Transport of Marine Pollutants

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1. INTRODUCTION

A review of marine pollutant transport processes is given, with the objective of introducing the basic concepts. The subject has great extent and detail, and is 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.

The basic concepts required in studying the diffusive/dispersive transport of pollutants will be described. One is often forced, however, to use more complicated theory and/or numerical models to assess these effects in the presence of more complex geometry, current systems or in deep basins. There is also an often empirical element in the theory due to the need for realistic determinations of diffusion coefficients via experiments. This presentation precludes such variations to the theme, providing information on basic physics and the tools that one often needs. In addition to pollutants, the transport of heat, salt and other ecological quantities (e.g. plankton, detritus, nutrients, oxygen etc.) in the sea are also governed by similar laws. A number of basic books on fluid dynamics (Batchelor, 1967), and transport processes (Csanady, 1973; Fischer *et al.*, 1979; Kullenberg, 1982) are advisable to complement these notes.

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.

1.1 FLUID MOTION

The equations governing fluid motion are briefly reviewed. The *continuity equation*

$$\frac{D\rho}{Dt} + \rho \nabla\cdot\vec{u} = 0 \qquad (1.1)$$

states the conservation of mass, where the *material derivative* is defined as

$$\frac{DX}{Dt} = \frac{\partial X}{\partial t} + \vec{u}\cdot\nabla X \ . \qquad (1.2)$$

for any variable X. An *incompressible fluid* is defined as one in which the density of material elements of the fluid does not change, i.e. equation (1.1) simplifies to

$$\nabla\cdot\vec{u} = 0 \ . \qquad (1.3)$$

The momentum equation

$$\frac{D\vec{u}}{Dt} + 2\Omega\times\vec{u} = \vec{g} - \frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla\cdot\underline{d} \ . \qquad (1.4)$$

expresses *Newton's Second Law of Motion* in an inertial (rotating) coordinate system on the earth, where Ω is the earth's angular velocity, p is the pressure, $\vec{g}$ is the gravitational acceleration and $\underline{d}$ is the deviatoric stress tensor (Batchelor, 1967).

The *thermodynamic equation* is derived from the *First and Second Laws of Thermodynamics*. For seawater, which is assumed to be incompressible, the thermodynamic equation is expressed as

$$\frac{DT}{Dt} = \nabla\cdot\kappa\nabla T + Q/c_p \qquad (1.5)$$

where $k=\kappa/(\rho c_p)$ is the *thermal diffusivity coefficient*, with κ being the thermal conductivity and c_p the *specific heat at constant pressure* for the fluid, and Q stands for heat sources (e.g. internal heating due to solar radiation or frictional dissipation). Neglecting the latter term yields

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T = \nabla\cdot k\nabla T \qquad (1.6)$$

1.2 DIFFUSION 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. Consider a *binary system* consisting of a mixture of two different fluids. The densities ρ_A and ρ_B represent the masses per unit volume of the mixture. The *concentration* of each constituent is defined as the mass of each constituent per unit mass of the mixture, $c_A = \rho_A/\rho$, and $c_B = \rho_B/\rho$.
Since the fluid density is $\rho = \rho_A + \rho_B$, we must have $c_A + c_B = 1$.

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

$$\vec{N}_A = \rho_A \vec{u}_A, \quad N_B = \rho_B \vec{u}_B \qquad (1.7.a,b)$$

where $\vec{u}_A$ and $\vec{u}_B$, are hypothetical velocities that an infinitesimal group (or cloud) of particles would have on the average, representing the momenta of each constituent. The total momentum (or total flux) of the mixture is

$$\begin{aligned} \rho\vec{u} &= \rho_A\vec{u}_A + \rho_B\vec{u}_B \\ &= c_A\vec{u}_A + c_B\vec{u}_B, \end{aligned} \qquad (1.8)$$

where the hydrodynamic velocity is defined as u.

The fluxes defined in (1.7.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 (1.7.a) as

$$\begin{aligned} \vec{N}_A &= \rho_A\vec{u}_A \\ &= \rho_A(\vec{u}_A-\vec{u}) + \rho_A\vec{u} \end{aligned} \qquad (1.9)$$

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

$$\rho_A(\vec{u}_A-\vec{u}) = - D_{AB}\,\nabla\rho_A \qquad (1.10)$$

for constituent A, where the diffusion coefficient D_{AB} characterizes the diffusivity of constituent A in medium.

We consider a *fixed* control volume V enclosed by a surface S with outward normal $\hat{n}$, and write a statement of the conservation of mass for each constituent:

$$\frac{\partial}{\partial t}\int_V \rho_A dV = -\int_S \vec{N}_A\cdot\hat{n}\,dS + \int_V r_A dV, \qquad (1.11)$$

where r_A is the rate of production of constituent A due

to possible chemical interactions. Since the total mass of the mixture should be conserved,

$$r_A + r_B = 0, \tag{1.12}$$

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

Using (1.9), (1.10), (1.1), the divergence theorem, and assuming that $\rho \approx$ constant yields

$$\frac{Dc_A}{Dt} = \nabla \cdot D_{AB} \nabla c_A + \frac{r_A}{\rho}$$

and

$$\frac{Dc_B}{Dt} = \nabla \cdot D_{BA} \nabla c_B + \frac{r_B}{\rho} . \tag{1.13.a,b}$$

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 corresponding diffusion equations must be solved together with the continuity (1.1), the momentum (1.4) equations, and an equation of state incorporating the effects of the two constituents and temperature, salinity of sea-water on density:

$$\rho = \rho(p, T, S, c_A, c_B) \tag{1.14}$$

Furthermore, the energy equation (1.5), and a diffusion equation (similar to (1.13.a)) for salinity (a third constituent) must also complement the above equations in order to be able to solve the system.

It is however, quite common that the mixture of interest is a weak (dilute) solution of one of the constituents (say $c_A << c_B$). Then, we can assume $c = c_A << 1$ (yielding $c_B \approx 1$, $\rho \approx$ constant), so that the second equation (1.13.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 (1.15) is decoupled from 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 (1.1) and (1.14) to determine the velocity field $\vec{u}(x,t)$. Consequently, for given velocity field, we seek solutions to equation (1.15).

1.3 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 result is the random motion of fluid "particles" consisting of lumps (eddies) of various sizes, superposed on the mean motion. 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 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 u and c in equation (1.15) we can write

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

and

$$c = \bar{c}(x,\ T^{-1}t) + c'(x,\ t) \qquad (1.16.a,b)$$

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

$$\bar{c} = \frac{1}{T}\int_0^T c\ dt \qquad (1.17)$$

and the primed quantities are the components with fluctuations that are typically more rapid than the turbulence time scale T. By definition, $\overline{c'} = \overline{c - \bar{c}} = 0$. 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 (1.1), momentum (1.4), energy (1.5) and diffusion (1.15) 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 be illustrative to average only one of these, that case being the diffusion equation.

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 (1.1) [which vanishes for homogeneous, incompressible fluids], of momentum (Reynolds' stresses) in the case of the

momentum equation (1.4), and of heat or concentration in the cases of the convective-diffusion equation (1.6 and 1.15).

We first put (1.15) into the flux form (making use of the continuity equation), substitute (1.16.a,b), and take averages. By making use of (1.17), we immediately obtain

$$\frac{\partial \bar{c}}{\partial t} + \nabla\cdot\bar{c}\bar{u} + \nabla\cdot\overline{c'\vec{u}'} = D\nabla^2\bar{c} + R \qquad (1.18)$$

i.e. the same as equation (1.15) with the exception of the term $\nabla\cdot\overline{c'\vec{u}'}$ 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 (1.18) actually suggests that it may represent the divergence of a flux in much the same way that the molecular flux divergence appears in (1.13). We can therefore define

$$\vec{N}_T = \rho\overline{c'\vec{u}'} \qquad (1.19)$$

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 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,

$$\overline{c'u'}_i = E_{ij}\frac{\partial \bar{c}}{\partial x_j} \qquad (1.20)$$

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 (i.e. the shallow water approximation) results in the common situation that the vertical stratification is far greater than 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 coordinates of the diffusivity tensor E_{ij}, which then reduces (1.20) to the special form

$$N_i = \rho\overline{c'u'}_i = -\rho E_i\frac{\partial \bar{c}}{\partial x_i} \qquad (1.21.a)$$

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

$$\vec{N}_T = \rho\overline{c'\vec{u}'} = -\rho(E\cdot\nabla)\bar{c} \qquad (1.21.b)$$

where $E = (E_x, E_y, E_z)$ are the turbulent diffusivities in the principal coordinates (x,y,z).

The turbulent mechanism of mixing (turbulent diffusion) is in fact much more effective than the molecular diffusion, so that typically $E_x, E_y, E_z >> D$, as a result of which the molecular diffusion term in (1.18) can be neglected. Substituting (1.21.b) in (1.18) and dropping the overbar notation, we obtain the turbulent diffusion equation

$$\frac{\partial c}{\partial t} + \vec{u}\cdot\nabla c = \frac{\partial}{\partial x}(E_x\frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(E_y\frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(E_z\frac{\partial c}{\partial z}) + R \ . \qquad (1.22)$$

The sources or sinks of concentration are represented by R. In some cases, this term stands for the decay or decomposition of a non-conservative pollutant due to extraneous influences. A linear form representing first order decay processes is

$$R = -kc \ . \qquad (1.23)$$

In the case of homogeneous turbulence, the diffusivities are constants in space and time, and we have a simpler version of the turbulent diffusion equation:

$$\frac{\partial c}{\partial t} + \vec{u}\cdot\nabla c = E_x\frac{\partial^2 c}{\partial x^2} + E_y\frac{\partial^2 c}{\partial y^2} + E_z\frac{\partial^2 c}{\partial z^2} - kc \ . \qquad (1.24)$$

1.4 RELATIVE AND APPARENT DIFFUSION

In reality, turbulence constitutes a random field of motion, and therefore the *ensemble averaged* equations would be appropriate. We have so far circumvented this difficulty by empirically representing these effects within the bulk turbulent diffusivity coefficients in time averaged equations.

Even in the case of homogeneous, stationary turbulence, an initial release of concentration will diffuse at a rate which depends on the size of the patch, so that the constant coefficients in (1.24) are not 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. As the patch size grows, larger eddies will begin to influence it, and distribute the material in a more efficient way.

In addition, each random 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 we 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.

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

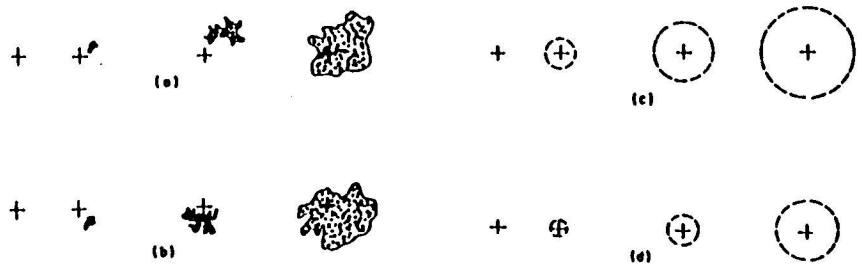

FIGURE 1.1 Turbulent diffusion from a small source. (a,b) Random spread of two identical clouds, (c) Spread of the ensemble mean, (d) Spred of the ensemble mean obtained by shifting the origin to the centeroid of each realization. (After Fischer *et al.* 1979)

$$\sigma_s^2 = \frac{\int_{-\infty}^{+\infty} cs^2\, ds}{\int_{-\infty}^{+\infty} c\, ds} \qquad (1.25)$$

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 length scales (standard deviations) of the diffusing cloud. It can be verified, through multiplication of equation (1.22) with x^2, y^2, z^2 respectively and through integration by parts that

$$E_s = \frac{1}{2}\frac{d\sigma_s^2}{dt} \qquad (1.26)$$

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)

$$\sigma_s^2 = \hat{\sigma}_s^2 + m_s^2 \qquad (1.27)$$

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 (1.26). 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 1.26), and the solution of (1.24) 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, for then the diffusion is proportional to eddy sizes. Fischer *et al.* (1979) show that in this case the Fickian diffusion equation (1.23) is valid with respect to relative coordinates shifted to the instantaneous center of mass of the cloud, provided that the diffusivities are prescribed as

$$E = \frac{1}{2}\frac{d\sigma^2}{dt} = \alpha\, \sigma^{4/3} \,. \qquad (1.29)$$

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.

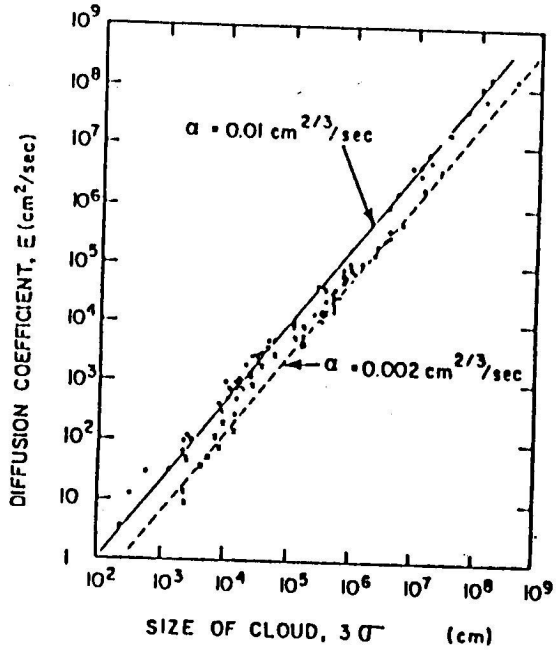

FIGURE 1.7 The turbulent diffusion coefficient as a function of patch size (After Okubo, 1974).

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 considerable latitude in Csanady (1973) and Fischer *et al.* (1979). In the following sections, we will mainly consider the cases in which the diffusivities are assumed to be constant.

2. SIMPLE MODELS OF TURBULENT DIFFUSION AND TRANSPORT

In this Section, solutions to the convective diffusion equation will be obtained 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).

Equation (1.25) is in general not very easy to solve under general flow situations, often due to the variable coefficients introduced by the velocity field u(x,t) determined by the equations of motion. An alternative approach is to lump the variability of the velocity field into the turbulent diffusivity coefficients, yielding *dispersion* equations to be demonstrated later in Section 3.

We consider a simple class of problems in which the velocity field is constant with speed U arbitrarily aligned with the x-axis. This case is analogous to the diffusion in a solid, when the equations are transformed to the coordinates fixed with respect to the uniform bodily motion of the fluid. We will assume homogeneous, non-isotropic turbulence and a non-conservative constituent which decays linearly. Namely, we consider the equation

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

We define the coordinate transformations

$$X = \left(\frac{E}{E_x}\right)^{1/2}(x-Ut), \quad Y = \left(\frac{E}{E_y}\right)^{1/2} y, \quad Z = \left(\frac{E}{E_z}\right)^{1/2} z,$$
$$T = t, \tag{2.2.a-d}$$

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

$$\frac{\partial c}{\partial t} + U \frac{\partial c}{\partial x} = \left(\frac{\partial X}{\partial t}\frac{\partial c}{\partial X} + \frac{\partial T}{\partial t}\frac{\partial c}{\partial T}\right) + U\left(\frac{\partial X}{\partial t}\frac{\partial c}{\partial X} + \frac{\partial T}{\partial t}\frac{\partial c}{\partial T}\right)$$
$$= -\left(\frac{E}{E_x}\right)^{1/2} U \frac{\partial c}{\partial X} + \frac{\partial c}{\partial T} + U\left(\frac{E}{E_x}\right)^{1/2} \frac{\partial c}{\partial X} = \frac{\partial c}{\partial T}, \tag{2.3}$$

and the terms on the right hand side are transformed as

$$E_x \frac{\partial^2 c}{\partial x^2} = E_x \frac{\partial X}{\partial x}\frac{\partial}{\partial X}\left(\frac{\partial X}{\partial x}\frac{\partial c}{\partial X}\right) = E_x \frac{\partial^2 c}{\partial X^2} \tag{2.4}$$

We also set the yet undetermined constant E equal to

$$E^3 = E_x E_y E_z \tag{2.5}$$

i.e. one of the *invariants* of the anisotropic diffusivity tensor. With these transformations (2.1) becomes

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

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 $x = x' = (x',y',z')$ released at some initial instant $t = 0$. We seek the solution to (2.9) with the initial condition

$$c(x,0) = \frac{M}{\rho}\,\delta(x-x')\,\delta(y-y')\,\delta(z-z') = \frac{M}{\rho}\,\delta(\vec{x}-\vec{x}') \qquad (2.10)$$

where M is the total mass of the substance introduced and ρ is the density of the receiving fluid. Here $\delta(x-x')$ is the *Dirac delta "function"* with the important properties of

$$\int_{-\infty}^{+\infty} \delta(x)\,dx = 1$$

$$\int_{-\infty}^{+\infty} F(x')\delta(x-x')dx = F(x) \qquad (2.11.a\text{-}c)$$

$$\int_{-\infty}^{+\infty} e^{ikx}\, dk = 2\pi\, \delta(x) \ .$$

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 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 $\alpha \rightarrow 0$, 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)

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

yielding the mass of the substance introduced, in agreement with the definition of concentration.

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, θ, ϕ) centered at the relative origin of the source and dropping the

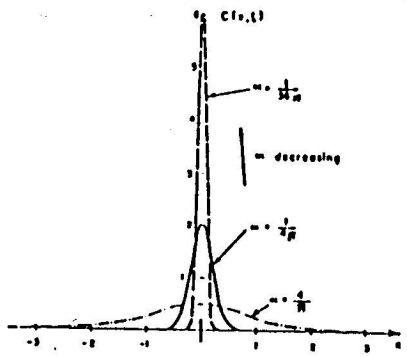

FIGURE 2.1 $f_\alpha(x)=(\alpha\pi)^{-1/2} \exp[-(x)^2/\alpha]$, the set of functions which reduce to the delta function as α-0.

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

$$c = \xi^{-m} f(\eta) \qquad (2.14)$$

in the transformed coordinates

$$\eta = \frac{r^2}{4Et} , \qquad \xi = 4Et . \qquad (2.15)$$

The transformation to the original variables are

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

and the corresponding cross-derivatives are

$$\frac{\partial \xi}{\partial t} = 4E , \quad \frac{\partial \eta}{\partial t} = - \frac{r^2}{4Et^2} = - 4E \frac{\eta}{\xi} ,$$
$$\frac{\partial \xi}{\partial r} = 0 , \quad \frac{\partial \eta}{\partial r} = \frac{2r}{4Et} = 2 \frac{\eta}{r} = 2(\frac{\eta}{\xi})^{1/2} , . \qquad (2.17.a-d)$$

The individual terms in (2.13) are then calculated as

$$\frac{\partial c}{\partial t} = \frac{\partial c}{\partial \xi} \frac{\partial \xi}{\partial t} + \frac{\partial c}{\partial \eta} \frac{\partial \eta}{\partial t}$$
$$= - 4E\xi^{-m-1} (\eta f_\eta + mf) \qquad (2.18)$$

and

$$\frac{1}{r^2} \frac{\partial c}{\partial r} (r^2 \frac{\partial c}{\partial r}) = \eta^{-1}\xi^{-1} \frac{\partial \eta}{\partial r} \frac{\partial}{\partial \eta} (\eta\xi \frac{\partial \eta}{\partial r} \frac{\partial c}{\partial \eta})$$
$$= \xi^{-m-1} (\eta f_{\eta\eta} + \frac{3}{2} f_\eta) \qquad (2.19)$$

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

With these substitutions we transform the partial differential equation (2.13) into the ordinary differential equation

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

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

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

(2.20) directly integrates to

$$g = f_H + f = A\,\eta^{-3/2}\ . \qquad (2.22)$$

Integrating once more with use of integration factors yields

$$f = B\,e^{-\eta} + A\,e^{-\eta}\int \eta^{-3/2}\,e^{\eta}\,d\eta, \qquad (2.23)$$

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

For small values of $\eta = r^2/(4Et)$ (i.e. as $t \to \infty$), the second term grows with a trend of $t^{3/2}$. Since the initial concentration should decay with time through diffusion, this solution can not be accepted and therefore we set A = 0.

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

$$\begin{aligned}\frac{M}{\rho} &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} c(r)\,dr\,r\,d\phi\,r\sin\phi\,d\theta \\ &= 4\pi\int_0^{\infty} r^2\,c(r)\,dr \\ &= 4\pi\int_0^{\infty} \eta\xi\,\frac{f(\eta)}{\xi^{3/2}}\,\frac{1}{2}\,(\frac{\xi}{\eta})^{1/2}\,d\eta \\ &= 2\pi B\int_0^{\infty} \eta^{1/2}\,e^{-\eta}\,d\eta = \pi^{3/2}\,B\ .\end{aligned} \qquad (2.24)$$

Therefore the solution of the problem becomes

$$c(r,t) = \frac{(M/\rho)}{(4\pi Et)^{3/2}}\exp(-\frac{r^2}{4Et}) \qquad (2.25)$$

or writing in Cartesian coordinates

$$c(x,y,z,t) = \frac{(M/\rho)}{(4\pi Et)^{3/2}}\exp-\,(\frac{(x-x')^2+(y-y')^2+(z-z')^2}{4Et})\ . \qquad (2.26)$$

The instantaneous point source solution (2.25) decays as $t^{-3/2}$ and goes to zero everywhere as $t \rightarrow \infty$. 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 $\alpha = 4Et$. The shape of the function with respect to the radial 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 as a result of the three-dimensionality of the problem. At any time, the constant concentration surfaces (of say $c=c_o$) are spheres.

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

$$c=\frac{M/\rho}{(4\pi Et)^{3/2}}\exp-\left[\frac{(x-x'-Ut)^2}{4E_x t}+\frac{(y-y')^2}{4E_y t}+\frac{(z-z')^2}{4E_z t}+kt\right] \qquad (2.27)$$

where $E^3=E_xE_yE_z$. In this case, the constant concentration surfaces are ellipsoids.

The variance (cf. equation 1.26) defined with respect to the center of the patch is

$$\sigma_s^2 = \frac{\int_{-\infty}^{+\infty} c\,\bar{s}^2\,d\bar{s}}{\int_{-\infty}^{+\infty} c\,d\bar{s}} \qquad (2.28)$$

where $\bar{s}$ stands for any of the shifted coordinates $\bar{x}=x-x'-Ut$ or $\bar{y}=y-y'$ or $\bar{z}=z-z'$ in equation (2.27). Noting that

$$\frac{\int_{-\infty}^{+\infty} r^2\exp(-r^2/a)\,dr}{\int_{-\infty}^{+\infty}\exp(-r^2/a)\,dr} = \frac{(\pi a)^{1/2}\,a/2}{(\pi a)^{1/2}} = a/2 \qquad (2.29)$$

(2.28) evaluates to (for each axis)

$$\sigma_x = (2E_x t)^{1/2},$$
$$\sigma_y = (2E_y t)^{1/2},$$
$$\sigma_z = (2E_z t)^{1/2} \qquad (2.30.a\text{-}c)$$

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 (1.27).

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

$$c(x,0) = C(x) = C(x,y,z) \ . \tag{2.31}$$

Consider the simple diffusion equation (2.9) written as

$$L(c) = 0; \quad L = \frac{\partial}{\partial t} - E\nabla^2 \ . \tag{2.32}$$

Let $\tilde{c}(x',t)$ be the basic solution of (2.32) for an instantaneous point source $\tilde{c}(x,0)=\delta(x-x')\delta(y-y')\delta(z-z')$ disregarding the dimensional coefficient M/ρ in (2.10). The solution to (2.32) with the initial condition (2.31) is constructed as

$$c(x,t) = \int_{-\infty}^{+\infty}\int\int\int C(x')\ \tilde{c}(x-x',t)\ dx'dy'dz' \tag{2.33}$$

where $\tilde{c}$ is (2.26) normalised with M/ρ. The proof is given as follows. Operating on (2.31) yields

$$L(c) = \int_{-\infty}^{+\infty}\int\int\int C(x')\ L(\tilde{c})\ dx'\ dy'\ dz' = 0 \tag{2.34}$$

since L operates on x and t only and $\tilde{c}$ satisfies (2.32). Evaluating (2.33) at t=0, we obtain from (2.10)

$$c(x,0) = \int_{-\infty}^{+\infty}\int\int\int C(x')\ \delta(x-x')\ dx'\ dy'\ dz' = C(x) \tag{2.35}$$

by virtue of (2.11.b). The expression in (2.34) 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

$$c(x,0) = (m'/\rho)\ \delta(x-x'')\ \delta(y-y'') \tag{2.36}$$

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

$$m' = M\,\delta(z-z'),$$
$$\int_{-\infty}^{+\infty} m'\,dz = M, \qquad (2.37.a\text{-}c)$$
$$m'\,dz = dM,$$

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

$$c(x,t)=\int\int\int_{-\infty}^{+\infty} \frac{m'}{\rho(4\pi Et)^{3/2}}\exp-\left(\frac{\tilde{r}^2}{4Et}\right)\delta(x'-x'')\delta(y'-y'')dx'dy'dz' \qquad (2.38)$$

where $\tilde{r}^2 = (x-x')^2+(y-y')^2+(z-z')^2$.
Using (2.11.b) and integrating further yields the two-dimensional solution

$$c(x,t) = \frac{m'}{\rho 4\pi Et}\exp-\left[\frac{(x-x'')^2+(y-y'')^2}{4Et}\right] \qquad (2.39)$$

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 (2.38) and (2.37). 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.

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

$$\sigma_x = \sigma_y = (2Et)^{1/2} \qquad (2.40)$$

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

2.4 INSTANTANEOUS PLANE SOURCE

We next consider an *instantaneous plane source*

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

where m'' represents the source strength

$$m'' = m' \, \delta(y-y''), \tag{2.42}$$

in comparison to (2.36). The solution can again be obtained by the same technique outlined in Section 2.2 as

$$c(x,t) = \int_{-\infty}^{+\infty}\int\int \frac{m''}{\rho(4\pi Et)^{3/2}} \exp-\left(\frac{\tilde{r}^2}{4Et}\right) \delta(x'-x'') \, dx' \, dy' \, dz' \tag{2.43}$$

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

$$c(x,t) = \frac{m''}{\rho(4\pi Et)^{1/2}} \exp - \frac{(x-x'')^2}{4Et} \tag{2.44}$$

The one dimensional solution can also be obtained from a summation of the two dimensional solutions. The solution decays as $t^{-1/2}$ at large times, i.e. slower than the two and three dimensional instantaneous sources. The variance for the solution is again $\sigma_x = (2Et)^{1/2}$.

2.5 CONTINUOUS POINT SOURCE

We can use the above methods to construct 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, with summation of delta function inputs with respect to time. However, due to the complex time dependence of the basic solutions, we must apply the summation directly on the general case (2.27).

Consider the *continuous point source*, starting from an initial time $t=t_o$ and continuing up to time $t=t_1$, (Fig. 2.2) with a rate of mass injection $Q = dM/dt$. 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 $d\tau$.

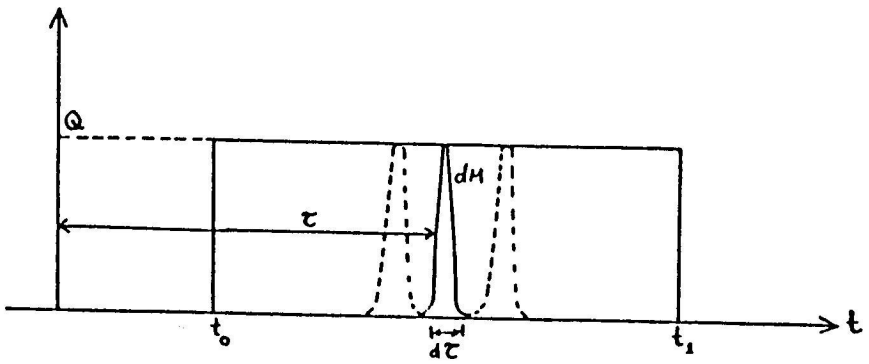

FIGURE 2.2 Idealization of the continuous point source as a series of instantaneous point sources.

We assume that the source is located at the origin x=y=z=0. The solution can be constructed as

$$c = \int_{to}^{t_*} c_1(x, t-\tau)\, dM = \int_{to}^{t_*} q\, c_1(x, t-\tau)\, d\tau \qquad (2.45)$$

where c_1 denotes the solution for the instateneous solution (i.e. equation 2.27) divided by M, and t_* the upper limit of integration in time. If we are interested in the solution for the time interval $t_o<t<t_1$ (*during* continuous injection), we must integrate (2.45) 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 (2.45) must be integrated up to $t_*=t_1$. Defining

$$\lambda^2=\frac{E_x}{E_y}\gamma_y^2, \quad \mu^2=\frac{E_x}{E_z}\gamma_z^2, \quad E^3=E_xE_yE_z \qquad (2.46)$$

and substituting (2.27), the solution (2.45) is written as

$$c=\int_{to}^{t_*} \frac{Q}{\rho[4\pi E(t-\tau)]^{3/2}} \exp-\frac{[x-U(t-\tau)]^2+\lambda^2+\mu^2}{4E_x(t-\tau)}d\tau \qquad (2.47)$$

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

$$r^2 = x^2+\lambda^2+\mu^2, \qquad \zeta = \frac{r}{2[E_x(t-\tau)]^{1/2}}$$

$$\nu = xU/(2E_x), \qquad \Omega = (U^2+4kE_x)^{1/2}, \qquad (2.48.a\text{-}e)$$

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

equation (2.47) can alternatively be written as

$$c=\frac{Q}{2\rho\pi^{3/2}(E_yE_z)^{1/2}r}e^{\nu}\int_{\zeta_o}^{\zeta_*}\exp-[\zeta^2+\frac{\beta^2}{\zeta^2}]\,d\zeta \qquad (2.49)$$

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

In order to integrate (2.49) we define

$$p = \zeta + \frac{\beta}{\zeta}, \qquad q = \zeta - \frac{\beta}{\zeta} \qquad (2.50.a, b)$$

and consequently

$$p^2 - q^2 = 4\beta \ , \quad \frac{\beta}{\zeta^2} = \frac{p - q}{p + q} \tag{2.50.c,d}$$

Differentiating (2.50.a,b) gives

$$\frac{dp}{d\zeta} = 2 - \frac{p}{\zeta} = 1 - \frac{\beta}{\zeta^2} = \frac{2q}{p+q}, \qquad \frac{dq}{d\zeta} = 2 - \frac{q}{\zeta} = 1 - \frac{\beta}{\zeta^2} = \frac{2p}{p+q}, \tag{2.51.a,b}$$

and therefore

$$p\,dp = q\,dq \ . \tag{2.52}$$

The integral in (2.56) can be formed into

$$\int \exp -(\zeta^2 + \frac{\beta^2}{\zeta^2})\,d\zeta = \frac{1}{2}\int [\exp(-p^2+2\beta)+\exp(-q^2-2\beta)]\,d\zeta \tag{2.53}$$

or, using (2.51.a,b)

$$\frac{1}{4}\int (\frac{p}{q}+1)\exp(-p^2+2\beta)\,dp + \frac{1}{4}\int (\frac{q}{p}+1)\exp(-q^2+2\beta)\,dq \tag{2.54}$$

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

$$\frac{1}{2}\int \exp(-p^2+2\beta)\,dp + \frac{1}{2}\int \exp(-q^2-2\beta)\,dq \tag{2.55}$$

As a result, the solution (2.49) becomes

$$c=\frac{Qe^{\nu}}{8\pi\rho(EyEx)^{1/2}r}[e^{+2\beta}(\operatorname{erfc} p)\Big|_{p_o}^{p_o} + e^{-2\beta}(\operatorname{erfc} q)\Big|_{q_o}^{q_o}] \tag{2.56}$$

where evaluations are between the limits $p_o=p(\zeta_o)$, $q_o=q(\zeta_o)$, $p_*=p(\zeta_*)$, $q_*=q(\zeta_*)$.

Note that the transient solution (2.56) in the special case U=K=0 (β=0) becomes

$$c = \frac{Q}{4\pi\rho(EyEz)^{1/2}r}[\operatorname{erfc}\frac{r}{2[Ex(t-to)]} + \operatorname{erfc}\frac{r}{2[Ex(t-t*)]}] \tag{2.57}$$

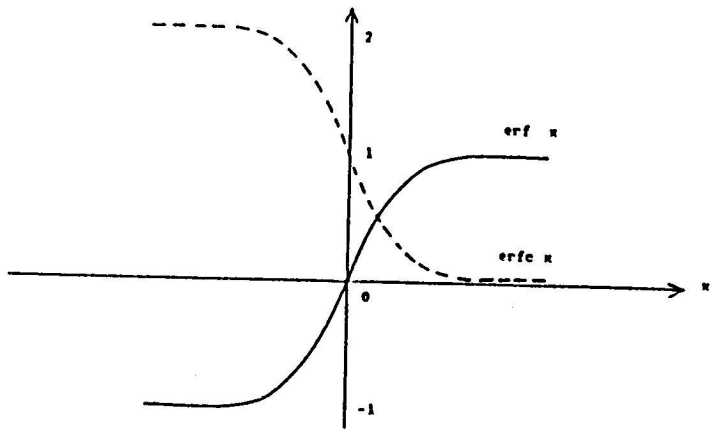

FIGURE 2.3 Error function and complementary error function.

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

$$\text{erf } u = \frac{2}{\sqrt{\pi}} \int_0^u \exp -s^2 \, ds \qquad (2.58.a)$$

and the *complementary error function* as

$$\text{erfc } u = 1 - \text{erf } u \qquad (2.58.b)$$

which are sketched in Fig. 2.3.

In the case of continuous injection, it is possible to have a steady solutions, which is obtained by letting $t_H = t$, $t_0 - \infty$ in (2.56). The lower limit of the integral (corresponding to $\tau = t_0$) becomes $\xi_0 = 0$ and the upper limit $\xi_0 - \infty$ in this case, and a definite integral results, yielding the steady state solution

$$c = \frac{Q}{\rho 4\pi (E_y E_z)^{1/2} r} \exp -[2\beta - \nu] \qquad (2.59.a)$$

Consider the case k=0, then (2.59.a) becomes

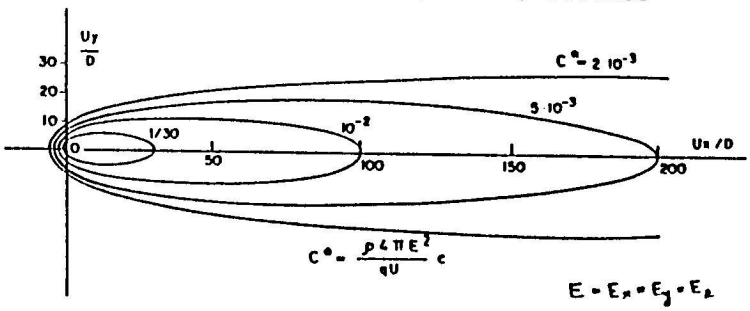

FIGURE 2.4 Solution for a continuous point source

$$c = \frac{Q}{\rho 4\pi (E_y E_z)^{1/2} r} \exp -\left[\frac{U(r-x)}{2E_x}\right] \qquad (2.59.b)$$

These solutions are shown in Fig 2.4. At long distances away from the origin along the x-axis, i.e. for $x>>\lambda$ and $x>>\mu$, we can simplify and (2.48.a) to

$$r = (x^2+\lambda^2+\mu^2)^{1/2} = x\left(1 + \frac{\lambda^2+\mu^2}{x^2}\right)^{1/2} \approx x + \frac{1}{2}\frac{\lambda^2+\mu^2}{x} \qquad (2.60)$$

so that (2.59.b) can be approximated as

$$c = \frac{Q}{\rho 4\pi (E_y E_z)^{1/2} x} \exp - \left[\frac{U}{4x}\left(\frac{y^2}{E_y} + \frac{z^2}{E_z}\right)\right] \qquad (2.61)$$

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 $\bar{t}=x/U$; which upon substitution into (2.68) yields the familiar (two dimensional) instantaneous line source solution (2.44) with $m'U=Q$, $\bar{t}=t$, in this case the line source being oriented along x. It can be verified that this is equivalent to the solution of the system

$$U\frac{\partial c}{\partial x} = E_y\frac{\partial^2 c}{\partial y^2} + E_z\frac{\partial^2 c}{\partial z^2} \qquad (2.62)$$

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 an injection rate of $q' = dm'/dt$ can be obtained either by summation of continuous point source solutions in space or the summation of instantaneous line source solutions in time. With the definitions

$$r^2=x^2+\lambda^2, \quad \lambda^2=\frac{E_y}{E_y}\gamma y^2, \quad \xi=\Omega^2(t-\tau) \qquad (2.63.a\text{-}c)$$

and ν, Ω, β as defined in (2.48.c-e), the summation of instantaneous line sources yields (Harleman, 1970)

$$c = \frac{q' e^{\nu}}{4\pi\rho (E_x E_y)^{1/2}} \int_{\xi_o}^{\xi_o} \frac{1}{\xi} \exp -\left[\xi+\frac{\beta^2}{\xi}\right] d\xi \qquad (2.64)$$

where $\xi_o=\xi(\tau=t_o)$ and $\xi_*=\xi(\tau=t_*)$.

This general form can be integrated numerically. Note that in the case $t_u = t$, $\epsilon_o = 0$.

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

$$c = \frac{q' e^{\nu}}{2\pi\rho(E_x E_y)^{1/2}} K_o(2\beta) \tag{2.65}$$

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 (2.65) as

$$c = \frac{q'}{4\rho(\pi\beta E_x E_y)^{1/2}} \exp -[2\beta - \nu] \tag{2.66}$$

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 $q'' = dm''/dt$. Defining

$$r = x, \qquad \gamma = \Omega \left(\frac{t-\tau}{4E_x}\right)^{1/2} \tag{2.67.a,b}$$

and γ, Ω, β as in (2.48.c-e) the solution can be obtained by the methods outlined above, resulting in

$$c = \frac{2q'' e^{\nu}}{\rho\pi^{1/2}\Omega} \int_{\gamma_o}^{\gamma} \exp -[\gamma^2 + \frac{\beta^2}{\gamma^2}]\, d\gamma \,. \tag{2.68}$$

Comparing with (2.49) and (2.56) the solution is evaluated as

$$c = \frac{q'' e^{\nu}}{2\rho\Omega} - [\exp(+2\beta)(\operatorname{erfc} p)\Big|_{p_o}^{p} + \exp(-2\beta)(\operatorname{erfc} q)\Big|_{q_o}^{q}] \tag{2.69}$$

where p, q, p_o, q_o, p_u, q_u are defined the same way as in (2.57.a,b) replacing ξ by γ.

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 consider the case of an instantaneous line source confined in $-h<z<h$ at $x'=0$, $y'=0$. For brevity, we consider the isotropic, conservative non-convective case. In this case, the solution (2.38) is modified accordingly, to

$$c = \int_{-h}^{+h} \frac{m'}{\rho(4\pi Et)^{3/2}} \exp - \frac{\hat{r}^2}{4Et}\, dz' \qquad (2.70)$$

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

$$\mu(z') = \frac{(z-z')}{(4Et)^{1/2}}, \qquad dz' = -(4Et)^{1/2}\, d\mu \qquad (2.71.a,b)$$

yields the solution

$$c = \frac{m'}{\rho\pi^{3/2}(4Et)} \exp - \frac{x^2+y^2}{4Et} \int_{\mu(+h)}^{\mu(-h)} \exp - \mu^2\, d\mu \qquad (2.71.c)$$

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

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

2.9 INFLUENCE OF BOUNDARIES

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

$$\hat{n} \cdot \nabla c = 0 \qquad (2.72)$$

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

In some simple cases, the solution with this boundary condition is equivalent to superposition of mirror images with respect to the boundary of the 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

$$c = \frac{M}{\rho(4\pi Et)^{3/2}} \exp - \frac{y^2+z^2}{4Et} \left[\exp - \frac{(x-L)^2}{4Et} + \exp - \frac{(x+L)^2}{4Et}\right] \qquad (2.73)$$

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 located next to the boundary, the concentration is increased to twice the value of the unbounded solution. In more complicated cases, the solution is obtained through superposition or other mathematical techniques. Consider an initial vertical distribution $c_o(z)$ in a two dimensional uniform flow with finite depth as shown in Fig 2.5. The initial condition is

$$c(x,z,0) = c_o(z)\, \delta(x) \qquad (2.74)$$

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

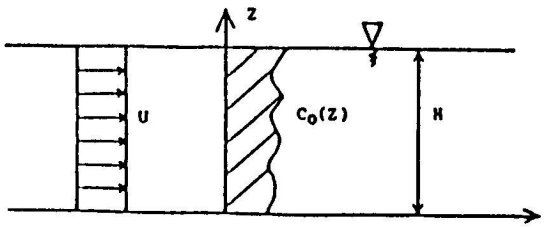

FIGURE 2.5 Diffusion in confined flow

$$X = x - Ut \tag{2.75}$$

can be written as

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial X^2} + E_y \frac{\partial^2 c}{\partial z^2} . \tag{2.76}$$

The boundary conditions are

$$\frac{\partial c}{\partial z} = 0, \qquad \text{on} \quad z = 0, H, \tag{2.77}$$

by virtue of (2.72). A Fourier cosine series solution

$$c = \sum_{n=0}^{\infty} \phi_n(X,t) \cos \frac{n\pi z}{H} \tag{2.78}$$

is assumed, satisfying the boundary conditions (2.77). The solution satisfying (2.76) is then obtained as follows

$$c = \frac{1}{(4\pi E_x t)^{1/2}} \exp - \frac{(x-Ut)^2}{4E_x t} \sum_{n=0}^{\infty} a_n \exp -(\lambda_n^2 t) \cos \frac{n\pi z}{H} \tag{2.79.a}$$

where

$$\lambda_n^2 = (n\pi/H)^2 E_z \tag{2.79.b}$$

and

$$a_o = \frac{1}{H} \int_0^H c_o(z)\, dz, \quad n=0 \tag{2.79.c,d}$$

$$a_n = \frac{2}{H} \int_0^H c_o(z) \cos \frac{n\pi z}{H}\, dz, \quad n=1,2,\ldots.$$

Note that each term in the series solution (2.79.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 times ($t>>H^2/(\pi^2E_z)$), the solution is

$$c = \frac{a_0}{(4\pi E_x t)^{1/2}} \exp - \frac{(x-Ut)^2}{4E_x t} \qquad (2.80)$$

i.e. uniformly distributed with depth and equivalent to that of an instantaneous plane source with strength $a_0=m''/\rho$ (cf. equation 2.44).

2.10 INFLUENCE OF VARIABLE DIFFUSION COEFFICENTS

As noted in Section 1.4, the assumption of constant diffusivity is actually inappropriate shortly after the release of a small 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) in the case of continuous line sources located on solid boundaries.

For these more advanced 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

The dramatic effects of velocity shear will first be demonstrated by a simple solution due to Okubo and Karweit (1969) who considered the linear velocity profile

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

for the x-component of velocity and obtained a solution to equation (1.25) for an instantaneous point source at x=0, y=0, z=0 and time t=0. The solution was obtained as

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

where

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

$$E_\xi = E_x (1 + \phi^2 t^2) \tag{3.3.b}$$

$$E^3 = E_\xi E_y E_z \tag{3.3.c}$$

and

$$\phi^2 = (\alpha^2 E_y + \beta^2 E_z)/(12 E_x) \tag{3.3.d}$$

It can be seen from the above that shortly after the release $(\phi t)^2 << 1$ the influence of shear is unimportant and the solution is very similar to the case without shear in (2.27). On the other hand, for large time $(\phi t)^2 >> 1$, the peak concentration decays as $t^{-5/2}$, much faster than the uniform flow solution with $t^{-3/2}$ decay. 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

$$E_\xi \approx E_x (\phi t)^2 = \frac{1}{2} \frac{\partial \sigma_\xi^2}{\partial t} \tag{3.4}$$

which yields

$$\sigma_\xi^2 = \frac{2}{3} E_x \phi^2 t^3 \tag{3.5}$$

and (3.4) can alternatively be expressed as

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

which is analogous to the "4/3 Law" (cf. 1.29) 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.

The shear flow dispersion behaviour differs considerably when the flow is confined between boundaries, for example in a shallow sea, where the no flux condition (2.72) applies at the bottom and the free surface. 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). We start with equation (1.25), or alternatively,

$$\frac{\partial c}{\partial t} + \nabla \cdot \vec{u} c + \frac{\partial}{\partial z} w c = \frac{\partial}{\partial z} E_z \frac{\partial c}{\partial z} + T - Kc \tag{3.7}$$

where use has been made of the continuity equation (1.3) 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 $T=\nabla\cdot E_H\cdot\nabla c$. We assume that the horizontal velocity and concentration can be separated into vertically averaged and fluctuating (deviation from the vertical average) components

$$c = \bar{c} + c'' \qquad u = \bar{\vec{u}} + u'' \tag{3.8.a,b}$$

where for instance

$$\bar{c} = \frac{1}{H}\int_{-h}^{\eta} c\, dz\ . \tag{3.9}$$

The free surface and the bottom are respectively defined at $z=\eta$ and $z=-h$, bounding a total depth $H=\eta+h$. Integrating the continuity equation (1.3) in the vertical yields

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

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

$$\frac{\partial \bar{c}}{\partial t} + \bar{\vec{u}}\cdot\nabla\bar{c} = -\frac{1}{H}\nabla\cdot H\overline{\vec{u}''c''} + \bar{T} - k\bar{c} \tag{3.11}$$

Subtracting (3.11) from (3.7) gives

$$\frac{\partial c''}{\partial t} + \bar{\vec{u}}\cdot\nabla c'' + \vec{u}''\cdot\nabla c'' + w\frac{\partial c''}{\partial z} + \vec{u}''\cdot\nabla\bar{c} = \frac{\partial}{\partial z}E_z\frac{\partial c''}{\partial z} + T'' + \frac{1}{H}\nabla\cdot H\overline{\vec{u}''c''} - kc''\ . \tag{3.12}$$

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 $\bar{c}$, 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

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

which is much easier to integrate.

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

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

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

$$O(1) + O(1) + O(1) + O(\frac{\mu}{\delta}) + O(\frac{1}{\epsilon}) = O(\frac{E_z}{HU}\frac{1}{\delta}) + O(\frac{E_H}{LU}) + O(1) + O(\frac{kL}{U}), \tag{3.15}$$

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 hand side and the first term in the right hand side (the terms of $O(\epsilon^{-1})$ and $O(\delta^{-1})$) dominate, yielding (3.13).

Equation (3.13) can be integrated twice, resulting in

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

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

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

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 $\bar{c}''(0)$ 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 (1.21), 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 tensor*.

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

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

where

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

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 (in principal coordinates), and $\hat{E}_{ij}$ is the total dispersion tensor. The dispersion coefficients K_{ij} depend 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). Since the vertical assymmetries of the current and concentration profiles contributing to (3.19) are predominant, it is natural to expect that $\hat{E}_{ij} \approx K_{ij}$ and therefore to neglect the turbulent diffusivity. Note that if the depth variations are small, we can write (3.20) as

$$\frac{\partial c}{\partial t} + \hat{u}\cdot\nabla c = \nabla\cdot\underline{\hat{E}}\cdot\nabla c - Kc \tag{3.22}$$

The reader is referred to Fischer *et al.* (1979) and Nihoul and Adam (1974) for examples of two-dimensional dispersion.

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

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x} A(K_x + \bar{E}_x)\frac{\partial \bar{c}}{\partial x} \tag{3.23}$$

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).

$$K_x = - \frac{1}{A \frac{\partial \bar{c}}{\partial \varepsilon}} \int_A \overline{u'' c''} \, dA \qquad (3.24)$$

is defined as the *longitudinal dispersion coefficient* where

$$\varepsilon = x - \bar{u} t \qquad (3.25)$$

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 shear flow in a pipe, taking the laminar equivalent of (3.26) written in cylindrical coordinates, from which c'' is calculated for laminar velocity profiles. Then he determined the longitudinal dispersion coefficient from (3.24), yielding

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

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 analogy*, which states that the transfer of mass, heat, momentum and turbulence are exactly analogous, he was able to relate the concentration and velocity profiles to the turbulent diffusivity, and obtained

$$E_L = K_x + E_x = 10.1 \, R \, u_* \qquad (3.28)$$

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

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

where $E_L = K_x + E_x$ and

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

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

$$\eta = z/h, \quad \phi = u^*/\sigma_u, \quad e = E_z/E_z, \tag{3.32.a-c}$$

where

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

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

we can also express (3.30) as

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

where

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

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

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

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 (3.12) balance the left hand side of (3.13) 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, a number of other effects modify the 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

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

where 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.

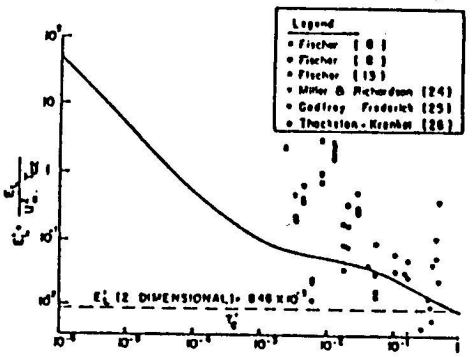

FIGURE 3.1 Longitudinal Dispersion coefficient in a rectangular channel (After Taylor, 1974).

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. 3.1. 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 as

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

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

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

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 (1965) investigated the dispersion coefficient in two dimensional oscillatory flow, but because he used equation (3.13) without due concern for the unsteady terms (for the limit $T \to \infty$), he obtained a longitudinal dispersion coefficient that is one half the value for steady unidirectional flow. 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

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

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

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

where

$$T_c = h^2/E_z \qquad (3.41.b)$$

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

$$\langle E_L \rangle_t = (E_L)_s + \langle E_L \rangle_o \qquad (3.42)$$

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

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

and

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

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

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

(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

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

and

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

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, $U_o=0$) and obtained an analytical solution from which an expression for $\langle E_L \rangle$ is obtained:

$$\langle E_L \rangle = E_o \, f(T') \qquad (3.46)$$

where

$$T' = T/T_c = T\,E_z/h^2$$

and (3.47)

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

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.3.2.a, where the ratio $\langle E_L \rangle / E_o$ 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_o on the left hand side of (3.46) by

$$E_o = \alpha\, I \sigma_u^2 h^2 / E_z = \alpha\, I \sigma_u^2 T \qquad (3.49)$$

assuming E_o, 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. Nevertheless, by combining (3.46), (3.49) and (3.50) we obtain

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

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

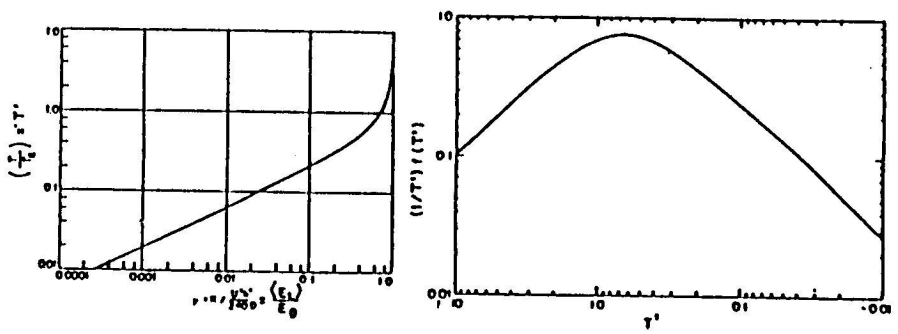

FIGURE 3.2 (a) Oscillatory flow dispersion coefficient, function f(T') (Holley *et al.*, 1970), and (b) the normalized function g(T') due to Fischer *et al.* (1979).

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. 3.2.b.

In all of the analyses discussed above, it has commonly been assumed 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 causing phase shifts which depend on position in the fluid, and which 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 analogous to (3.51), although the dependence on T' is modified compared to the Holley *et al.* (1970) solution. The results are plotted in Fig.3.3 where it is shown that a maximum value of $\langle E_L \rangle$ is obtained atcertain values of T_c depending on the period T.

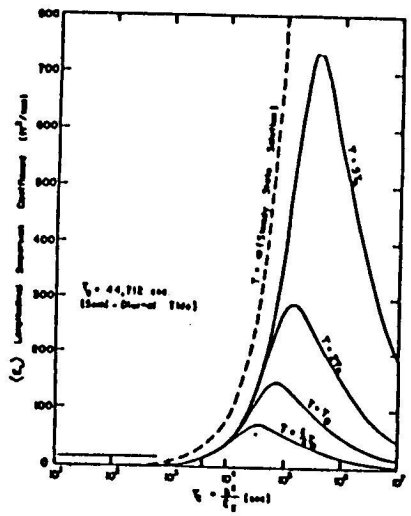

FIGURE 3.3 Oscillatory flow dispersion coefficient for different values of the period T (Taylor, 1974).

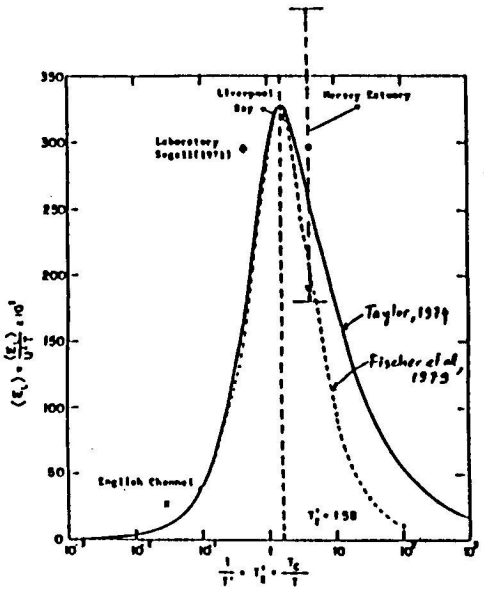

FIGURE 3.3 Normalized oscillatory flow dispersion coefficient (After Taylor, 1974 and Fischer *et al.*, 1979).

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

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

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 Fischer *et al.* (1979) based on the solution of Holley *et al.* (1970) in comparison to Taylor's (1974) results, as shown in Fig. 3.4. 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 rectangular 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. 3.4 for different values of the ratio T_{cz}/T_{cy}. Taylor has found that by varying $T_c'=T_{cz}/T_{cy}$ (cf. equation 3.38) in the

range 10^{-5} to 1, the peak value of the dispersion cofficient corresponding to Fig. 3.4 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

$$u = u_o \sin(mz) \cos(\omega t) \tag{3.53}$$

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

$$\langle E_L \rangle = \frac{1}{4} \left(\frac{u_o^2}{\omega}\right) \left(\frac{\kappa_e}{1+\kappa_e^2}\right) \tag{3.54.a}$$

where

$$\kappa_e = E_v m^2/\omega \ . \tag{3.54.b}$$

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=π/m, where the velocities vanish, i.e. a flow with a vertical extent and oscillation period of

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

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

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

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.3.4, 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.

$$\langle E_L \rangle \approx \left(\frac{mu_o}{2\omega}\right)^2 E_z, \quad \text{for } \kappa_e << 1 \tag{3.57.a}$$

and

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

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 steady flow dispersion, 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 conclude 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. The terms *suspended matter*, *suspended solids*, *suspended sediments*, *gelbstoff* or *seston* are widely applied to refer to these concentrations of solids. 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 previous approximations of Section 1.2 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. We modify (1.7.a), (1.9) and (1.10) to write

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

where the first term describes the diffusive flux and the second term the convective flux of suspended matter. Following the earlier developments of Section 1.2, we derive the turbulent diffusion equation

$$\frac{\partial c}{\partial t} + \vec{u}\cdot\nabla c - \frac{\partial w_s c}{\partial z} = \nabla\cdot\vec{E}\cdot\nabla c - \kappa c \tag{4.2}$$

in analogy with (1.25) or (3.22). The boundary conditions at a solid boundary are also modified as compared to (2.72). Since the velocity and the flux of material normal to the surface must vanish ($u=0$ and $N\cdot\hat{n}=0$) in (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 ($\hat{n}=\hat{k}$) becomes

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

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. 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

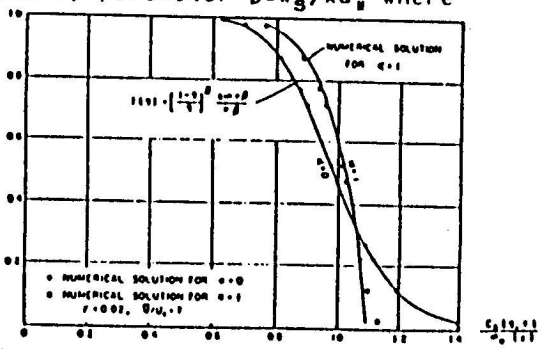

FIGURE 4.1 Vertical distribution of suspended matter for $\beta=0.1$ and at $\tau=0.5$ (After Sayre, 1970).

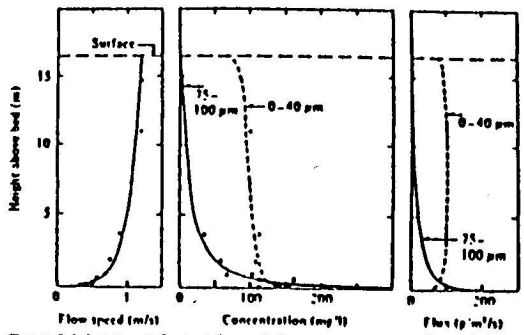

FIGURE 4.2 Profiles of velocity, concentration and flux of suspended sediments in the Thames estuary (After McCave, 1979).

κ=0.41 is Von Karman's constant. The concentration profile becomes time-independent (in the convected coordinates) after an initial time of τ>0.5, and is self similar. Sayre's solutions for τ>0.5, β=1, α=0 and α=1 are shown in Fig. 4.1. Jobson and Sayre (1970) verified their solutions with experimental data. 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.

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 vertical averaging following section 3.1 yields (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

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

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

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

In estimating the dispersion tensor E, Nihoul and Adam (1974) assume low concentrations of fine sediment and therefore neglect the influence of these terms in (4.6) 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 produces nonuniform distributions. It should therefore be expected that, in general the dispersion coefficient should be a function of settling velocity. Sayre(1969) and Sumer (1974) have taken the settling terms into account and have calculated the dispersion coefficient (normalized with respect to the neutrally buoyant case) as a function of the settling velocity as shown in Fig.4.3. With increasing settling velocity (e.g. sediment size), the dispersion is increased with respect to the neutrally buoyant case.

For completing the description of horizontal dispersion in (4.4), the flux term Q must be specified. This is often done

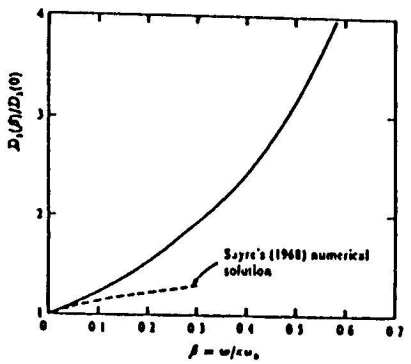

FIGURE 4.3 Longitudinal dispersion coefficient for suspended matter (normalized with respect to neutrally buoyant substances) as a function of B (After Sumer, 1979).

empirically and, neglecting the surface fluxes, Q represents the deposition losses to the bottom or reentrainment from the bottom into the flow. A model of practical importance (Sayre, 1969) is given by (4.3.c) and (4.5).

The flux terms should be different for the different processes of deposition and resuspension. For the 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. 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

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

In many estuaries, a turbidity maximum and a corresponding region of high deposition is found in the mid-reaches of the estuary, where the bed shear stress decreases 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 (1968)

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

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($\tau>\tau_c$). 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.

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 source/sink function (4.10) has been utilized by Ozsoy (1977, 1986) to model suspended sediment transport and deposition on the seaward side of a tidal inlet. During the ebb tide, the flow is in the form of a quasi-steady jet, with pronounced lateral diffusion. Then, using the jet velocity distribution obtained by Ozsoy and Unluata(1982), equation (4.4) with (4.10) is solved for the horizontal diffusion within the jet (Fig.4.4.a). Ambient concentrations, lateral entrainment into the jet, depth variations, bottom friction and settling velocity are taken into account. The contours of bottom deposition rate seaward of the inlet are computed via (4.11). In Fig.4.4.b, the inlet velocity is critical

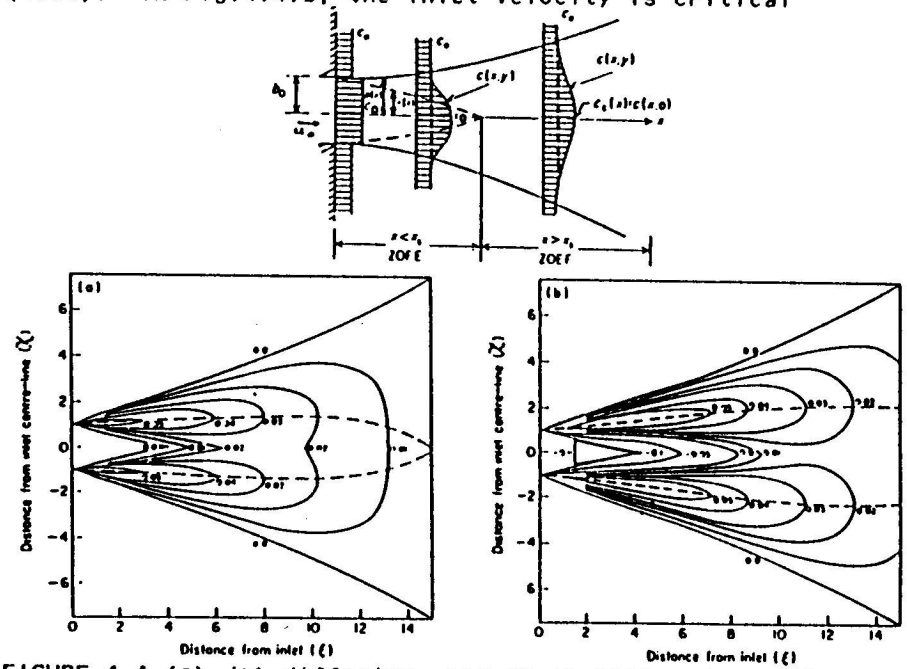

FIGURE 4.4 (a) Jet diffusion, and (b,c) bottom deposition of sediments near a tidal inlet (After Ozsoy, 1986).

$u_o=u_c$, 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. In the second case (Fig. 4.4.c), the inlet velocity exceeds the critical velocity ($u_o=1.4u_c$), and the material eroded at the jet core is deposited in the bar system encircling the mouth. The implications on tidal inlet morphology and river deltas are discussed in Ozsoy (1986). Wang (1984) has applied Ozsoy's model (although without due reference to the original solution provided by Ozsoy, 1977) to the dynamics and growth of a river delta.

Sediment diffusion and dispersion is an emerging field of study deserving much attention. It must however be stressed that the subject is a complicated one requiring considerable empirical guidance. Many aspects of sediment transport, such as the bed-load mode of transport have not been described within the limited scope of this course. 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, 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, the weather conditions etc. 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. 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.

Since estuarine processes are quite complicated, they are the subjects of detailed theory in their own right. 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).

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, transport processes in an estuary are highly dependent on the hydrodynamic and mixing characteristics, and therefore we venture for a brief review of the 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 turbulence, 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. According to a well known formula due to Munk and Anderson (1948), the vertical diffusivity decreases with increasing stratification and increases with increasing vertical shear. Fischer *et al.* (1979), however, caution for indiscriminate use of such formulas, since many other processes that need empirical definition can influence the diffusion processes.

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 (3.23) 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

$$A(x)\frac{\partial c}{\partial t} + Q_f\frac{\partial c}{\partial x} = \frac{\partial}{\partial x} A(x)(K_x+E_x)\frac{\partial c}{\partial x} \quad . \qquad (5.1)$$

Here, K_x is the longitudinal dispersion coefficient which must now be evaluated from (3.24) based on the different conditions of stratification, velocity distribution, transverse mixing etc., as summarized above.

In principle, the use of equation (5.1) 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 (5.1) 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 (5.1) 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 is idealized as a rectangular plug intruding the estuary. Over one tidal cycle, only a proportion of material introduced on the ocean side during flood will return to the ocean during the subsequent ebb-flow, leading to trapping within the estuary. The residual circulation 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

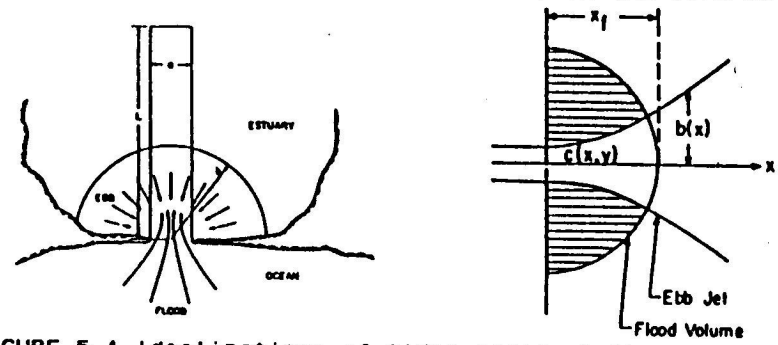

FIGURE 5.1 Idealizations of tidal residual flow near entrances (a) Stommel and Farmer (1952), (b) Ozsoy (1977)

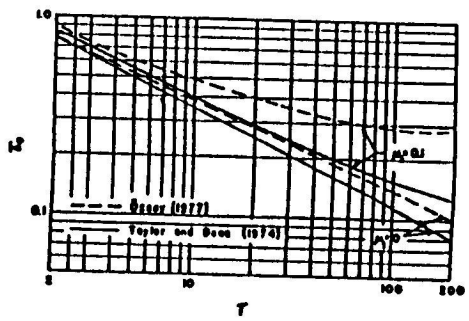

FIGURE 5.2 Ocean mixing coefficient as a function of bottom friction and tidal excursion (After Ozsoy, 1977).

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 Ozsoy and Unluata (1982) and Ozsoy (1986), allowing the calculation of exchange. 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 Ozsoy (1977) and Mehta and Ozsoy (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.

These concepts of tidal exchange at an entrance region has been applied by Ozsoy (1977) to the exchange of a pollutant between a bay and the ocean. 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

$$c_{if}^{n} = \gamma_o \, c_{ie}^{n-1} \tag{5.2}$$

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

$$c_{ie}^{n} = \gamma_b c_{if}^{n} + (1-\gamma_b) c_{be}^{n-1} \tag{5.3}$$

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, Ozsoy (1977) obtained the recursion formula

$$c_{be}^{n} = A_1 c_{be}^{n-1} + A_2 c_{be}^{n-2} \tag{5.4.a}$$

where

$$A_1 = 1 + \gamma_o\gamma_b - \frac{(1-\gamma_b)k}{(1-k/2)} \tag{5.4.b}$$

$$A_2 = \frac{(1-\gamma_b)\gamma_o(1+k/2)}{(1-k/2)} - \gamma_o \tag{5.4.c}$$

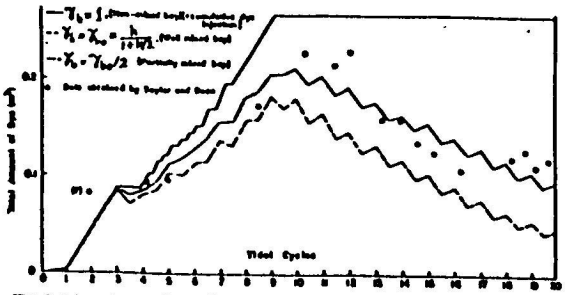

FIGURE 5.3 Total dye in Card Sound, experimental values (points) by Taylor and Dean (1974), and calculations by Ozsoy (1977)

and where

$$k = \Omega/V = 2a_o/h_b \qquad (5.4.d)$$

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.

Ozsoy (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 (5.4.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 completely mixed with the incoming tidal waters during flood, it is shown that γ_b should have the value $\gamma_b=k/(1+k/2)=\gamma_{bo}$. 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 $\gamma_b=\gamma_{bo}/2$ have yielded reasonable agreement with observations of Taylor and Dean (1974), which were obtained by integrating the dye concentration over the bay volume.

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 material in the mainstream flow and the fraction caught in the trap zones are seperated from each other. Shijf and Schonfeld (1953) and Okubo (1973) have studied tidal trapping, and have found that it may significantly contribute to dispersion 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*

$$T_{cv} = h^2/E_V, \quad \text{and} \quad T_{ch} = w^2/E_H \tag{5.5.a,b}$$

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

$$T_r = 0.4\ L^2/E_L \tag{5.6}$$

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):

$$T_f = V_f/Q_f \tag{5.7}$$

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

$$V_f = \int_V \frac{S_o - S}{S_o}\, dV = \int_V f\, dV = fV\ . \tag{5.8}$$

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, and $f=(S_o-S)/S_o$ 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

$$(V_P + V_R)S = V_P\, S_o\ . \tag{5.9.a}$$

where S is the mean salinity in the estuary, and the mean freshness is therefore $f=V_R/P$ where $P=V_P+V_R$ is the tidal prism. Then the tidal prism flushing time is

$$T_t = \frac{fV}{Q_f} = \frac{fV}{V_R/T} = \frac{V}{P}\,T \qquad (5.9.b)$$

with T being the tidal period. Since neither the entire estuary, nor the ebb-water on the ocean side are 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)

$$T_p = \rho cV/q \qquad (5.10)$$

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 $M_o = \rho V$. 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

$$\lim_{\tau \to \infty} M(\tau) = M_o \qquad (5.11)$$

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

$$\int_o^\infty \Psi(\tau)\, d\tau = 1 \qquad (5.12)$$

which is related to the cumulative function through

$$\Psi(\tau) = \frac{1}{M_o}\,\frac{dM(\tau)}{d\tau}\,. \qquad (5.13)$$

Secondly, consider a steady state volume flux F_o 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,

$$\lim_{\tau \to \infty} F(\tau) = F_o \qquad (5.14)$$

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

$$\int_0^\infty \Phi(\tau)\, d\tau = 1 \,. \qquad (5.15)$$

This frequency function is then

$$\Phi(\tau) = \frac{1}{F_o} \frac{dF(\tau)}{d\tau} \,. \qquad (5.16)$$

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

$$F_o - F(\tau) = M_o \Psi(\tau) = \frac{dM(\tau)}{d\tau} \,, \qquad (5.17)$$

or with the aid of (5.14)

$$\Phi(\tau) = - \frac{M_o}{F_o} \frac{d\Psi(\tau)}{d\tau} \,. \qquad (5.18)$$

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

$$\Psi(0) = \frac{F_o}{M_o} \,. \qquad (5.19)$$

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

$$\tau_o = \frac{M_o}{F_o} \,. \qquad (5.20)$$

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

$$\tau_t = \int_0^\infty \tau \Phi(\tau)\, d\tau = \frac{M_o}{F_o} = \tau_o \qquad (5.21)$$

which is integrated by making use of (5.18). Therefore, the average transit time and turn-over time equivalent. 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

$$\tau_a = \int_0^\infty \tau \Psi(\tau)\, d\tau = \frac{1}{M_o} \int_0^\infty \tau\, dM(\tau) \,. \qquad (5.22)$$

Since it is shown that $\tau_t = \tau_o$, 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, the sufficient condition (from 5.19, 5.21 and 5.22) is

$$\Psi(\tau) = \Phi(\tau) = \frac{1}{\tau_a} \exp(-\tau/\tau_a) \,. \qquad (5.23)$$

$\tau_a > \tau_t$:
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 (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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