (2.45)$$

The diffusivity E therefore measures the rate of increase of the influenced region.

A better measure of the spread in each direction is obtained from (2.32) yielding

$$\sigma_x = \sigma_y = (2Et)^{1/2} \qquad (2.46)$$

i.e. the same as in the case of the point source solution

It is worth remarking at this point that (2.44) could also be obtained by directly solving the two-dimensional equivalent of the diffusion equation (2.9), and using the similarity techniques of Section 2.1.

2.4 INSTANTANEOUS PLANE SOURCE

We next consider an *instantaneous plane source*

$$c(x,0) = (m''/\rho)\ \delta(x-x''') \qquad (2.47)$$

where m'' represents the source strength

$$m'' = m'\ \delta(y-y''),$$

$$m''\ dy\ dz = m'\ dz = M \qquad (2.48.a,b)$$

in comparison to (2.38) and (2.10). The solution can again be obtained by the same technique outlined in Section 2.2 as

$$c(x,t) = \iiint_{-\infty}^{+\infty} \frac{m''}{\rho(4\pi Et)^{3/2}} \exp-\left(\frac{\tilde{r}^2}{4Et}\right) \delta(x'-x''')\ dx'\ dy'\ dz' \qquad (2.49.a)$$

where $\tilde{r}^2 = (x-x')^2 + (y-y')^2 + (z-z')^2$.
Then we have

$$c(x,t) = \iint_{-\infty}^{+\infty} \frac{m''}{\rho(4\pi Et)^{3/2}} \exp -\left(\frac{\hat{r}^2}{4Et}\right) dy'\ dz' \qquad (2.49.b)$$

where $\hat{r}^2 = (x-x''')^2 + (y-y')^2 + (z-z')^2$
and making use of (2.43) and (2.47) this reduces to

$$c(x,t) = \int_{-\infty}^{+\infty} \frac{m''}{\rho 4\pi Et} \exp-\left(\frac{(x-x''')^2+(y-y')^2}{4Et}\right) dy' \qquad (2.49.c)$$

from which the solution is obtained as

$$c(x,t) = \frac{m''}{\rho(4\pi Et)^{1/2}} \exp - \frac{(x-x''')^2}{4Et} \qquad (2.50)$$

It can be noted from (2.49.c) that the one dimensional solution (2.50) is a summation of the two dimensional solutions (i.e. line sources along the y-axis. In this case, the solution decays as $t^{-1/2}$ at large times, i.e. slower than the two and three dimensional instantenous sources. The variance for the solution is again $\sigma_x=(2\Gamma t)^{1/2}$.

2. 5 CONTINUOUS POINT SOURCE

We can use the methods outlined above, for constructing solutions for *continuous sources* i.e. sources from which a substance is injected continuously, either for a certain period or for an infinite time. The construction technique of Section 2.2 is applicable in these cases, except that we must now define delta function inputs with respect to time and must sum their influences. However, note that since the time **t** appears in more than one term in the general (non-isotropic, non-conservative moving fluid) basic solution (2.31), we can no longer do the summation on the simplest case of (2.29) and consequently back transform the variables. Instead, we must do the summation directly on the general case (2.31). This will be better understood through the following example.

Consider the *continuous point source*, in which a substance is injected continuously, starting from an initial time $t=t_0$ up to time $t=t_1$, (Fig. 2.3) with a rate of mass injection

$$q = \frac{dM}{dt} . \qquad (2.51)$$

We idealize the situation as a summation of an infinite number of point sources progressing in time, each with a mass injection of **dM** per unit time increment **dτ**. We assume that the source is located at the origin x=y=z=0 for brevity. Then, the solution can be constructed as

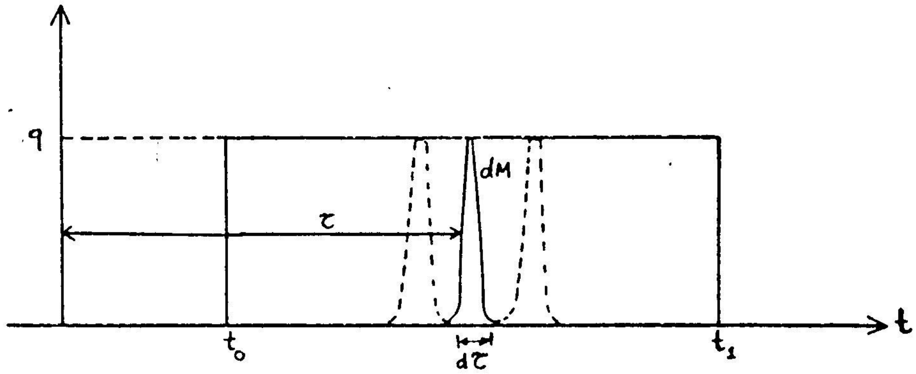

FIGURE 2.3 Idealization of the continuous point source as a series of instantaneous point sources.

$$c = \int_{to}^{t_*} c_1(x,t-\tau)\, dM = \int_{to}^{t_*} q\, c_1(x,t-\tau)\, d\tau \qquad (2.52)$$

where c_1 denotes the solution for the instateneous solution (i.e. equation 2.29) divided by M, and t_* the upper limit of integration in time. If we are interested in the solution for the time interval $t_0<t<t_1$ (*during* continuous injection), we must integrate (2.52) up to $t_*=t$. On the other hand, if we are interested in $t>t_1$ (i.e. *after* the continuous source is stopped) equation (2.52) must be integrated up to $t_*=t_1$. Defining

$$\lambda^2=\frac{E_x}{E_y}y^2, \quad \mu^2=\frac{E_x}{E_z}z^2, \quad E^3=E_xE_yE_z \qquad (2.53)$$

and substituting (2.31) and (2.51), the solution (2.52) is written as

$$c=\int_{to}^{t_*}\frac{q}{\rho[4\pi E(t-\tau)]^{372}}\exp-\frac{[x-U(t-\tau)]^2+\lambda^2+\mu^2}{4E_x(t-\tau)}d\tau \qquad (2.54)$$

Note that a continuous point source with varying injection rate q(t) can also be taken into account by taking $q=q(t-\tau)$ in this equation. With the following definitions of

$$r^2 = x^2+\lambda^2+\mu^2, \qquad \zeta = \frac{r}{2[E_x(t-\tau)]^{372}} \qquad (2.55.a-e)$$

$$\nu = xU/(2E_x), \quad \Omega = (U^2+4KE_x)^{1/2},$$

$$\beta=r\Omega/(4E_x)$$

equation (2.54) can alternatively be written as

$$c=\frac{}{2\rho\pi^{372}}\frac{q\,e^{\nu}}{(E_yE_z)^{372}}\frac{}{r}\int_{\zeta o}^{\zeta_*}\exp-[\zeta^2+\frac{\beta^2}{\zeta^2}]\,d\zeta \qquad (2.56)$$

where $\zeta_0=\zeta(\tau=t_0)$ and $\zeta_*=\zeta(\tau=t_*)$.
Note that in the case $t_*=t$ (i.e. $t<t_1$),
$\zeta_*=\infty$.

In order to integrate (2.56) we define

$$p = \zeta + \frac{\beta}{\zeta}, \qquad q = \zeta - \frac{\beta}{\zeta} \qquad (2.57.a,b)$$

and consequently

$$p^2 - q^2 = 4\beta , \quad \frac{\beta}{\zeta^2} = \frac{p - q}{p + q} \qquad (2.57.c,d)$$

Differentiating (2.57.a,b) gives

$$\frac{dp}{d\zeta} = 2 - \frac{p}{\zeta} = 1 - \frac{\beta}{\zeta^2} = \frac{2q}{p+q},$$

$$\frac{dq}{d\zeta} = 2 - \frac{q}{\zeta} = 1 - \frac{\beta}{\zeta^2} = \frac{2p}{p+q}, \qquad (2.58.a,b)$$

and therefore

$$p\ dp = q\ dq\ . \qquad (2.59)$$

The integrand in (2.56) can be formed into

$$\int \exp -(\zeta^2 + \frac{\beta^2}{\zeta^2})\ d\zeta$$

$$= \frac{1}{2} \int [\exp(-p^2+2\beta)+\exp(-q^2-2\beta)]\ d\zeta \qquad (2.60)$$

and the integral can therefore be expressed alternatively, using (2.58.a,b)

$$\frac{1}{4} \int (\frac{p}{q}+1)\exp(-p^2+2\beta)\ dp + \frac{1}{4} \int (\frac{q}{p}+1)\exp(-q^2+2\beta)\ dq \qquad (2.61)$$

which, with the help of (2.59) and (2.57.c) becomes

$$\frac{1}{2} \int \exp(-p^2+2\beta)\ dp + \frac{1}{2} \int \exp(-q^2-2\beta)\ dq \qquad (2.62)$$

As a result, the solution (2.56) becomes

$$c=\frac{qe^{\nu}}{8\pi\rho(EyEx)^{1/2}r}[e^{+2\beta}(\mathrm{erfc}\ p)\Big|_{p_*}^{p_0}+e^{-2\beta}(\mathrm{erfc}\ q)\Big|_{q_*}^{q_0}] \qquad (2.63)$$

where evaluations are between the limits $p_0=p(\zeta_0)$, $q_0=q(\zeta_0)$, $p_*=p(\zeta_*)$, $q_*=q(\zeta_*)$.

Note that the transient solution (2.63) in the special case U=K=0 (β=0) becomes

$$c = \frac{q}{4\pi\rho(EyEz)^{1/2}r}[\mathrm{erfc}\frac{r}{2[Ex(t-to)]}+\mathrm{erfc}\frac{r}{2[Ex(t-t*)]}] \qquad (2.64.a)$$

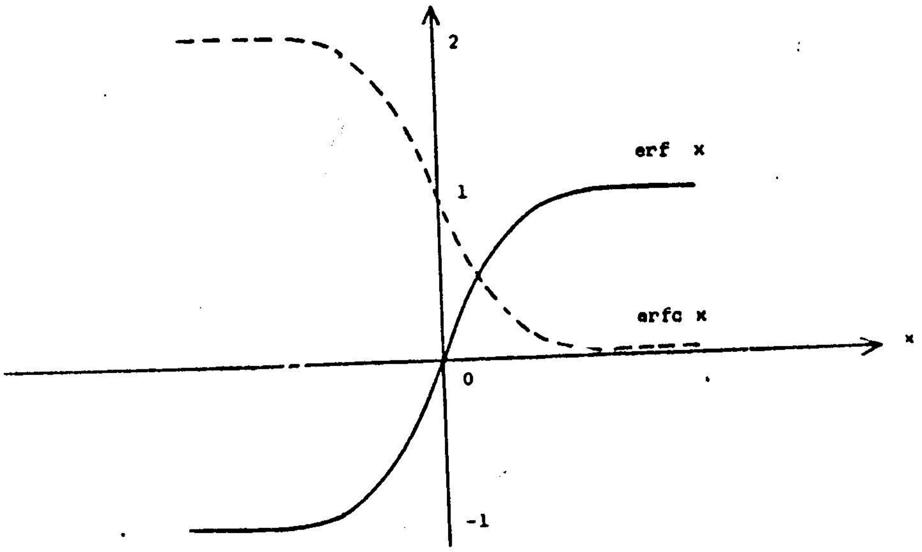

FIGURE 2.4 Error function and complementary error function.

and if $t_0=0$, $t_*=t$, simplifies to

$$c = \frac{q}{4\pi\rho(E_yE_z)^{1/2}r}\,\mathrm{erfc}\left(\frac{r}{2(E_xt)^{1/2}}\right) \qquad (2.64.b)$$

In the above, the *error function* is defined as

$$\mathrm{erf}\ u = \frac{2}{\pi^{1/2}}\int_0^u \exp -s^2\,ds \qquad (2.65.a)$$

and the *complementary error function* as

$$\mathrm{erfc}\ u = 1 - \mathrm{erf}\ u \qquad (2.65.b)$$

which are sketched in Fig. 2.4.

When considering instantaneous sources, we have noted that we could not have any steady solutions, since in these cases we had $c \to 0$ as $t \to \infty$. In the case of continuous injection, it is possible to have a steady solution, which is obtained by letting $t_*=t$, $t_0 \to \infty$ in (2.50). The lower limit of the integral (corresponding to $\tau=t_0$) becomes $\zeta_0=0$ and the upper limit $\zeta_* \to \infty$ in this case, and a definite integral results, yielding the steady state solution

$$c = \frac{q}{\rho 4\pi(E_yE_z)^{1/2}r}\,\exp -[2B-\nu] \qquad (2.66.a)$$

Consider the case K=0, then (2.66.a) becomes

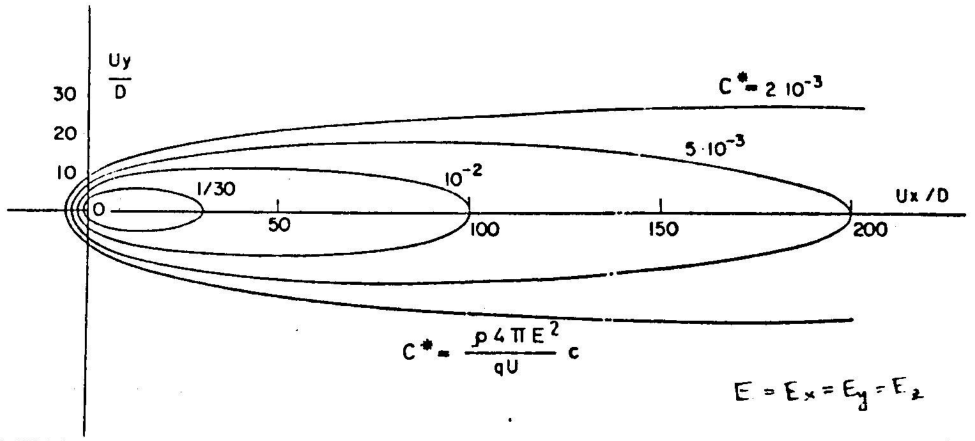

FIGURE 2.5 Solution for a continuous point source (After Csanady, 1973).

$$c = \frac{q}{\rho 4\pi (E_y E_z)^{1/2} r} \exp -\left[\frac{U(r-x)}{2E_x}\right] \qquad (2.66.b)$$

These solutions are shown in Fig 2.5. At long distances away from the origin along the x-axis, i.e. for $x \gg \lambda$ and $x \gg \mu$, we can simplify (2.53.a,b) and (2.55.a) to

$$r = (x^2+\lambda^2+\mu^2) = x\left(1 + \frac{\lambda^2+\mu^2}{x^2}\right) \approx x + \frac{1}{2}\frac{\lambda^2+\mu^2}{x} \qquad (2.67)$$

so that (2.66.b) can be expressed as

$$c = \frac{q}{\rho 4\pi (E_y E_z)^{1/2} x} \exp - \left[\frac{U}{4x}\left(\frac{y^2}{E_y} + \frac{z^2}{E_z}\right)\right] \qquad (2.68)$$

i.e. the distribution becomes two dimensional at large x.

At large distances along the x-axis the solution has *boundary layer* structure, with diffusion occuring transverse to the flow, and negligible diffusion along x. A particle released at the origin is swept to any point x in a time duration of $\tilde{t}=x/U$; which upon substitution into (2.68) yields the familiar (two dimensional) instantaneous line source solution (2.44) with $m'U=q$, $\tilde{t}=t$, in this case the line source being oriented along x. It can be verified that this is equivalent to the solution of the system

$$U\frac{\partial c}{\partial x} = E_y \frac{\partial^2 c}{\partial y^2} + E_z \frac{\partial^2 c}{\partial z^2} \qquad (2.69)$$

i.e. the steady 2-D convective diffusion equation equivalent to the time dependent case with $\tilde{t}=x/U$, and the diffusivity along the x-axis being neglected (the boundary layer approximation).

2.6 CONTINUOUS LINE SOURCE

Solutions for the case of a *continuous line source* aligned with the z-axis (at x=0, y=0) with a time rate of injection

$$q' = \frac{dm'}{d\tau} \qquad (2.70)$$

can be obtained either by summation of continuous point source solutions in space or the summation of instantaneous line source solutions in time. The latter yields an integral form in anology to (2.48) and with the definitions

$$r^2=x^2+\lambda^2, \quad \lambda^2=\frac{E_x}{E_y}y^2, \quad \varepsilon=\Omega^2(t-\tau) \qquad (2.71.a\text{-}c)$$

and ν, Ω, β as defined in (2.55.c-e), the solution is written as (Harleman, 1970)

$$c = \frac{q'e^{\nu}}{4\pi\rho(E_xE_y)^{1/2}} \int_{\varepsilon_*}^{\varepsilon_o} \frac{1}{\varepsilon} \exp -[\varepsilon+\frac{\beta^2}{\varepsilon}]\, d\varepsilon \qquad (2.72)$$

where $\varepsilon_o=\varepsilon(\tau=t_o)$ and $\varepsilon_*=\varepsilon(\tau=t_*)$.
Note that in the case $t_*=t$, $\varepsilon_*=0$.

The steady state solution is obtained by letting $t_o \rightarrow \infty$. In the case $t_*=t$, this is

$$c = \frac{q'e^{\nu}}{2\pi\rho(E_xE_y)^{1/2}} K_o(2\beta) \qquad (2.73)$$

where K_o is the modified Bessel function of the second kind and order zero. For large values of r (i.e. $\beta>>1/2$) we can approximate (2.73) as

$$c = \frac{q'}{4\rho(\pi\beta E_xE_y)^{1/2}} \exp -[2\beta - \nu] \qquad (2.74)$$

2.7 CONTINUOUS PLANE SOURCE

Consider a continuous plane source (an assemblage of continuous line sources or instantaneous plane sources) in the y-z plane positioned at the origin x=0. Let the strength of the source be

$$q'' = \frac{dm''}{dt} . \qquad (2.75)$$

In analogy with the previous Section, the solution is obtained as

$$c = \int_{to}^{t_*} \frac{q''}{\rho(4\pi E_x(t-\tau))} \exp[- \frac{[x-U(t-\tau)]^2}{4E_x(t-\tau)} + k(t-\tau)]\, d\tau \qquad (2.76)$$

or defining

$$r = x, \qquad y = \Omega \left(\frac{t-\tau}{4E_x}\right)^{1/2}$$

and y, Ω, β as in (2.55.c-e) we can write (2.77.a,b)

$$c = \frac{2q''e^{\nu}}{\rho\pi\ \Omega} \int_{y_*}^{y_o} \exp -\left[y^2 + \frac{\beta^2}{y^2}\right] dy \tag{2.78}$$

or in analogy with (2.63) as

$$c = \frac{q''e^{\nu}}{2\rho\Omega}\left[\exp(+2\beta)(\mathrm{erfc}\ p)\Big|_{p_*}^{p_o} + \exp(-2\beta)(\mathrm{erfc}\ q)\Big|_{q_*}^{q_o}\right] \tag{2.79}$$

where p, q, p_o, q_o, p_*, q_* are defined the same way as in (2.57.a,b) replacing ξ by y.

2.8 INFLUENCE OF FINITE SOURCE DIMENSIONS

The influence of finite source dimensions can in principle be accounted for through the superposition techniques outlined above. As an example, we will only consider the case of a finite length instantaneous line source confined in $-h<z<h$ and in the x-y plane (at $x'=0$, $y'=0$). For brevity, we consider the isotropic, conservative non-convective case. In this case the solution (1.115) is modified accordingly, to

$$c = \int_{-h}^{+h} \frac{m'}{\rho(4\pi Et)^{3/2}} \exp - \frac{\hat{r}^2}{4Et}\, dz' \tag{2.80}$$

where $\hat{r}^2 = x^2+y^2+(z-z')^2$. Making the substitutions

$$\mu(z') = \frac{(z-z')}{(4Et)^{1/2}}, \qquad dz' = -(4Et)^{1/2}\, d\mu \tag{2.81.a,b}$$

yields the solution

$$c = \frac{m'}{\rho\pi^{3/2} 4Et} \exp - \frac{x^2+y^2}{4Et} \int_{\mu(+h)}^{\mu(-h)} \exp - \mu^2\, d\mu \tag{2.81.c}$$

$$= \frac{m'}{8\rho\pi Et} \exp - \frac{x^2+y^2}{4Et} \left[\mathrm{erf}\ \frac{z+h}{(4Et)^{1/2}} - \mathrm{erf}\ \frac{z-h}{(4Et)^{1/2}}\right]$$

as the solution. Note that the solution is symmetric about z 0, since erf(-r)=erf(+r).

Other solutions for finite sources of different geometry and time dependence can likewise be obtained through the techniques outlined so far.

2.9 INFLUENCE OF BOUNDARIES

On impervious boundaries the flux must vanish normal to the boundary surface,

$$\hat{n}\cdot\nabla c = 0 \qquad (2.82)$$

where $\hat{n}$ in the unit normal to such a surface.

In some simple cases, it is possible to regard this situation of vanishing gradient at a boundary through superposing mirror images with respect to the boundary of the otherwise unbounded solutions. To illustrate this method consider an instantaneous point source positioned at $y'=z'=0$ and $x=L$ where x is measured perpendicular to a boundary at $x=0$ and in the y,z plane. The solution is

$$c=\frac{M}{\rho(4\pi Et)^{3/2}}\exp-\frac{y^2+z^2}{4Et}\left[\exp-\frac{(x-L)^2}{4Et}+\exp-\frac{(x+L)^2}{4Et}\right] \qquad (2.83)$$

where the second term is due to an image at $x=-L$. Note that the solution is symmetric with respect to $x=0$ and if the source is close to the boundary, the concentration is considerably increased (increased to twice the unbounded solution if $L=0$). In more complicated cases of distributed initial concentrations and multiple boundaries, it is in principle possible to use these superposition techniques, or more convenient mathematical techniques. As an example, we will consider an initial vertical distribution $c_o(z)$ specified in a two dimensional uniform flow with finite depth as shown in Fig 2.6. The initial condition is

$$c(x,z,0) = c_o(z)\ \delta(x) \qquad (2.84)$$

The diffusion pattern is governed by a convective diffusion equation, which, upon transforming the x coordinate as

$$X = x - Ut \qquad (2.85)$$

can be written as

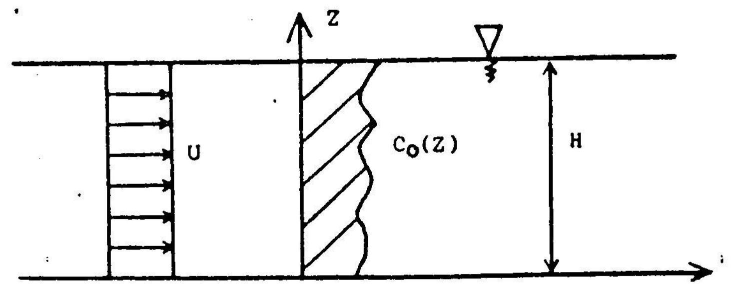

FIGURE 2.6 Diffusion in confined flow

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial z^2} \ . \tag{2.86}$$

The boundary conditions are

$$\frac{\partial c}{\partial z} = 0, \qquad \text{on} \quad z = 0,\ H, \tag{2.87}$$

by virtue of (1.154). A Fourier cosine series solution

$$c = \sum_{n=0}^{\infty} \Phi_n(X,t) \cos \frac{n\pi z}{H} \tag{2.88}$$

is assumed, satisfying the boundary conditions (1.159.a,b). It is left as an exercise to verify that the solution is

$$c = \frac{1}{(4\pi E_x t)^{1/2}} \exp - \frac{(x-Ut)^2}{4E_x t} \sum_{n=0}^{\infty} a_n \exp-(\lambda_n^2 t) \cos \frac{n\pi z}{H} \tag{2.89.a}$$

where

$$\lambda_n^2 = (n\pi/H)^2\ E_z \tag{2.89.b}$$

and

$$a_0 = \frac{1}{H} \int_0^H c_0(z)\ dz, \quad n=0$$

$$a_n = \frac{2}{H} \int_0^H c_0(z) \cos \frac{n\pi z}{H}\ dz, \quad n=1,2,\ldots. \tag{2.89.c,d}$$

Note that each term in the series solution (1.161.a) decays in a time of $T_n = 1/\lambda_n^2 = (H/n\pi)^2/E_z$ approximately, except the term $n=0$, which survives as a dominant term. Therefore, at large time $(t \gg H^2/(\pi^2 E_z))$, the solution is

$$c = \frac{a_0}{(4\pi E_x t)^{1/2}} \exp - \frac{(x-Ut)^2}{4E_x t} \tag{2.90}$$

i.e. uniformly distributed with depth and equivalent to that of an instantaneous plane source with strength $a_0 = m''/\rho$ (cf. equation 1.122).

2.10 INFLUENCE OF VARIABLE DIFFUSION COEFFICENTS

As noted in Section 1.6, the assumption of constant diffusivity is actually inappropriate shortly after the release of a small (as compared to eddy sizes) source. Another reason for variable diffusivities can be the presence of a solid boundary, because near the boundaries the structure of the turbulence is modified and eddies decrease in size. Furthermore, the texture of the boundaries can also be important, since the turbulence field near a flat surface will differ from that near a rough surface. Modifications of the solutions which describe the initial growth stages and diffusion near boundaries have been obtained by various investigators, for example by Joseph and Sendner (1958), and Okubo(1962) in the case of instantaneous line sources, Walters(1962), Sutton(1953) and Smith (1957) in the case of continuous point souces, and Pasquill (1962) n the case of continuous line sources located on solid boundaries.

For these more advenced diffusion theories, the reader can consult Slade(1968), Frenkiel and Munn(1974), Csanady(1973) and Fischer *et al.* (1979).

3. SHEAR FLOW DISPERSION

3.1 INFLUENCE OF VELOCITY SHEAR

We have so far considered uniform velocities. The shear in a velocity profile can have dramatic influences on the diffusion pattern. These effects will first be demonstratad by a simple solution in the case of linear trends in the velocity profile. Okubo and Karweit (1969) considered the velocity profile

$$u = U + \alpha y + \beta z \qquad (3.1)$$

where u represents the x-component of velocity (the other components being zero) and obtained a solution to equation (1.68) for an instataneous point source at x=0, y=0, z=0 at time t=0. The solution obtained by Okubo and Karweit (1969) (after Harleman, 1970) is

$$c = \frac{M}{\rho(4\pi E t)^{3/2}} \exp -\left(\frac{\varepsilon^2}{4E_\varepsilon t} + \frac{y^2}{4E_y t} + \frac{z^2}{4E_z t} + kt\right) \qquad (3.2)$$

where

$$\varepsilon = x - Ut - \frac{1}{2}(\alpha y + \beta z)t, \qquad (3.3.a)$$

$$E_\varepsilon = E_x\,(1 + \Phi^2 t^2) \qquad (3.3.b)$$

$$E^3 = E_\varepsilon E_y E_z \qquad (3.3.c)$$

and

$$\Phi^2 = (\alpha^2 E_y + \beta^2 E_z)/(12E_x) \qquad (3.3.d)$$

It can be seen from the above that shortly after the release $(\Phi t)^2 \ll 1$ the influence of shear is unimportant and the solution is very similar to the case without shear in (1.101). On the other hand, for large time $(\Phi t)^2 \gg 1$, it is noted that the peak concentration decays as $t^{-5/2}$ instead of the $t^{-3/2}$ decay in the case of unsheared flow, i.e. much faster than the uniform flow solution. In effect and by virtue of (3.3.b) the effective diffusivity is considerably increased for large time, due to the elongating influence of shear. Also note that for large time we can approximate (3.3.b) as

$$E_\varepsilon \approx E_x\,(\Phi t)^2 = \frac{1}{2}\frac{\partial \sigma_\varepsilon^2}{\partial t} \qquad (3.4)$$

which yields

$$\sigma_\varepsilon^2 \doteq \frac{2}{3} E_x\,\Phi^2 t^3 \qquad (3.5)$$

and (3.4) can alternatively be expressed as

$$E_\xi \approx \left(\frac{3\Phi}{2E_x}\right)^{2/3} \sigma_\xi^{4/3} \qquad (3.6)$$

which is analogous to the "4/3 Law" (cf. 1.72) for relative diffusion but arises in the much different context of shear flow.

The above example displays the important and convenient result that the effect of shear can be incorporated into "*dispersion coefficients*" in anology to the diffusivities.

In contrast to the shear dispersion in an infinite medium displayed above, the behaviour of the solutions differ considerably when the flow is confined between boundaries. For example in a shallow sea, the flow and the diffusion processes are confined between the bottom and the free surface, where the no flux condition (2.82) applies. The convective-diffusion equation can be averaged in the vertical, and as to be shown briefly, the dipersion of the mean concentration field can be represented in analogy to the Fickian diffusivities. In shear flow the spreading of a patch occurs due to both turbulent diffusion and its distortion due to shear. When the equations are averaged vertically, it is therefore reasonable to expect that the distortion (elongation) due to shear appears equivalent to much increased effective diffusivities.

The following method is based on the early analyses of Taylor (1953, 1954), Aris (1956), Elder (1959), Bowden(1965) and Fischer(1967). The formulation of the shallow water equations will closely follow that of Nihoul and Adam(1974). More detailed discussion can be found in Fischer *et al.* (1979). We start with equation (1.68), alternatively written as

$$\frac{\partial c}{\partial t} + \nabla\cdot\vec{u}c + \frac{\partial}{\partial z}wc = \frac{\partial}{\partial z}E_z\frac{\partial c}{\partial z} + T - kc \qquad (3.7)$$

where use has been made of the continuity equation (1.6) and $\nabla=(\partial/\partial x,\ \partial/\partial y)$ and $\vec{u}=(u,\ v)$ stand for the horizontal components of the gradient and the velocity vectors, w is the vertical velocity and T represents the horizontal diffusion terms $T=\nabla\bullet E_H\bullet\nabla c$. We assume that the horizontal velocity and concentration can be separated into vertically averaged and fluctuating (deviation from the vertical average) components

$$\begin{aligned} c &= \bar{c} + c'' \\ \vec{u} &= \bar{\vec{u}} + \vec{u}'' \end{aligned} \qquad (3.8.a,b)$$

where for instance

$$\bar{c} = \frac{1}{H}\int_{-h}^{\eta} c\ dz\ . \qquad (3.9)$$

The free surface and the bottom are respectively defined as $z=\eta$ and $z=-h$, bounding a total depth $H=\eta+h$.
Integrating the continuity equation (1.6) in the vertical yields

$$\frac{\partial H}{\partial t} + \nabla \cdot H\bar{\vec{u}} = 0. \qquad (3.10)$$

Then, integrating (3.7) in the vertical and making use of (3.10), we have

$$\frac{\partial \bar{c}}{\partial t} + \bar{\vec{u}} \cdot \nabla \bar{c} = -\frac{1}{H}\nabla \cdot H\overline{\vec{u}''c''} + \bar{T} - K\bar{c} \qquad (3.11)$$

Subtracting (3.11) from (3.7) gives

$$\begin{aligned} \frac{\partial c''}{\partial t} + \bar{\vec{u}} \cdot \nabla c'' + \vec{u}'' \cdot \nabla c'' + w\frac{\partial c''}{\partial z} + \vec{u}'' \cdot \nabla \bar{c} \\ = \frac{\partial}{\partial z}E_z\frac{\partial c''}{\partial z} + T'' + \frac{1}{H}\nabla \cdot H\overline{\vec{u}''c''} - Kc'' . \end{aligned} \qquad (3.12)$$

We assume $\vec{u}$ (and therefore $\bar{\vec{u}}$ and $\vec{u}''$) are known; equation (3.12) can then be solved for c''. With the correlation $\overline{\vec{u}''c''}$ determined, the dispersion equation (3.11) can then be solved for c, using some simplifying assumptions first introduced by Taylor (1953). Through an order of magnitude analysis it can be shown that the basic balance in (3.12) is

$$\vec{u}'' \cdot \nabla \bar{c} = \frac{\partial}{\partial z}E_z\frac{\partial c''}{\partial z}, \qquad (3.13)$$

which is much easier to integrate.

The basic assumptions are that $c'' \ll c$, $|\vec{u}''| = O(|\bar{\vec{u}}|)$, $w = O(|u''|H/L)$, where H is the depth and L is the horizontal scale. Defining

$$c''/\bar{c} = O(\epsilon), \qquad |\vec{u}''/\bar{\vec{u}}| = O(1)$$
$$w/|\vec{u}''| = O(\mu), \qquad H/L = O(\delta) \qquad (3.14.a\text{-}d)$$

where ϵ, μ, δ are small numbers $\ll O(1)$. The orders of each term (written in the same sequence as 3.12) are

$$\begin{aligned} O(1) + O(1) + O(1) + O(\frac{\mu}{\delta}) + O(\frac{1}{\epsilon}) \\ = O(\frac{E_z}{HU}\frac{1}{\delta}) + O(\frac{E_H}{LU}) + O(1) + O(\frac{KL}{U}), \end{aligned} \qquad (3.15)$$

where U is a velocity scale and E_H stands for the horizontal diffusivites E_x, E_y. Shear dispersion effects obviously become important only when diffusion time scales are comparable with convection time scales i.e. E_z and $E_H = O(HU)$. The decay term $O(KL/U)$ is often small or at most $O(1)$. Therefore the last term on the left of $O(\epsilon^{-1})$ and $O(\delta^{-1})$) dominate, yielding (3.13).

Equation (3.13) can be integrated twice, resulting in

$$c''(z) - c''(0) = \left(\int_{-h}^{z} \frac{1}{E_z} \int_{-h}^{z} \vec{u}''\, dz'\, dz''\right) \bullet \nabla\bar{c} \,. \tag{3.16}$$

Then the dispersive flux term on the right hand side of (3.11) becomes

$$\begin{aligned} S &= -\frac{1}{H} \nabla\bullet\, \overline{H\vec{u}''c''} \\ &= -\frac{1}{H} \nabla\bullet \int_{-h}^{\eta} \vec{u}'' \int_{-h}^{z} \frac{1}{E_z} \int_{-h}^{z''} \vec{u}''\, dz'\, dz'' \bullet\nabla\bar{c}\, dz \\ &= -\frac{1}{H} \frac{\partial}{\partial x_i} \int_{-h}^{\eta} u_i'' \int_{-h}^{z} \frac{1}{E_z} \int_{-h}^{z''} u_j''\, dz' dz'' dz\, \frac{\partial\bar{c}}{\partial x_j}, \end{aligned} \tag{3.17}$$

the last expression being written in indical notation, with x_i for $i=1,2$ representing x and y directions respectively.

Note that the integration of the second term on the left hand side of (3.16) does not contribute to (3.17) since $c''(0)$ is constant.

The form of (3.17) suggests that we can express this term in linear proportion to the local gradients of mean concentration in analogy to the Fickian expression (1.63), i.e.

$$S = \frac{1}{H} \frac{\partial}{\partial x_i} H K_{ij} \frac{\partial\bar{c}}{\partial x_j} \tag{3.18}$$

so that we can write

$$K_{ij} = -\frac{1}{H} \int_{-h}^{\eta} u_i'' \int_{-h}^{z} \frac{1}{E_z} \int_{-h}^{z''} u_j''\, dz'\, dz''\, dz \tag{3.19}$$

where K_{ij} is the horizontal *dispersion tenscr*.

Note that the dispersion terms in (3.18) are generally anistropic, depending on the three dimensional structure cf the integrated velocity components. Making the substitution (3.17) and dropping overbars, equation (3.11) describing the dispersion of vertically averaged concentration c becomes

$$\frac{\partial c}{\partial t} + \vec{u}\bullet\nabla c = \frac{1}{H} \nabla\bullet\, H\hat{\underline{E}}\nabla\bullet c - kc \tag{3.20}$$

where

$$\underline{E} = \hat{E}_{ij} = K_{ij} + E_i \, \delta_{ij} \qquad (3.21)$$

for i=1,2 where K_{ij} is the dispersion tensor, E_i stand for the vertical averages of the horizontal turbulent diffusivities Ex and Ey, and $\hat{E}_{ij}$ is the total dispersion tensor. Note that (3.21) is written with respect to the principle coordinates of the turbulent diffusivities, although in general $\underline{E}=E_{ij}$ is also a tensor, in any general coordinate system.

The turbulent diffusivities were assumed to be constant in the earlier developments. On the other hand, the dispersion coefficients K_{ij} are not constant in general, depending on the variable current distributions, and therefore it is often not possible to write either K_{ij} or $\hat{E}_{ij}$ in principle coordinates, since the orientation of these coordinates are subject to change with horizontal position. We must therefore use the full anisotropic form of (3.20) to investigate dispersion problems in two dimensions.

It is often true in practice that the dispersion coefficients are much larger than the horizontal turbulent diffusion coefficients, since the vertical assymmetries of the current and concentration profiles that are accounted for in (3.19) become predominant. We can therefore expect that $\hat{E}_{ij} \approx K_{ij}$ and neglect the turbulent diffusivity.Note that if the depth variations are small (i.e. $H^{-1}\nabla H \ll L^{-1}$ where L is a horizontal scale) we can write (3.20) as

$$\frac{\partial c}{\partial t} + \vec{u} \bullet \nabla c = \nabla \bullet \hat{\underline{E}} \bullet \nabla c - kc \qquad (3.22)$$

An interesting example of two-dimensional dispersion is discussed by Fischer *et al.* (1979), who idealized the currents on the continental shelf as shown in Fig.3.1.a. The dispersion tensor is evaluated from (3.19) as

$$K = \frac{H^2}{192 E_z} \begin{vmatrix} 8\, U_0^2/5 & 5\, U_0 V_0 \\ 5\, U_0 V_0 & 16\, V_0^2 \end{vmatrix} \qquad (3.23)$$

An example calculation for this case with currents of the order of 5 cm/s is shown in Fig.3.1.b. After five days the concentration released from an instanteneous point source moves along the shelf and is dispersed into an elongated elliptical shape inclined with respect to the shelf area.

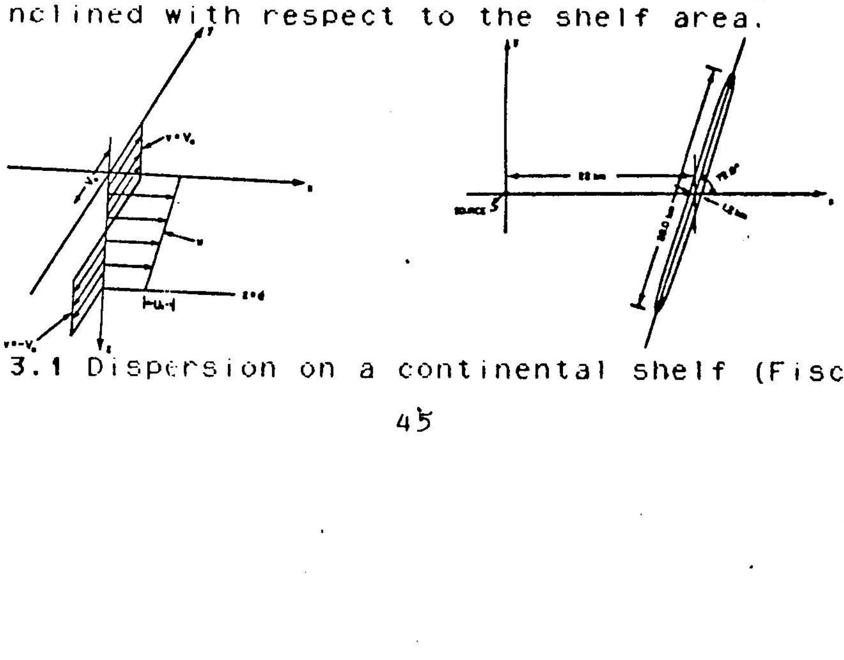

FIGURE 3.1 Dispersion on a continental shelf (Fischer, 1978).

3.2 LONGITUDINAL DISPERSION

If we consider unidirectional steady flows in the x-direction that are bounded in a cross sectional area of A, and neglect the decay term, it can be verified that the corresponding equation (3.20) becomes

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x} A(K_x+\bar{E}_x)\frac{\partial \bar{c}}{\partial x} \qquad (3.24)$$

where u and c are respectively the sectionally averaged velocity and concentration, $\bar{E}_x$ the sectional averaged longitudinal turbulent diffusivity (in the flow direction).

$$K_x = -\frac{1}{A\frac{\partial \bar{c}}{\partial \xi}}\int_A \overline{u''c''}\,dA \qquad (3.25.a)$$

is defined as the *longitudinal dispersion coefficient* where

$$\xi = x - u\,t \qquad (3.25.b)$$

and c" is solved from

$$u''\frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial y} E_y\frac{\partial c''}{\partial y} + \frac{\partial}{\partial z} E_z\frac{\partial c''}{\partial z}\,, \qquad (3.26)$$

in analogy to (3.13).

With this approach, Taylor (1953) solved the dispersion problem for laminar shear flow in a pipe (the diffusion coefficient was taken to represent molecular diffusion). Accordingly, he solved the equivalent of (3.26) written in cylindrical coordinates, determined c" for known laminar velocity profiles in circular tube, then determined the longitudinal dispersion coefficient from (3.25) as

$$K_x = \frac{R^2 u_m^2}{192 D_r} \qquad (3.27)$$

where R is the radius of the tube, u_m the centerline velocity and D_r the radial molecular diffusivity. In his later work, Taylor (1954) extended his analysis to the turbulent shear flow in a pipe. Using the *Reynolds anology*, which states that the transfer of mass, heat, momentum and turbulence are exactly analogous, he was able to relate both concentration and velocity profiles to the turbulent diffusivity, and obtained

$$E_L = K_x + \bar{E}_x = 10.1\,R\,u_* \qquad (3.28)$$

where u_* is the *shear velocity* (defined as $u_* = (\tau/\rho)^{1/2}$, τ being the shear stress).

Note that (3.27) and (3.28) constitute two different ways of writing the dispersion coefficient. The difference implies (considering the turbulent equivalent of (3.27)) that the cross-stream turbulent diffusivity can be expressed as $E_r = \alpha R u_*$, where α is constant. In fact Taylor (1954) obtained (3.28) as $E_L = (10.04+0.06) h u_*$ ($\alpha = 0.06$), showing the negligible contribution of the turbulent diffusivity.

Elder (1959) applied the same technique to two dimensional unidirectional flow with infinitely wide horizontal extent and constant depth h. In this case (3.24) becomes

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = E_L \frac{\partial^2 c}{\partial x^2} , \tag{3.29}$$

where $E_L = K_x + E_x$ and

$$K_x = -\frac{1}{h} \int_{\omega}^{h} u'' \int_0^z \frac{1}{E_z} \int_0^{z''} u'' \, dz' \, dz'' \, dz \tag{3.30}$$

and for a logarithmic velocity profile

$$E_L = 5.93 \, h u_* . \tag{3.31}$$

is obtained. Note that if we use the non-dimensional variables

$$\nu = z/h, \quad \phi = u''/\sigma_u, \quad \epsilon = E_z/\overline{E}_z, \tag{3.32.a-c}$$

where

$$\sigma_u^2 = \overline{u''^2} = \frac{1}{h} \int_0^h u''^2 \, dz,$$

$$\overline{E}_z = \frac{1}{h} \int_0^h E_z \, dz , \tag{3.32.d,e}$$

we can also express (3.30) as

$$K_x = \frac{h^2 \sigma_u^2}{E_z} I \tag{3.33}$$

where

$$I = -\int_0^1 \phi \int_0^{\eta} \frac{1}{\epsilon} \int_0^{\eta''} \phi \, d\eta' \, d\eta'' \, d\eta \tag{3.34}$$

Fischer *at al.* (1979) note that the dimensionless integral I has values of 0.05-0.1 for most practical flows, so that it may suffice to take I=0.1. The rms amplitude of the velocity deviation from the mean is lumped into the parameter σ_u, and E_z is the mean vertical diffusivity in (3.33).

Bowden (1965) considered various velocity and vertical eddy diffusivity distributions and showed that for those cases considered, values of E_L/hu_* (cf. equation 3.29) ranged between 5.9-25. On the other hand, observations in natural water courses of limited width indicated considerably higher values: For example Fischer (1967) reported values of E_L/hu_* in the range 50-700, and to account for the large difference with theory, it was proposed that lateral (transverse) shear effects not considered so far could have caused the disperancy. Fischer(1967) has in fact argued that, since the transverse mixing time scale in wide channels should be larger than the vertical mixing time scales, transverse shear could have a more predominant effect on longitudinal dispersion. This is an apparent paradox, since with increasing widths we do not apparently obtain the case of the infinitely wide channel (the two dimensional case), but has since been resolved through both theory and experiments.

With this motive, Fischer (1967) considered the lateral shear acting on the vertically averaged velocities and first, averaged the velocity distribution vertically as

$$\tilde{u}''(y) = \frac{1}{h(y)} \int_{-h(y)}^{0} u''(y,z)\, dz = \frac{q''(y)}{h(y)} \qquad (3.35)$$

where u'' is the deviation of the velocity field from the cross-sectional average u, and $h(y)$ is the lateral depth variations. By requiring that the T'' terms in equation (1.75) balance the left hand side of (1.76) instead of the vertical diffusion terms, the longitudinal dispersion coefficient is then calculated as

$$E_L = -\frac{1}{A} \int_0^w q''(y) \int_0^y \frac{1}{E_y h(y'')} \int_0^{y''} q''(y')\, dy'\, dy''\, dy \qquad (3.36)$$

where E_y is the transverse eddy diffusivity, w is the width and A the cross-sectional area of the channel.

In actual water courses, there are number of effects modifying dispersion, such as the actual three-dimensional channel cross-sections, secondary flows, channel irregularities etc., so that some empirical judgement enters the dispersion formulations. Considering these effects, Fischer (1975) gives an estimate of the longitudinal dispersion coefficient in analogy to (3.31) as

$$E_L = 0.0011 \frac{\bar{u}^2 w^2}{h u_*} \qquad (3.37)$$

where $\bar{u}$, w, h are the mean velocity, width and depth of the channel and u_* the friction velocity. Reasonable agreement with observations is reported (Fischer *et al.*, 1979).

In laterally confined flows such as in rivers, estuaries and continental shelves, the transverse mixing effects are important and should be taken into consideration.

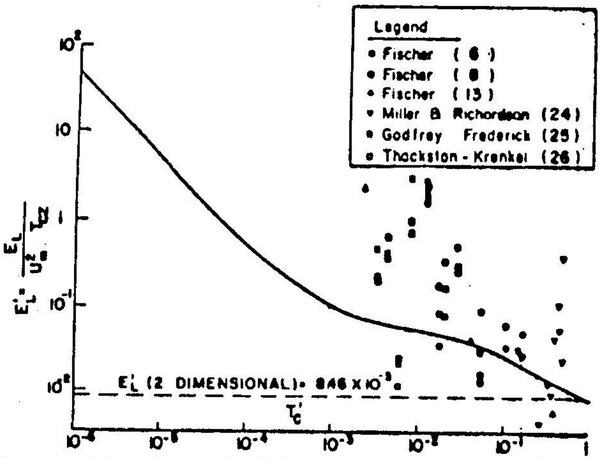

FIGURE 3.2 Longitudinal Dispersion coefficient in a rectangular channel (After Taylor, 1974).

While Fischer's analysis accounting for transverse mixing indicates that these effects can increase the dispersion, it provides little insight into the problem of longitudinal dispersion due to three-dimensional velocity and concentration distributions. Taylor (1974) has considered the turbulent flow constrained by both horizontal and vertical boundaries of rectangular cross-section, and has obtained exact solutions for velocity and concentration distributions, from which the longitudinal dispersion is calculated (from 3.25). Although an oversimplifying assumption of constant turbulent diffusivities has been used, Taylor's(1974) results show increasing dispersion effects for increasing aspect ratios as displayed in Fig. 3.2 . Here, the non-dimesional variables are defined as

$$E_L' = \frac{E_L}{U_m^2 T_{cz}} = \frac{E_L}{U_m^2 h^2/E_z}$$

$$T_c' = \frac{T_{cz}}{T_{cy}} = \frac{h^2/E_z}{w^2/E_y} = \frac{h^2 E_y}{w^2 E_z} \qquad (3.38.a,b)$$

where U_m is the maximum (centerline) velocity, h is the height and w is the width of the channel, and T_{cz} and T_{cy} are respectively the vertical and lateral mixing time scales.

The infinitely wide channel case (two-dimensional flow) is shown by the dotted lines Fig. 3.2 and corresponds to $E_L = 8.46 \times 10^{-3} U_m^2 h^2/E_z$ (which is in analogy to (3.31), but has a different form due to the assumption of constant E_z). Note that the dispersion coefficient for the rectangular section (solid line) does not approach the two-dimensional solution as $w \to \infty$ ($T_c' \to 0$) and in fact differs by a large factor from this case. The three-dimensional problem includes the lateral shear effect, which is present no matter how wide the channel, while the two-dimensional problem has no such effect by definition Comparison with various field and laboratory data indicates the increasing trend with increasing T_c' values, in spite of the different flow geometries and subjective evaluations of the diffusion coefficients.

3.3 DISPERSION IN OSCILLATORY SHEAR FLOW

The analysis of dispersion in oscillatory shear flow is more complex than the steady unidirectional flows considered above, mainly due to two reasons. Firstly, the unsteady and convective terms in (3.12) must be kept in addition to those already appearing in (3.13). Secondly, oscillatory motions create phase lags between concentration and velocity distributions both in space and time. However, assuming a single frequency of oscillation and by averaging the equations both vertically and in time, a mean dispersion coefficient in analogy to Taylor's(1954) hypothesis for unidirectional flows can be defined. The equivalent longitudinal dispersion coefficient for oscillatory flow can be defined as

$$\langle E_L \rangle = \frac{1}{\frac{\partial \bar{c}}{\partial \xi}} \langle \overline{u''c''} \rangle \qquad (3.39.a)$$

where the velocity and concentration are decomposed into vertically averaged and deviational components

$$\begin{aligned} c &= \bar{c}(t) + c''(z,t) \\ u &= \bar{u}(t) + u''(z,t) \end{aligned} \qquad (3.39.b,c)$$

following the notation of the earlier section, and where

$$\xi = x - \int_0^t \bar{u}(t')\,dt' \qquad (3.39.d)$$

represents a coordinate transformation to the time and space averaged center of the patch. The angled brackets imply time averaging

$$\langle X \rangle = \frac{1}{T}\int_0^T X\,dt \qquad (3.39.e)$$

where T is the period of the oscillation.

Bowden (965) investigated the dispersion coefficient in two dimensional oscillatory flow, but because he used equation (3.13) without due concern for the unsteady terms (this is the limit of $T \rightarrow \infty$, i.e. infinitely long period oscillations), he obtained a result that is similar to steady flow. The longitudinal dispersion coefficient found by Bowden is one half the value of the coefficient obtained for steady unidirectional flow with the same velocity shear profile and the same constant vertical eddy diffusivity. The ratio of 1/2 arises because of the phase shift in time between velocity and concentration.

Okubo (1967) investigated the same problem, specifying a shear profile with velocity increasing linearly in the vertical and which has both fluctuating and steady components

$$u = \left(\frac{z}{h}\right) \left(U_o + U \sin \frac{2\pi}{T} t\right) \tag{3.40}$$

where U_O and U are surface velocity amplitudes and T the period of the oscillation. Okubo obtained solutions through Aris' (1956) method of moments, and for this case he expressed the dispersion as a functional representation of

$$\langle E_L \rangle = f(U_o, U, h, T, T_c) \tag{3.41.a}$$

where

$$T_c = h^2/E_z \tag{3.41.b}$$

is the time scale of vertical mixing. He showed that the effects of steady and oscillatory parts of the motion on the longitudinal dispersion are additive (superposed) such that

$$\langle E_L \rangle_t = (E_L)_s + \langle E_L \rangle_o \tag{3.42}$$

where the subscripts t, s and o denote the total, steady and oscillatory contributions respectively. Okubo (1967) obtained two limits for his solution:

$$\langle E_L \rangle_t = \frac{U_o^2 T_c}{120} \left[1 + \frac{120}{4\pi^2} \left(\frac{U\,T}{U_o T_c}\right)^2\right], \text{ for } T \ll T_c$$

and

$$\langle E_L \rangle_t = \frac{U_o^2 T_c}{120} \left[1 + \frac{120}{236} \left(\frac{U}{U_o}\right)^2\right], \text{ for } T \gg T_c \tag{3.43.a,b}$$

When the flow is steady (U=0) the equivalent value is

$$(E_L)_s = \frac{U_o^2 T_c}{120} \tag{3.44}$$

(the solution for this case of steady flow with linear profile can also be found in Fischer *et al.*, 1979, p.85). On the other hand, the oscillatory flow dispersion coefficient in the case of equal amplitudes with the steady case ($U=U_o$) as related to (3.44) are

$$\frac{\langle E_L \rangle_o}{(E_L)_s} = 3.04 \left(\frac{T}{T_c}\right)^2, \text{ for } T \ll T_c, \tag{3.45.a}$$

and

$$\frac{\langle E_L \rangle_o}{(E_L)_s} = 0.51, \qquad \text{for } T \gg T_c\ . \tag{3.45.b}$$

This result indicates that for $T \ll T_c$, the dispersion coefficient is proportional to T^2, whereas for $T \gg T_c$ it is a constant about one half the value of the steady case.

This behaviour is expected, since for long periods of oscillation, the diffusion process is similar to that in steady flow, where an initial patch has sufficient time to diffuse before the flow reverses. On the other hand, in the limit $T \to 0$ (rapid oscillations), the diffusing patch returns to its original position rapidly before any diffusion can take place, and therefore cannot respond to the shear in the velocity profile, making the oscillatory dispersion coefficient vanish in this limit. (A discussion ot these limits is given in Fischer *et al.*, 1979, p.95).

Later, Holley *et al.* (1970) considered the same problem with the linear velocity profile (3.40) (without the steady component, $U_0=0$) and obtained an analytical solution from which they could find an expression for $\langle E_L \rangle$. Their functional form is

$$\langle E_L \rangle = E_0 \; f(T') \qquad (3.46)$$

where

$$T' = T/T_c = T \; E_z/h^2 \qquad (3.47)$$

and

$$E_0 = \frac{U^2 T_c}{240} \qquad (3.48)$$

which is the constant value of $\langle E_L \rangle$ for the limit $T \gg T_c$ (i.e. one half of 3.44). The function (3.46) is shown in Fig.3.3.a, where the ratio $\langle E_L \rangle / E_0$ is plotted against T'. In applying the results to estuaries, Fischer *et al.* (1979, p.235), make an analogy to (3.31), and use some empirical judgement to replace E_0 on the left hand side of (3.46) by

$$\begin{aligned} E_0 &= \alpha \; I \sigma_u{}^2 h^2/E_z \\ &= \alpha \; I \sigma_u{}^2 T \end{aligned} \qquad (3.49)$$

assuming E_0, the limit of (3.46) for $T \gg T_c$, to be proportional to the steady dispersion coefficient. In fact for a linear velocity profile (3.40) it is found that (Fischer, *et al.*, 1979, p.93, Table 4.1)

$$\sigma_u{}^2 = U^2/24 \text{ and } I = 1/10 \qquad (3.50)$$

so that (3.44) results in the case of steady flow. Comparing with (3.48) the proportionality constant is found as $\alpha = 1/2$, and therefore (3.49) reduces to (3.48). It should be noted that in their analogy, Fischer *et al.* (1979) have erroneously omitted this proportionality constant, which should be included. Neverthless, by combining (3.46), (3.49) and (3.50) we obtain

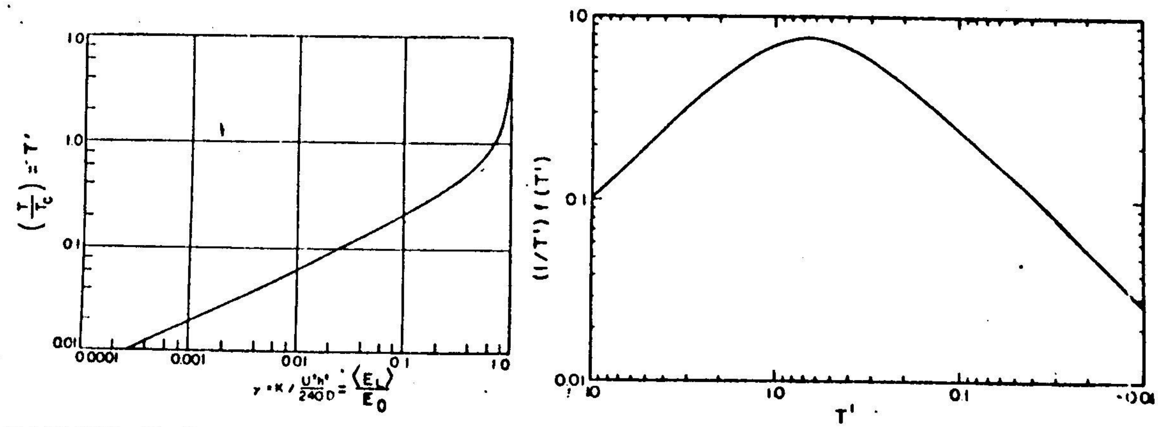

FIGURE 3.3 (a) Oscillatory flow dispersion coefficient, function **f(T')** (Holley *et al.*, 1970), and (b) the normalized function **g(T')** due to Fischer *et al.* (1979).

$$\langle E_L \rangle = \alpha I \sigma_u{}^2 T \, \frac{f(T')}{T'} = \frac{U^2 T}{240} \, \frac{f(T')}{T'} \, , \qquad (3.51)$$

which is in fact the same as (3.46), written differently. Fischer *et al.* (1979) suggest using the first equality in (3.51) empirically for velocity distributions other than the case considered above. For example in a wide and shallow estuary, they suggest using the time scale $T_c = w^2/E_H$ corresponding to lateral mixing, rather than that for vertical mixing, since then the lateral shear is expected to dominate the dispersion. The function $g(T') = (T')^{-1} f(T')$ is shown in Fig. 3.3.b.

In none of the analyses discussed above, it was attempted to solve for the actual velocity distribution in oscillatory flow. It has commonly been accepted that the velocity profile at each instant is the same as an equivalent steady flow. In reality, the velocity distribution is also subject to a convective-diffusion equation of its own, where the turbulent diffusion of momentum in the direction transverse to the flow must be taken into account. In fact, the diffusion of the momentum in oscillatory flow gives rise to *shear waves* in the fluid, just as concentration waves in the case of diffusion equation which propagate in the transverse direction giving causing phase shifts which depend on position in the fluid. These phase shifts are important in the correlations of u'' and c'' in equation (3.39.a).

These influences of simultaneous diffusion of momentum and concentration were accounted for the first time by Taylor (1974), who solved both equations and rigorously constructed the oscillatory longitudinal dispersion coefficient from (3.39.a). In his analyses, Taylor used constant turbulent diffusivity coefficients for both momentum and concentration.

Taylor's (1974) oscillatory flow dispersion coefficient is anologous to (3.51), although the dependence on T' is modified compared to the Holley *et al.* (1970) solution. The results are plotted in Fig.3.4 as a function of T_c and for different values of T. It may be noted that a maximum value of $\langle E_L \rangle$ is obtained for certain values of T_c depending on the period T.

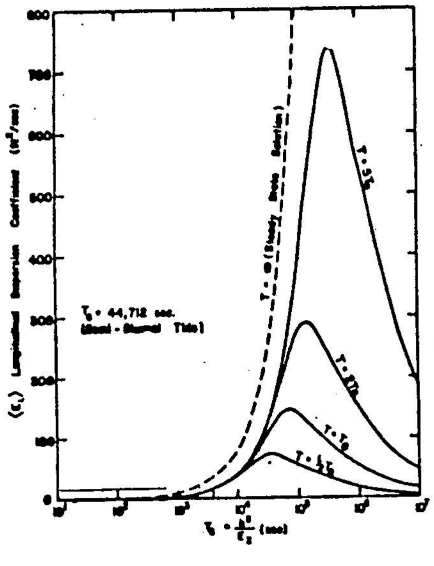

FIGURE 3.4 Oscillatory flow dispersion coefficient for different values of the period T (Taylor, 1974).

Taylor (1974) also showed that it is not appropriate to normalise the oscilatory flow dispersion coefficient with respect to the steady flow dispersion, for they are two different processes. When the variables are normalized as

$$\langle E_L' \rangle = \frac{\langle E_L \rangle}{U^2 T} \quad \text{and } T_z' = (T')^{-1} = \frac{T_c}{T} \qquad (3.52)$$

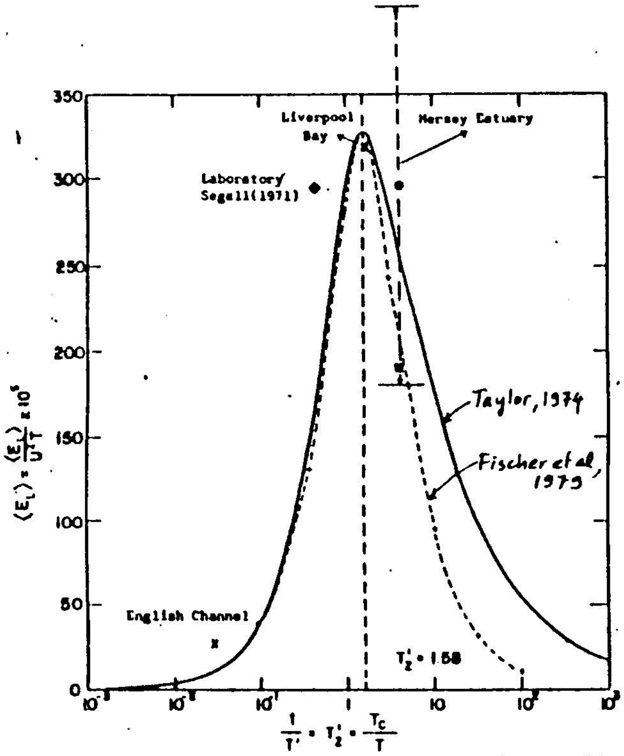

FIGURE 3.5 Normalized oscillatory flow dispersion coefficient (After Taylor, 1974 and Fischer *et al.*, 1979).

a single curve results as shown in Fig 3.5. The maximum dispersion occurs for $T=T_c/1.58=0.63T_c$, i.e. when the oscillation period is of the same order as the transverse mixing time ($T'=0.63$). Experimental verification of the results as obtained by Taylor (1974) are also superposed.

It is quite interesting to plot the empirical formulation of the Fischer *et al.* (1979) based on the solution of Holley *et al.* (1970) in comparison to Taylor's (1974) results, as shown in Fig. 3.5. It is noted that the agreement of the two versions of the oscillatory dispersion coefficient is quite good for $T>T_c$ ($T_z'<1$). On the other hand, the two solutions differ considerably for the range $T<T_c$ ($T_z'>1$), for the phase distribution of concentration and velocity profiles begin to play important roles, which are not accounted for in the former solution.

Taylor (1974) has further considered the oscillating flow in a channel of rectengular cross-section. The main results are the shifting of the period of oscillation for which maximum dispersion occurs and rather small modifications in the functional form displayed in Fig.3.5 for different values of theratio T_{cz}/T_{cy}. Taylor has found that by varying $T_c' \equiv T_{cz}/T_{cy}$ (cf. equation 3.38) in the range 10^{-5} to 1, the peak value of the dispersion cofficient corresponding to Fig. 3.5 changes by about 15 % and the value of $T_z'=1/T'$ at which the peak occurs varies between 1.58 - 4.5.

Oscillatory shear flow dispersion with applications on horizontal mixing in the ocean have been investigated by Young *et al.* (1982). Considering a periodic shear flow velocity

$$u = u_0 \sin(mz) \cos(\omega t) \qquad (3.53)$$

in an infinite domain, they solve for the concentration distribution and obtain a dispersion coefficient

$$\langle E_L \rangle = \frac{1}{4} \left(\frac{u_0^2}{\omega}\right) \left(\frac{\kappa_*}{1+\kappa_*^2}\right) \qquad (3.54.a)$$

where

$$\kappa_* = E_v m^2/\omega \; . \qquad (3.54.b)$$

Since the velocity field is periodic in z, the results can also be interpreted for an equivalent flow between horizontal boundaries placed at $z=0$ and $z=\pi/m$, where the velocities vanish, i.e. a flow with a vertcal extent and oscillation period of

$$h = \pi/m \quad \text{and} \quad T = 2\pi/\omega \qquad (3.55)$$

respectively. The dispersion coefficient in (3.54.a) can then be put into the form

$$\frac{\langle E_L \rangle}{u_0^2 T} = \frac{1}{16} \left(\frac{T'}{1+(\pi T'/2)^2}\right) \qquad (3.56)$$

where $T' = E_v T/h^2 = T/T_c$ as defined in (3.52.b). This solution also gives a maximum value at $T' = 2/\pi = 0.64$ where the value of the function is $\langle E_L \rangle / u_o^2 T = 0.04$. It can be observed that the form of the solution is similar to those presented earlier in Fig.3.5, coinciding better with the functional form of Holley *et al.* (1970), but the magnitude of the calculated values are about one order larger than that plotted in the same figure. This is because the original solution is obtained for unconfined flow, and the characteristic velocity u_o largely differs from that defined earlier for confined flows, the similarity only being established through heuristic arguments.

The important result in the case of infinite domain, just like in the confined flow case, is that two different limits are obtained for oscillatory shear flow dispersion, i.e.

$$\langle E_L \rangle \approx \left(\frac{m u_o}{2\omega}\right)^2 E_z, \quad \text{for } \kappa_* \ll 1 \qquad (3.57.a)$$

and

$$\langle E_L \rangle \approx \left(\frac{u_o}{2m}\right)^2 E_z^{-1}, \quad \text{for } \kappa_* \gg 1. \qquad (3.57.b)$$

The first case corresponds to rapid oscillations with high vertical wavenumber and vanishes in the limit $\kappa_* \to 0$. Young and Rhines (1982) note the similarity of this case to the "Okubo (1967) mechanism". In this limit, the dispersion is directly proportional to E_z. The second case corresponds to long period oscillations and is analogous to Taylor's (1953) initial theory of dispersion for steady flow, where the dispersion effect is inversely proportional to E_z.

Young *et al.* (1982) also construct dispersion coefficients for a random velocity field, from observed and empirical models of the shear spectrum in the ocean. They arrive at the conclusion that shear dispersion by an internal-wave field is dominated by the Okubo (1967) mechanism, rather than the Taylor(1953) mechanism, since they show a dependence on E_z.

The transition from the internal-wave shear dispersion regime to the meso-scale stirring regime caused by eddying motions in the ocean is also discussed by Young *et al.* They find the important result that meso-scale stirring begins influencing the dispersion at horizontal scales as small as 100m.

4. SUSPENDED SEDIMENTS

4.1 TURBULENT DIFFUSION OF SUSPENDED MATTER

In natural water bodies, such as estuaries, rivers, lakes and the ocean, suspended matter is quite common and is often distinguished by its yellowish colour. The terms *suspended matter, suspended solids, suspended sediments, gelbstoff* or *seston* are widely applied to refer to these concentrations of solids which appear in a mixture with water. The concentration of suspended matter is likewise defined as its mass per unit mass of the mixture. Since the concentrations are often smaller than that of the main constituent of water, suspended sediment often does not influence the density of the mixture; so that we can use the approximations (1.55.a-c) in its definition. However, the distinguishing property of suspended matter is that individual particles are often heavier (denser) than water. As a result, they sink in the vertical, characterized by the *settling velocity* w_s, which differs from the vertical velocity w of the fluid particles. In other words, the sediment particles move relative to the fluid in the vertical direction $\hat{k}$. We modify (1.42.a), (1.44) and (1.45) to write

$$\begin{aligned} N_A &= \rho_A\,(\vec{u}_A - w_s\,\hat{k}) \\ &= \rho_A(\vec{u}_A-\vec{u}) + \rho_A(\vec{u}-w_s\hat{k}) \qquad (4.1) \\ &= -D_{AB}\,\nabla\rho_A + \rho_A(\vec{u}-w_s\hat{k}), \end{aligned}$$

where the subscript A now denotes the sediment constituent. The first term describes the diffusive flux and the second term the convective flux. Following the earlier derivations and developing the turbulent equivalents, we arrive at the turbulent diffusion equation

$$\frac{\partial c}{\partial t} + \vec{u}\cdot\nabla c - \frac{\partial w_s c}{\partial z} = \nabla\cdot E\cdot\nabla c - kc \qquad (4.2)$$

in analogy with (1.68). The boundary conditions at a solid boundary are also modified as compared to (2.82). Since the velocity and the flux of material normal to the surface must vanish ($\vec{u}=0$ and $\vec{N}\cdot\hat{n}=0$), in analogy to (4.1) we have

$$(E\cdot\nabla c)\cdot\hat{n} + c\,(w_s\hat{k})\cdot\hat{n} = 0 \qquad (4.3.a)$$

which for a horizontal surface can be expressed as

$$E_z\,\frac{\partial c}{\partial z} + w_s c = 0\,. \qquad (4.3.b)$$

Note that in the above, we have assumed that no sediment can pass across a solid boundary. In free surface flows, (4.3.b) is valid at the surface, if no sediments are input from the atmosphere; or else if atmospheric inputs (such as aeolian dust, or other atmospheric pollutants) are important, we must set the right hand side of (4.3.b) equal to q, where q represents the atmospheric flux of such inputs. On the other hand, in applying (4.3.b) to the bottom boundary, we must account for the bottom deposition loss of sediments. While the flow in the interior is often turbulent, there exists a viscous sub-layer near the boundary. If the size of the settling particles is larger than the thickness of this layer they are reflected from the bottom. On the other hand, particles smaller than the viscous layer thickness tend to stay near the bottom to form a layer of *fluid mud* and are eventually deposited on the bottom. The following bottom boundary condition has therefore been suggested by Sayre (1969) and Jobson and Sayre (1970):

$$E_z \frac{\partial c}{\partial z} + (1-\alpha)w_s c + \gamma q = 0 \qquad (4.3.c)$$

where α represents the probability that a particle settling to the bottom is deposited there, and γq is the average rate of entrainment into the flow, q being the storage at the bed. Sayre (1969) and Jobson and Sayre (1970) have obtained analytical and numerical solutions to the two-dimensional version of equation (4.2) with the surface and bottom boundary conditions (4.3.b,c) respectively, and an initial condition of a vertical line source. The solutions are functions of $\eta=z/h$, $\tau=tE_z/h^2$, α and a settling velocity parameter $\beta=w_s/\kappa u_*$ where $\kappa=0.41$ is Von Karman's constant. The concentration profile becomes time-independent (in the convected coordinates) after an initial time of $\tau>0.5$, and is self similar. Sayre's solutions for $\tau>0.5$, $\beta=1$, $\alpha=0$ and $\alpha=1$ are shown in Fig. 4.1. Jobson and Sayre (1970) verified their solutions with experimental data and found good aggreement irrespective of the particular model used in parameterizing the transverse turbulent mixing.

Later, Sumer (1974) has obtained analytical solutions for the various ranges of parameters, and has shown that some of the special cases reduce to Sayre's solutions.

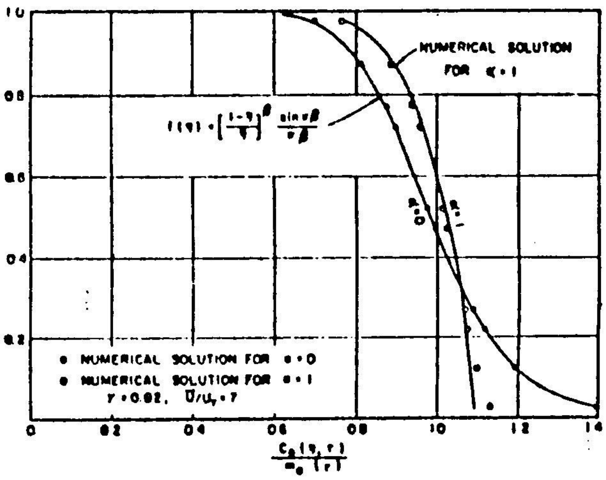

FIGURE 4.1 Vertical distribution of suspended matter for $\beta=0.1$ and at $\tau=0.5$ (After Sayre, 1970).

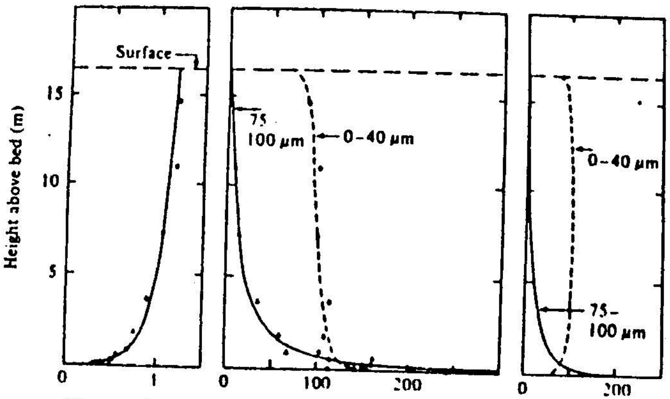

FIGURE 4.2 Profiles of velocity, concentration and flux of suspended sediments in the Thames estuary (After McCave, 1979).

In the above descriptions the settling velocity w_s is a function of sediment density, size and eddy viscosity, empirical values of which can be found in the literature. In situ values can be obtained through methods outlined in McCave (1979). Note, however, that w_s is different for each type of sediment (fine, coarse sand, silt, detritus, organic debris etc.) and separate equations with appropriate values of w_s are required to describe the diffusion of each size fraction. In reality, the settling of sediments in sea water is often influenced by flocculation (combining of small particles into larger aggregates through electrodynamic attraction). The probability of flocculation is a function of particle type, electrolytic strength (i.e. salinity), and velocity shear (Dyer, 1979).

Example measurements of suspended sediment profiles in an estuary are shown in Fig. 4.2. Coarser sediments are usually concentrated near the bottom, whereas fine sediments in suspension are more uniformly distributed in the vertical.

4.2 SHEAR FLOW DISPERSION

Considering the diffusion equation (4.2) in the presence of sediments, and averaging in the vertical following the same methods as in section 3.1, we obtain the two dimensional equation (Nihoul and Adam, 1974)

$$\frac{\partial c}{\partial t} + \vec{u}\cdot\nabla c = \frac{1}{H}\,\nabla\cdot H\hat{E}\cdot\nabla c + Q - Kc \qquad (4.4)$$

where ∇ represents the two dimensional gradient operator as in section 3.1, and

$$Q = \frac{1}{H}\left(E_z\frac{\partial c}{\partial z} + w_s c\right)\Bigg|_{z=-h}^{z=\nu} \qquad (4.5)$$

represents the total flux through the surface and the bottom. Subtracting the averaged equation (4.4) from (4.2) yields the same equation as (3.12) with the addition of the following terms on the right hand side

$$\mathrm{lhs}(3.12) = \mathrm{rhs}(3.12) + w_s \frac{\partial c''}{\partial z} - Q \qquad (4.6)$$

In estimating the dispersion tensor $\hat{E}$, Nihoul and Adam (1974) assume low concentrations of fine sediment and therefore neglect the influence of these terms in (4.6) just like some of the other terms neglected in section 3.1, and use the basic balance in (3.13) to derive the expression for K_{ij} in (3.19). Therefore the dispersion is assumed to be the same as that for neutrally buoyant concentrations.

On the other hand, the settling of suspended matter influences the concentration profiles as shown earlier and produce nonuniform distributions even for sufficiently long times after release. It should therefore be expected that, in general the dispersion coefficient should be a function of settling velocity. Only in the case of weak concentrations of fine suspended sediments, we can assume the dispersion coefficients are not influenced by the negative buoyancy of the sediment. Sayre(1969) and Sumer (1974) have taken the settling terms into account and have calculated the dispersion coefficient in the case of steady, unidirectional flow. The dependence of the dispersion coefficient (normalized with respect to the neutrally buoyant case) on the settling velocity is shown in Fig.4.3. With increasing settling velocity (e.g. sediment size), the dispersion is increased with respect to the neutrally bouyant case.

For completing the description of horizontal dispersion in (4.4), the flux term Q must be specified. This is often done empirically and, neglecting the surface fluxes, Q represents the deposition losses to the bottom or reentrainment from the bottom into the flow. One of the models of practical importance is that given by (4.3.c) and used by Sayre(1969).

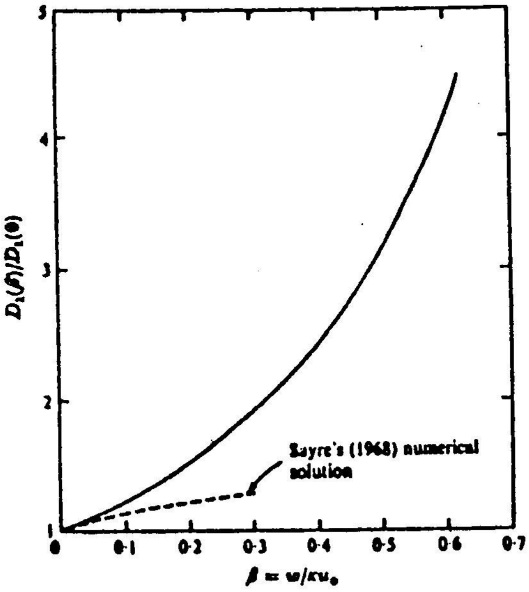

FIGURE 4.3 Longitudinal dispersion coefficient for suspended matter (normalized with respect to neutrally buoyant substances) as a function of β (After Sümer, 1979).

the flux terms for deposition and resuspension are expected to be different, since they are actually different processes. For deposition of cohesive sediments Krone (1962,1976) suggests (after McCave, 1979)

$$Q = - w_s c\ r\ \left(\frac{1-\tau/\tau_c}{1+t/t_c}\right) \qquad (4.7)$$

for $\tau<\tau_c$, where τ is the bed shear stress, τ_c the critical shear stress below which deposition occurs, t the time, t_c the "coagulation time" (the mean time between collisions of particles), and r the mean number of particles in a floc. The value of τ_c is reportedly on the order of 0.4-0.8 dynes/cm^2. This formula is actually of little practical use since the time t from the beginning of flocculation cannot be easily determined in nature. A further complication arises because the settling velocity is a function of concentration; when the sediment concentration is sufficiently high, $w_s=Kc^n$, where **K** and **n** are coefficients depending on sediment type and occasion, with $n=4/3$ suggested by Krone(1962) and $n=1$ or 2 suggested by Owen(1971). For low concentrations of sediments, w_s can often be taken as constant ($n=0$).

When both the rate of flocculation and the sediment concentration are low, the approximations $r=1$ and $t<<t_c$ can be made, upon which (4.7) reduces to

$$Q = - w_s c\ (1 - \tau/\tau_c) \qquad (4.8)$$

This expression explains some of the observed features in estuaries. For example, in many estuaries, a turbidity maximum and a corresponding region of high deposition is found in the mid-reaches of the estuary, where the near-bottom velocities (and bed shear stress) decrease due to opposing effects of river and open sea waters (e.g. near the tip of a salt wedge). In this bottom convergence region, sediment concentration increases and bottom shear vanishes, yielding high deposition rates according to (4.8).

In the case of resuspension of sediments from the bottom (erosion), a different formula applies according to Partheniades (1965)

$$Q = M\ (\tau/\tau_e - 1) \qquad (4.9)$$

where **M** is an erosion rate constant and τ_e the minimum required bed shear stress for erosion to take place.

The above relations are often difficult to use in modelling practice, mainly because they require the switching on and off of the deposition and erosion processes according to situation. Nihoul and Adam (1974) have adopted (4.8) for general modelling application, assuming that it applies for both deposition ($\tau<\tau_c$) and erosion($\tau>\tau_c$), representing it as a reversible process. Replacing $\tau=(\rho f/8)u^2$, where **f** is the Darcy-Weisbach bottom friction coefficient, they write

$$Q = w_s c \left(1 - \frac{u^2}{u_c^2}\right) \qquad (4.10)$$

Note that this source/sink function formulates the deposition/erosion as a completely reversible process, and gives equal rates of both deposition and erosion for the same values of settling velocity, concentration in the water column and flow velocity.

Nihoul and Adam (1974) have used (4.10) in (4.2) to model dispersion and settling of sediments near a dump site in a shallow sea with tidal flows. The mass m of sediments deposited on the bottom are calculated from

$$\frac{\partial m}{\partial t} = Q \; . \qquad (4.11)$$

The convenient form of the source/sink function (4.10) representig erosion and deposition processes at the bottom has been utilized by Özsoy (1977, 1986) to model suspended sediment transport and deposition due to an ebb-tidal jet in the seaward side of a tidal inlet. During the ebbing phase of the tide, the flow issuing from an inlet is in the form of a quasi-steady jet, with pronounced lateral diffusion effects (as compared to longitudinal diffusion). Then, using the velocity distribution in the tidal jet obtained by Özsoy and Ünlüata(1982),

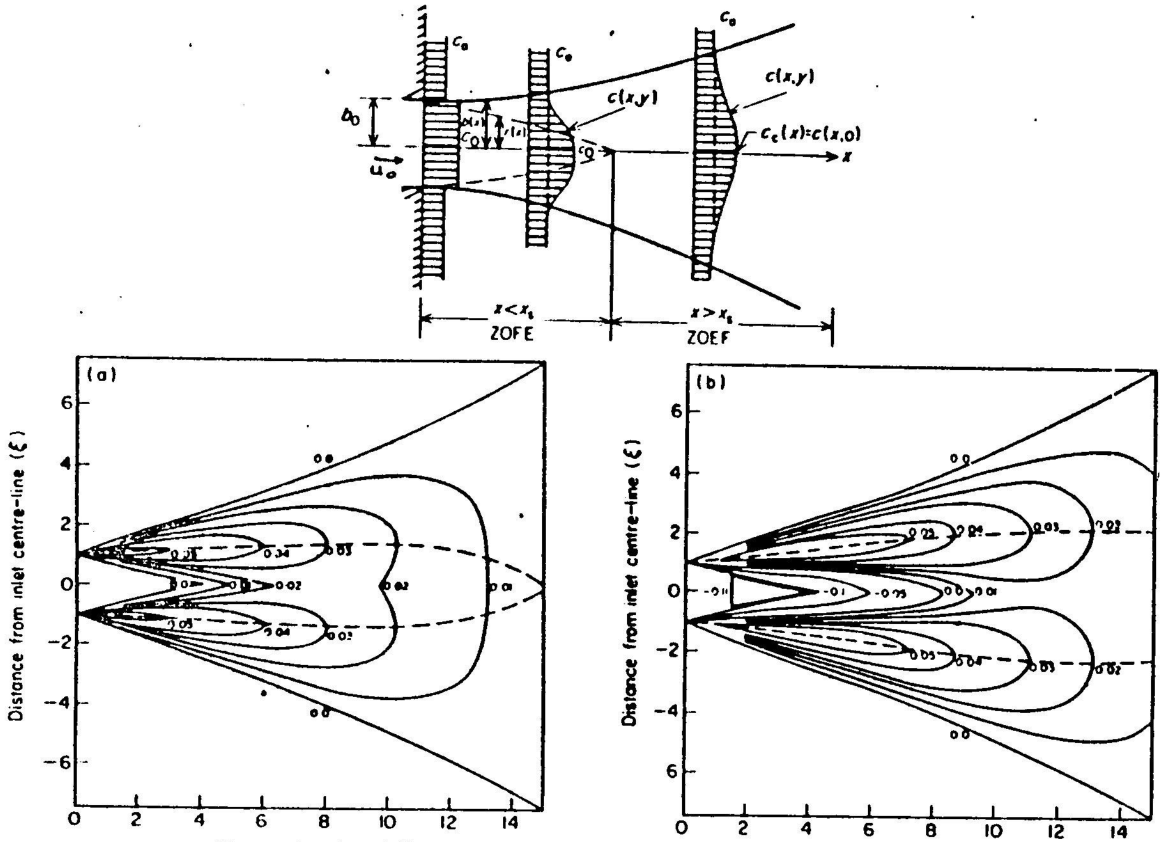

FIGURE 4.4 (a) Jet diffusion, and (b,c) bottom deposition of sediments near a tidal inlet (After Özsoy, 1986).

vertically averaged equations that are analogous to (4.4) and with the deposition and erosion term represented by (4.10) are solved for the horizontal diffusion within a jet (Fig.4.4.a) of either nautrally bouyant concentrations or suspended sediments. Ambient concentrations, lateral entrainment into the jet, depth variations, bottom friction and settling velocity are taken into account. The deposition/erosion rates seaward of the inlet are calculated via (4.11). The contours of bottom deposition rate seaward of the inlet are shown in Fig.4.4.b,c for two illustrative cases. In the first case (Fig.4.4.b), the inlet velocity is critical $u_o=u_c$, so that no deposition takes place at the jet core, where no diffusion or settling occurs. In the diffusion regions of the jet, diffusion and settling processes compete and yield maximum deposition rates at lateral lobes. These lateral lobes extend seaward and join together at some distance, corresponding to the building of transverse bars that are commonly observed near an inlet or estuary mouth. In the second case (Fig. 4.4.c), the inlet velocity exceeds the critical velocity by 40%. ($u_o=1.4u_c$). Erosion occurs at the jet core region, where deep scour holes can often be observed in actual inlets, presumably cut out during peak flows. The lateral lobes have higher deposition rates in this case and are elongated in form, producing evidence that the material eroded at the inlet mouth is deposited in the bar system encircling the mouth. Since the deposition and transport patterns are sensitive to settling velocity and inlet flow velocity, it is concluded that the material in the bars should be highly sorted. These implications on tidal inlet morphology and the applications to related engineering structures, tidal inlets and river deltas are discussed in Özsoy (1986). While the results are not directly applicable to river mouth sedimentation, mainly because of the buoyancy effects in river plumes, the model can be of some use in understanding the nearshore region of river mouths. For example, Wang (1984) has applied Özsoy's model (although without due reference to the original solution provided by Özsoy, 1977) to the dynamics of a river delta, in order to predict delta growth.

Sediment diffusion and dispersion is an emerging field of study which has drawn wide scale and much deserved attention. It must however be stressed that the subject is a complicated one requiring considerable empirical guidance. In addition, many aspects of sediment transport, such as bed-load and its relation to flow parameters and bottom texture have not been described here for they have been considered to be outside of our limited scope.

For further information, an expedient summary of marine sediment transport, its relationships with shelf circulation and implications on morphology can be found in Stanley and Swift (1976). The modelling of sediment transport on the continental shelf requires special attention, considering the specific nature of the circulation and dynamics on the shelf, and the state of the art is in a constantly developing stage, an introduction to which can be found in Smith (1977).

5. ESTUARINE TRANSPORT

5.1 INTRODUCTION

An estuary is a semi-enclosed coastal water body communicating with the sea through a mouth or entrance region and which is diluted considerably by the influence or river runoff in the interior region. Although this definition is quite general, it does not sufficiently describe an estuary, since the physical nature of each estuary differs considerably from another with respect to the varying influences of geometrical shape (depth and area distribution, sand bars, islands, channels, ruggedness of coasts etc.), amount of freshwater inflow, the nature of the restricted exchange at its connection with the sea, the degree of tidal influence etc. In addition to the above, the weather conditions can exert significant influences on estuarine circulation and modify the structure of an estuary considerably. As a result of these varying influences, each estuary has a different personality and the stratification and circulation in one estuary may differ greatly from another, so that only estuaries of the same type can be compared. There has been various attempts to classify estuaries, for example by Pritchard (1967) and Hansen and Rattray (1966), basically utilizing the salinity and the velocity ratios of surface values to mean cross sectional values. Generally, an estuary can be of *salt wedge type*, where fresh water on the surface and sea water at the bottom are sharply separated by a wedge, or *partially mixed type*, where vertical stratification is strong but an interface is not formed, or *well mixed type*, where vertical stratification is small. These classes arise as a result of the physical inputs and the mixing realized in an estuary.

Estuarine processes are quite complicated, due to varying influences of stratification, tidal mixing, wind mixing etc., and a subject of detailed theory in its own right, which can not be discussed in detail in the present scope. However, the general hydrodynamic, thermodynamic and mass conservation laws of Section 1 can, in principle, be applied to estuaries, with further specific assumptions and reductions required. The various aspects of estuarine processes can be found in a number of specialized books such as Ippen (1966), Dyer (1973), Officer (1976), Kjerfve (1978), McDowell and O'Connor (1977), etc.

Our purpose here is not to describe in detail the hydrodynamic and mixing characteristics in estuaries, but rather how these characteristics influence the transport and dispersion of a substance in solution, e.g. a pollutant. On the other hand, the transport processes in an estuary are highly dependent on the hydrodynamic and mixing characteristics, and therefore we venture for a brief rewiew of influencing factors.

5.2 ESTUARINE MIXING

The processes of estuarine mixing will be briefly summarized, following Fischer *et al.* (1979), but keeping the scope much more concise within the present context. Various mechanisms are considered, which are often superposed in real estuaries.

Wind mixing:
Wind drift and mixing is often important in shallow and wide estuaries. The surface stress exerted by the wind constitutes a force at the surface, which is redistributed over the water column through the vertical diffusion of momentum. In salt-wedge type estuaries (two layer stratification), the wind induced driving force influences only the upper layer, and causes entrainment processes at the interface. On the other hand, in well-mixed estuaries, the wind force is distributed over the whole depth, so that it influences shallow regions more than deep regions. A residual wind-induced circulation can therefore be driven in estuaries with large depth variations, which can influence the dispersion patterns (Fischer *et al*, 1979).

Influence of stratification on mixing:
One of the most important factors to be considered in estuaries is the inhibiting influence of stratification on turbulance, and hence on vertical mixing. As compared to the homogeneous cases considered earlier, an extra amount of energy is required for vertical mixing in order to overcome the potential energy of stratification. In estuaries, this energy is derived from boundary and internal shear. One of the various formulas describing the effect of stratification on vertical diffusion is due to Munk and Anderson (1948):

$$E_v = E_o\ (1 + 3.33\ Ri)^{-3/2} \tag{5.1}$$

where E_o is the value in the absence of stratification, and

$$Ri = (g/\rho)\ (\partial\rho/\partial z)/(\partial u/\partial z)^2 \tag{5.2}$$

is the *gradient Richardson Number*, $\rho=\rho(z)$ and $u=u(z)$ being the density and the horizontal velocity respectively. As indicated by (5.1), the vertical diffusivity (of either momentum or concentration) decreases with increasing stratification and increases with increasing vertical shear. Fischer *et al*. (1979), however, caution for indiscriminate use of (5.1) in predicting vertical diffusion, since many other processes that need empirical definition can influence diffusion processes.

In most estuaries, there is an influence of river water entering from the head of the estuary and the sea water entering from the mouth, so that there is both horizontal and vertical stratification. Fischer *et al* (1979) provide a classification of estuaries based on the two parameters of *estuarine Richardson Number* and *densimetric Froude Number*, which incorporate the geometric scales, the fresh water discharge and the density difference between river and sea water. By superposing these two dimensionless parameters on Hansen and Rattray's (1966) classification diagram, they can find the dilution ratio of the salinity in the estuary.

In addition, in an estuary of elongated form, the cross section is often not uniform in the longitudinal direction and depth variations in the transverse direction are important. While the opposing influences of river and sea water generate depth dependent vertical circulation, this circulation is modified by transverse mixing and lateral depth variations. Sumer and Fischer (1977) (after Fischer *et al*, 1979) have made some laboratory investigations with lateral depth variations and vertical stratification in which they have shown that density stratification influences transverse circulation and mixing to a greater extent than vertical mixing. In real estuaries, they expect these influences to play important roles.

Longitudinal Dispersion:
Assuming an estuary with longitudinal variations of cross sectional area **A(x)**, and a flow induced by fresh water inflow $u=Q_f/A$, where Q_f is the river discharge, equation (3.24) derived in section 3 should in principle be applicable to describe the longitudinal dispersion in an estuary, i.e. considering steady flows due to river discharge alone, we have

$$A(x)\frac{\partial c}{\partial t} + Q_f\frac{\partial c}{\partial x} = \frac{\partial}{\partial x} A(x)(K_x+\bar{E}_x)\frac{\partial c}{\partial x} . \qquad (5.3)$$

Here, K_x is the longitudinal dispersion coefficient which must now be evaluated from (3.25) based on the different conditions of stratification, velocity distribution, transverse mixing etc., as summarized above.

In principle, the use of equation (5.3) with appropriate values of the longitudinal dispersion coefficient, should describe the dispersion processes in an estuary. However, as noted above, K_x is modified due to a number of influences. A method often suggested was to obtain K_x from the observed longitudinal salinity distributions, since the cross sectionally averaged salinities also obey (5.3) with the unsteady term omitted for equilibrium conditions, and hence could be used as a tracer. On the other hand, Fischer *et al* (1979) admit that, in spite of the considerable developments in the last 25-30 years since these ideas were suggested, there is still no general predictive method to obtain the dispersion coefficient in estuaries. Nevertheless, equation (5.3) has often been used in estuaries with experimentally determined values of the dispersion coefficients, with examples provided by Officer (1976) and Fischer *et al* (1979).

Tidal dispersion:
In the above sub-sections, the influence of oscillatory shear flows, such as that occurs due to tidal propogation in estuaries have not been considered. In the presence of stratification and residual circulations, such analyses are

tedious and produce little of practical use, although an understanding of various contributions can be reached (cf. Dyer (1973) and Fischer *et al* (1979)).

On the other hand, the longitudinal dispersion in well mixed estuaries due to tidal oscillations alone can be estimated through the methods outlined for oscillatory shear flows in section 3. Fischer *et al* (1979) have taken this route, but considering the dominant influence of transverse mixing have formulated (3.51) such that the transverse mixing time have been used instead of the vertical mixing time. We have already discussed these aspects of the applications in section 3.

Tidal pumping:
The tidal oscillatory flow in estuaries often gives rise to a net steady circulation, which only becomes apparent after averaging the currents over the period of oscillation. These residual circulations arise mainly due to the nonlinear terms in the equations of motion which yield mean currents when averaged: convection and turbulent bottom friction and their interactions with bottom topography. Examples of residual circulations in estuaries are given by Stommel and Farmer (1952), Bowden and Gilligan (1971), Van de Kreeke (1975,1978) etc. These residual circulations contribute effectively to the longitudinal dispersion and exchange processes.

Stommel and Farmer (1952) have considered the residual circulations near the mouth of an estuary. As shown in Fig. 5.1.a, the ebb flow in the estuary is in the form of a sink flow converging towards the mouth, and the volume of water ejected out of the estuary is in the form of a semi-circle. During flood flow, the water entering from the sea can be idealized as a rectangular plug intruding the estuary. If we take a time average covering both phases of the tide, then a residual circulation with two cells on both sides of the centerline will result and therefore only a proportion of material introduced on the ocean side during flood will return to the ocean during ebb-flow. This leads to trapping within the estuary. Stommel and Farmer (1952) applied this concept to the salinity budget in the estuary instead of the mixing of a pollutant, but the concept equally applies to the exchange of a pollutant through an estuary mouth. The residual circulation

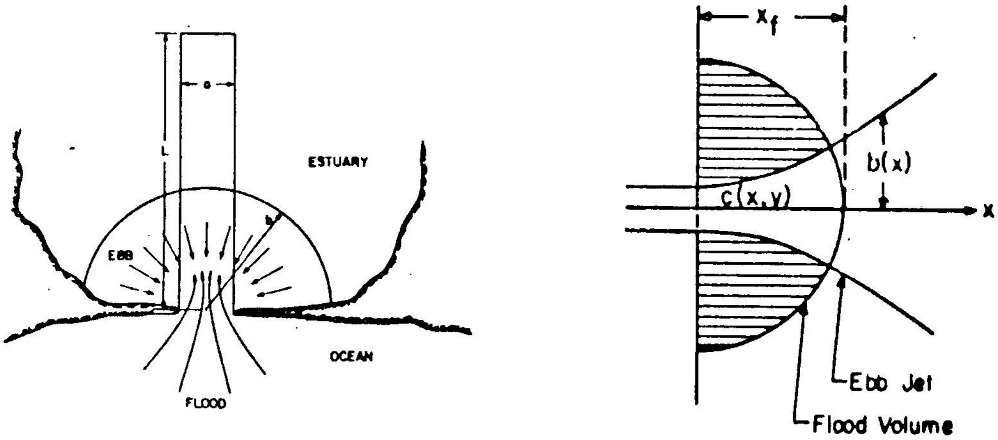

FIGURE 5.1 Idealizations of tidal residual flow near entrances (a) Stommel and Farmer (1952), (b) Ozsoy (1977)

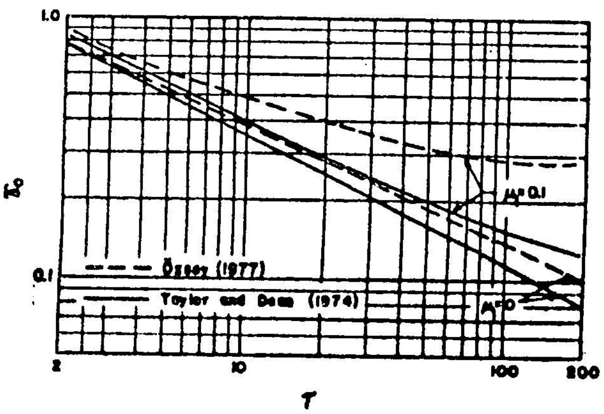

FIGURE 5.2 Ocean mixing coefficient as a function of bottom friction and tidal excursion (After Özsoy, 1977).

represented for the estuary side in Fig. 5.1.a is in fact also valid for the ocean side of the estuary mouth, reversing the roles of flood and ebb (mirror image of Fig.5.1.a with respect to the mouth region).

The flood flow represented in Fig.5.1.a (or alternatively the ebb-flow on the ocean side) is actually in the form of a turbulent jet as shown in Fig.5.1.b, rather than the idealized form of a slug. The hydrodynamic and mass transport characteristics of such jets have been investigated by Özsoy and Ünlüata (1982) and Özsoy (1986), incorparating the influences of lateral entrainment, bottom friction and topography. Therefore, the actual distribution of a pollutant in the jet and its integrated amount within the volume returned during the following sink flow can be determined in detail. An ocean mixing coefficient γ_o, defined as the ratio of the average concentrations passing through the mouth during the respective flood and ebb phases can therefore be defined and calculated as a function of bottom friction, mouth geometry and the ratio $\tau=Tu_o/2b_o$ of the tidal excursion length u_oT to the inlet width $2b_o$ (u_o is the mouth flow velocity, T the period of the tide). The ocean mixing coefficient thus calculated by Özsoy (1977) and Mehta and Özsoy (1978) for the case of constant depth is shown in Fig.5.2 as a function of a bottom friction parameter $\mu=fb_o/8h_o$ (f is the Darcy-Weisbach bottom friction coefficient and h_o is the depth) and the excursion length ratio τ. Taylor and Dean (1974) have considered the same problem earlier, but have found a different expression since they neglect lateral entrainment in the jet, as also shown in Fig.5.2.

These concepts of tidal exchange at an entrance region has been applied to the mixing of a pollutant in a bay with the ocean waters by Özsoy (1977), neglecting any fresh water influences. The tidal flow is idealized as a series of quasi-steady flows (with inlet velocity u_o during ebb and $-u_o$ during flood). The average concentrations at the inlet (entrance) during the ebb and flood flows are related as

$$c_{if}^{n} = \gamma_o \, c_{ie}^{n-1} \tag{5.4}$$

where the subscripts denote i=inlet, f=flood, e=ebb and the superscript n represents the n th tidal cycle starting with flood. The mixing on the bay side is assumed to be more complex due to its confined nature, where it is assumed that

$$c_{ie}^{n} = \gamma_b c_{if}^{n} + (1-\gamma_b) c_{be}^{n-1} \tag{5.5}$$

where b=bay, c_{be} the volume averaged bay concentration during ebb, and γ_b a coefficient describing the bay mixing, and varying in the range (0,1), so that the concentration of the ebb flow at the inlet is always between the values c_{if} and c_{be}, representing the inlet (flood) and bay (previous ebb) concentrations. Considering further the mass balance of the bay during the flood and ebb phases, Özsoy (1977) obtained the recursion formula

$$c_{be}^{n} = A_1 c_{be}^{n-1} + A_2 c_{be}^{n-2} \tag{5.6.a}$$

where

$$A_1 = 1 + \gamma_o \gamma_b - \frac{(1-\gamma_b)K}{(1-K/2)} \tag{5.6.b}$$

$$A_2 = \frac{(1-\gamma_b)\gamma_o(1+K/2)}{(1-K/2)} - \gamma_o \tag{5.6.c}$$

and where

$$K = \Omega/V = 2a_o/h_b \tag{5.6.d}$$

is the ratio of the tidal prism Ω to the mean bay volume V, a_o being the tidal amplitude and h_b the mean depth of the bay.

Özsoy (1977) applied this method to Card Sound in Florida, where a dye injection study had earlier been made by Taylor and Dean (1974). Using numerical values of the parameters and the recursion formula (5.6.a), reasonable estimates of the dye remaining in the bay were obtained, as shown in Fig. 5.3. In the case of no mixing in the bay, it is sufficient to take $\gamma_b=1$; on the other hand, if the bay waters are

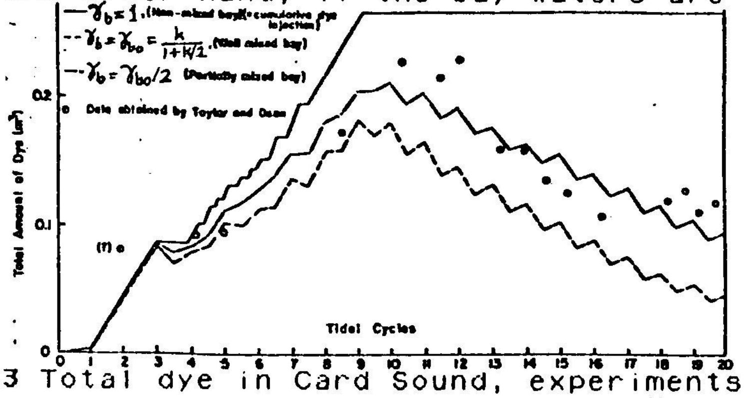

FIGURE 5.3 Total dye in Card Sound, experiments done by Taylor and Dean (1974), and calculated by Özsoy (1977)

completely mixed with the incoming tidal waters during flood, it is shown that y_b should have the value $y_b=K/(1+K/2)=y_{bo}$. These two limits bound the possible solutions that can be obtained for specific cases of bay mixing. An assumption of partial mixing in the bay with $y_b=y_{bo}/2$ have yielded reasonable agreement with observations of Taylor and Dean (1974), which were obtained by integrating the dye concentration over the bay volume at different times.

Tidal Trapping:
In estuaries with storage basins, or relatively stagnant regions of branching waterways or embayments along the coasts, tidal currents can cause a subtle and additional dispersive effect called tidal trapping. A patch of pollutant released in such a system may get partially trapped at the surrounding embayments or shallow banks during a certain phase of the tide and gets released into the mainstream flow some time later. This influence results in increased dispersion since the phase differences between the material in the mainstream flow and the fraction caught in the trap zones are seperated from each other and therefore the patch effectively spreads with an increased rate. Shijf and Schonfeld (1953) and Okubo (1973) have studied tidal trapping, and have found that it may contribute to dispersion in a greater way as compared to shear effects alone. Fischer *et al.* (1979) estimate that the trapping mechanism may play a major role in many estuaries.

5.3 CHARACTERISTIC TIME SCALES

There are various time scales characterising the various mechanisms of exchange and transport in estuaries. We have already seen in section 4, that two of the basic time scales are the *transverse mixing times*

$$T_{cv} = h^2/E_V, \quad \text{and } T_{ch} = w^2/E_H \qquad (5.7.a,b)$$

the former being for vertical and the latter for transverse horizontal (lateral) mixing.

Fischer *et al.* (1979) suggest another time scale based on empirical judgement and in analogy to the above, namely the *replacement time*, representing the time required for a slug of material initially concentrated at one end of the basin to reach approximately uniform concentration throughout the basin, given as

$$T_r = 0.4\ L^2/E_L \qquad (5.8)$$

where L is the length of the basin and E_L the longitudinal dispersion coefficient.

An important concept is the *flushing time* which is the average time spent by a tracer particle in the estuary, defined as the ratio of the fresh water volume in the estuary to the fresh water flux (Officer, 1976; Fischer *et al.*, 1979):

$$T_f = V_f/Q_f \qquad (5.9)$$

where Q_f is the fresh water volume flux and V_f is the total volume of fresh water in the estuary, calculated from

$$V_f = \int_V \frac{S_o-S}{S_o}\, dV = \int_V f dV = \bar{f}V . \qquad (5.10)$$

Here, S_o is the ocean salinity, S the salinity in the basin and V the volume of the basin, and f is the freshness defined as the fraction of fresh water at any point, i.e.

$$f = (S_o - S)/S_o \qquad (5.11)$$

and $\bar{f}$ is the mean freshness of the basin. Note that the above flushing time is defined for an estuary influenced by a fresh water inflow alone.

For a tidal estuary, the *tidal prism flushing time* (Officer, 1976) is obtained by letting V_P and V_R respectively represent the volumes of ocean and river water entering the estuary during a tidal cycle, and writing the salt balance at high tide

$$(V_P + V_R)S = V_P\, S_o \qquad (5.10.a)$$

where S is the mean salinity in the estuary, and the mean freshness is

$$f = \frac{S_o - S}{S_o} = \frac{V_R}{V_P + V_R} = \frac{V_R}{P} \qquad (5.10.b)$$

where $P=V_p+V_R$ is the tidal prism. Then the tidal prism flushing time is

$$T_t = \frac{fV}{Q_f} = \frac{fV}{VR/T} = \frac{V}{P}\, T \qquad (5.10.c)$$

with T being the tidal period. Since neither the entire estuary, nor the ebb-water on the ocean side is not usually completely mixed during each tidal cycle, T_t is generally smaller than T_f.

If we perform a dye experiment in an estuary we need another measure of *pollutant flushing time*. Considering a continuous release of rate q and steady-state conditions to prevail, this is given as (Officer,1976)

$$T_p = \rho c V/q \qquad (5.11)$$

where ρ and c are the mean estuarine density and concentration.

Instead of the flushing time the term *residence time* is also often employed. However there seems to be a confusion with respect to the terminology applied to the various time scales of exchange.

Realizing the often confused and misleading terminology, Bolin and Rodhe (1973) have reviewed these concepts, and have derived the basic time scales. Basing their analyses on rigorous foundations, they have defined the time scales based on the *age* τ of any fluid element in the reservoir (i.e. the time elapsed since the entry of that element in the reservoir). The total mass of the basin is $M_0 = \rho V$. A cumulative age·distribution function $M(\tau)$ gives the mass that has spent a time less or equal to τ in the reservoir. All material elements spend an infinite time or less in the basin, so that

$$\lim_{\tau \to \infty} M(\tau) = M_0 \qquad (5.12)$$

An age frequency distribution functon $\Psi(\tau)$ can then be defined and normalized such that

$$\int_0^\infty \Psi(\tau)\, d\tau = 1 \qquad (5.13)$$

which is related to the cumulative function as

$$\Psi(\tau) = \frac{1}{M_0} \frac{dM(\tau)}{d\tau} . \qquad (5.14)$$

Secondly, consider a steady state volume flux F_0 of material entering the basin or equivalently leaving the basin. A cumulative transit time function $F(\tau)$ is defined, giving the mass leaving the basin per unit time of those fluid elements which has spent a time of τ or less in the basin. Obviously,

$$\lim_{\tau \to \infty} F(\tau) = F_0 \qquad (5.15)$$

and again we define a frequency distribution of transit time $\Phi(\tau)$ such that

$$\int_0^\infty \Phi(\tau)\, d\tau = 1 . \qquad (5.16)$$

This frequency function is then

$$\Phi(\tau) = \frac{1}{F_0} \frac{dF(\tau)}{d\tau} . \qquad (5.17)$$

In the case of a steady-state balance, the two sets of functions are related through

$$F_0 - F(\tau) = M_0\,\Psi(\tau) = \frac{dM(\tau)}{d\tau}\,, \qquad (5.18)$$

or with the aid of (5.14)

$$\Phi(\tau) = -\frac{M_0}{F_0}\,\frac{d\Psi(\tau)}{d\tau}\,. \qquad (5.19)$$

Since $F(0)=0$, it follows from (5.18) that

$$\Phi(0) = \frac{F_0}{M_0}\,. \qquad (5.20)$$

Equipped with the above tools, Bolin and Rodhe (1973) defined the various time scales as follows:

The *turn over time* is the ratio of the total mass of the reservoir to the total flux

$$\tau_0 = \frac{M_0}{F_0}\,. \qquad (5.21)$$

The *average transit time* of particles leaving the basin (which is equal to the expected life time of newly incorporated particles) is given by

$$\tau_t = \int_0^\infty \tau\Phi(\tau)\,d\tau\,. \qquad (5.22.a)$$

Making use of (5.19) the above equation integrates to

$$\tau_t = \frac{M_0}{F_0} = \tau_0 \qquad (5.22.b)$$

hence making the average transit time and turn-over time equal to each other. An alternative name for both time scales is *residence time* as suggested by Bolin and Rodhe (1973), who note that this last term has often been misused.

Another time scale that can be defined is the *average age* of particles in the reservoir at any time, given by

$$\tau_a = \int_0^\infty \tau\Psi(\tau)\,\partial\tau = \frac{1}{M_0}\int_0^\infty \tau\,dM(\tau)\,. \qquad (5.23)$$

Since it is shown that $\tau_t=\tau_0$, there are basically two time scales τ_t and τ_a.
The relation between these two time scales is determined by the form of the frequency functions $\Psi(\tau)$ and $\Phi(\tau)$.
Three cases can be distinguished according to the ranges of these time scales:

$\tau_a < \tau_t$:
A reservoir with modest transport velocities and source and sink regions placed far apart belongs to this case (for example, a well-mixed, wide and elongated estuary).

$\tau_a = \tau_t$:
A well-mixed reservoir with isolated source/sink regions, such that all elements in the reservoir have equal probability of exiting at any time is characterised by this condition (for example, a well-mixed estuary of very small volume). Bolin and Rodhe (1973) note, however, that since any element in the basin is comprised of particles of all ages, it is impossible in this case to establish the frequency functions by direct observation. In this case, they derive the sufficient condition (from 5.22.a and 5.23)

$$\Psi(\tau) = \Phi(\tau) \qquad (5.24.a)$$

so that from (5.19) they derive the frequency functions

$$\Psi(\tau) = \Phi(\tau) = \frac{1}{\tau_a} \exp(-\tau/\tau_a) \, . \qquad (5.24.b)$$

$\tau_a > \tau_t$:
This case represents the situation in which most of the fluid particles entering the reservoir exit in a short time and those remaining particles stay in the reservoir for a much longer time. Such a case is possible if the source and sink regions are close to each other (short circuiting), so that any particles diffusing in the relatively stagnant major part of the basin are trapped in these regions (for example a salt-wedge or partially mixed estuary with stagnant regions).

Takeoka (1984a) developed these concepts further and redefined the residence time differently from Bolin and Rodhe (1973), producing two different residence times, one for the reservoir and one for the inlet. Takeoka's residence time is not the same as the average transit time, since he defined it as being the average time required for the particles to reach the outlet, which becomes a complement of the average age. These results were then applied to coastal seas in two important papers (1984a,b).

While the earlier definitions of time scales in this section apply to specific situations in estuaries, the latter more rigorous definitions outlined above apply to more general situations, involving larger basins with more structural variations. On the other hand, they require the determination of frequency functions through direct observations or various models.

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