

Boundary retention effects upon contaminant dispersion in parallel flows

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Mass transfer between a flowing region and an adjacent stationary medium can greatly alter the overall contaminant dispersion. Here, an extension is given of Taylor's (1953) method to encompass this class of complications. The only mathematical assumption made is that the mass flux transfer at the boundary depends linearly upon the concentration at earlier times. Expressions are derived for the longitudinal shear dispersion coefficient. Detailed results are presented for the effects both of reactions and of retention at the bed upon contaminant dispersion in turbulent open-channel flow.

1. Introduction

The problem of retention effects of dispersing contaminant at flow boundaries is common to many fluid flows and has several important applications in diverse fields such as biology, physiology, chromatography, chemistry and environment fluid mechanics.

The respiratory gas exchange between the body and its surroundings requires the inspired air to be heated to body temperature and humidified to saturation on its passage through the lung. This process and the removal of noxious gases (or particulate materials) involve mass transfer between the airstream and the walls of the respiratory tract. The analytical tool of gas chromatography employs a stationary gas phase deposited as a thin retentive layer on the inner wall of the tubular column. In a wide variety of problems of chemical engineering gaseous dispersion takes place with simultaneous chemical reaction. It is not uncommon for reactions carried out in a tubular reactor to be catalysed – deliberately or inadvertently – on the wall. The simple observation of a natural stream provides clear visual evidence how the contaminant is entrained into the dead zones which are caused by the meandering nature of streams and the long-term build-up of plant materials in the banks. Systems of less well-defined geometry are also frequently encountered, for example, an industrial pipe line in which stagnant fluid collects in the crevices of flanges, or at hollows of a corroded surface.

There are various forms of boundary conditions representing exchange between the main flow and the adjoining immobilized region. Some of these are listed in §1.1. A generalization of these boundary conditions is presented in §1.2.

1.1. *The variety of boundary conditions*

In the context of chromatography, Golay (1958) studied the dispersion of a gas flowing in a tubular column in which the inner walls of the column are coated with a thin uniform retentive layer. For the cases of rapid adsorption and desorption of

material, with concentration c , on and from the tube wall, the appropriate boundary condition at the tube wall is (Golay 1958, equation 8)

$$\frac{2D'}{r_0} \partial_r c = -k' \partial_t c, \quad \text{at } r = r_0, \quad (1.1)$$

where k' is the ratio of the amount of material adsorbed on the walls to that in the gas phase, and D' is the molecular diffusion coefficient.

The dispersion of a very reactive species (hydrogen atoms) in a gas flowing in a circular quartz tube, reported by Boddington & Clifford (1983), requires a further treatment that takes into account irreversible loss of the reactive species by reaction on the tube wall. In this situation the boundary condition at the tube wall is (Boddington & Clifford 1983, equations 1.6 and 1.7)

$$\frac{2D'}{r_0} \partial_r c = -\beta c - k' \partial_t c_s, \quad (1.2)$$

where β is the rate of loss of reactive species on the tube wall. The surface concentration, c_s , of the reactive species changes at a rate given by

$$k' \partial_t c_s = k_1 c - k_2 c_s; \quad (1.3a)$$

here k_1 and k_2 are the rate of adsorption and desorption at the tube wall, respectively. In the limit of no loss of reaction species on the walls (Boddington & Clifford 1983, §8),

$$k' = \frac{2k_1}{k_2 r_0}. \quad (1.3b)$$

Davidson & Schroter (1983) have studied the pattern of dispersion and uptake of an inhaled slug of tissue-soluble gas within a branching model of the bronchial wall, considered as an assembly of straight rigid tubes with absorbing wall of finite thickness. The airways are defined by two concentric circular cylinders. The inner cylinder defines the flowing gas phase while the annulus is the bronchial wall, considered for convenience as a stationary homogeneous liquid rather than a tissue compartment of unknown properties. The appropriate boundary condition at the gas-tissue interface is (Davidson & Schroter 1983, equation (2*a*, *b*))

$$D'_2 \partial_r c_2 = D'_1 \partial_r c_1. \quad (1.4)$$

Also, the injected solute is soluble in tissue, according to an approximately linear equilibrium relation at the gas-tissue interface

$$c_2 = k_0 c_1, \quad (1.5)$$

where c_1 and c_2 are solute concentration in the gas and the tissue respectively, for which the corresponding molecular diffusion coefficients are D'_1 and D'_2 , and k_0 is the solubility coefficient.

Fischer (1967) gave details of the variation of contaminant concentration, c , in an open-channel flow over its depth, and showed that at large times, the contaminant is concentrated near the bottom of the channel, and it is in this region that the differences between c and the value predicted are most marked. These observations suggest that the mechanism of the dispersion process in the region near the bed, such as the retentive (viscous sub-) layer, is important. To illustrate this effect of the viscous sublayer on longitudinal dispersion, Chatwin (1973) assumed that the flow

field is sharply divided into two layers of fluids with molecular diffusivities κ_1 and κ_2 and that contaminant can be exchanged between the two layers only by molecular diffusion (see also Elder 1959). Then the appropriate boundary condition across the sublayer surface is (Chatwin 1973, equation 3.5iv)

$$\kappa_1 \partial_y c = \kappa_2 \partial_y c, \quad \kappa_1 \ll \kappa_2. \quad (1.6)$$

The vertical mixing outside the retentive layer is dominated by turbulent velocity fluctuations, but within the retentive layer and sufficiently close to the bed the lateral mixing is essentially caused by molecular diffusion, since the velocity fluctuation falls to zero at the bed. This is difficult to quantify in view of the ignorance of the mechanics of the motion in the retentive layer. Purnama (1988) modelled the retentive layer as a random distribution of stagnant pocket of variable depths.

Storage in the retentive layer bears much the same relation to dispersion in two-dimensional flow as does storage in the dead zones to dispersion in the main flow part of a natural stream. In particular, for natural streams, the interstitial volume of the stone bed could have formed a dead zone for zero velocity in which temporary storage of the contaminant occurred. These dead water regions may significantly be isolated from the main stream. Valentine & Wood (1977) analysed numerically the effect of stationary eddy structure adjacent to the bed upon longitudinal dispersion in two-dimensional open-channel flow. The boundary condition at the bed requires an interchange of concentration between the dead zones and the main flow, and it is assumed that the mass transfer across the interface is proportional to the concentration difference across it, namely

$$\kappa' \partial_y c = \alpha(c - c_d), \quad (1.7)$$

here κ' is the eddy diffusivity, and the mean concentration in the dead zones c_d is governed by

$$\partial_t c_d = \gamma(c - c_d). \quad (1.8)$$

The exchange parameters α , γ relate to the relative volume of the dead zones and to the mixing process.

1.2. Unified treatment

A common phenomenon in all the cases described above is that the contaminant which migrates into the retentive layer is (more generally captured and) released some time after passage of the main part of the contaminant cloud. In this paper, the boundary retention effect upon the contaminant dispersion is analysed using an extension to the method used by Taylor (1953), with the assumption that the rate of contaminant flux across the retentive layer is proportional to the concentration at earlier times. This leads us to pose a provisional boundary condition, at the flow boundary ∂A ,

$$\kappa \mathbf{n} \cdot \nabla c = - \int_0^\infty J(\tau) c(t - \tau) d\tau \quad \text{on } \partial A, \quad (1.9)$$

where κ is the transverse diffusivity tensor, and the kernel $J(\tau)$ measures the diffusive effect of the time-lag between the contaminant concentrations across the retentive layer. Note that we do not prescribe the mechanisms of motion and dispersion within the retentive layer, but all these are embodied within $J(\tau)$. The retentive layer is a representation of all the dead zones within the river, on the bed, and along the banks, being spread into an equivalent uniform thickness on the river banks.

If we denote a Laplace transform by a hat, then a general form of the boundary condition (1.9) for the exchange between the flow and the surrounding immobilized medium is

$$\kappa \mathbf{n} \cdot \nabla \hat{c} = -\hat{J}(p) \hat{c} \quad \text{on } \partial A. \quad (1.10)$$

There is considerable freedom in the way that the boundary condition can be written. In particular, we can write

$$\kappa \mathbf{n} \cdot \nabla \hat{c} = -\hat{J}(0) \hat{c} - p \hat{I}(p) \hat{c} \quad \text{on } \partial A, \quad (1.11a)$$

where

$$\hat{I}(p) = \frac{\hat{J}(p) - \hat{J}(0)}{p}. \quad (1.11b)$$

The advantage is that for large p the new kernel $\hat{I}(p)$ is better behaved than $\hat{J}(p)$. Inverting the Laplace transform, we derive the boundary condition

$$\kappa \mathbf{n} \cdot \nabla c = -\hat{J}(0) c - \partial_t \int_0^\infty I(\tau) c(t-\tau) d\tau \quad \text{on } \partial A. \quad (1.12)$$

This particular formulation of the boundary conditions has the advantage of being an obvious generalization of the boundary conditions given in the previous subsection. For example, the Boddington & Clifford (1983) boundary conditions (1.2), (1.3) correspond to

$$\hat{J}(0) = \beta, \quad I(\tau) = k_1 \exp\left(-\frac{k_2}{k'} \tau\right). \quad (1.13a, b)$$

The dead-zones model (1.7), (1.8) has a similar exponential structure:

$$\hat{J}(0) = 0, \quad I(\tau) = \alpha \exp(-\gamma \tau). \quad (1.14a, b)$$

When the concentration within the retentive layer is governed by partial (rather than ordinary) differential equations the structure of $I(\tau)$ is more complicated (see Appendix). It would be straightforward to adapt the analysis presented in this paper to encompass other formulations of the boundary conditions.

2. Advection–diffusion equation

In keeping with the generality of the dispersion concept, we start our mathematical analysis with the advection–diffusion equation for the contaminant concentration $c(x, y, z, t)$:

$$\partial_t c + u \partial_x c - \nabla \cdot (\kappa \nabla c) = 0, \quad (2.1a)$$

with the boundary condition

$$\kappa \mathbf{n} \cdot \nabla c = -\beta c - \partial_t \int_0^\infty I(\tau) c(t-\tau) d\tau \quad \text{on } \partial A, \quad (2.1b)$$

where $u(y, z)$ is the longitudinal velocity directed along the x -axis, $\kappa(y, z)$ the transverse diffusivity tensor, ∇ the transverse gradient operator $(0, \partial_y, \partial_z)$, and \mathbf{n} the outward normal.

We have ignored direct longitudinal diffusion, on the assumption that after a short distance downstream it is dominated by shear dispersion (Taylor's 1953 Condition A). The term $-\beta c$ on the right-hand side of the defining boundary condition (2.1b) represents an irreversible (possibly catalysed) boundary reaction, which reflects the effect of contaminant removal. The case when $\beta = 0$ is usually referred to as the

dispersion of a passive (neutrally buoyant and chemically inert) contaminant. Subsequently, the case of $\beta \neq 0$ can be referred to as the dispersion of reaction (or chemically active) contaminant. In contrast, the second term on the right-hand side of (2.1*b*) represents a non-absorbing conservative boundary term, which measures the amount of contaminant held in the stationary medium.

In the steady state, (2.1*a*) admits an exponentially decaying solution $\exp(-\lambda x)$ with a corresponding non-negative asymptotic profile $\psi(y, z)$ for the concentration variation across the entire flow:

$$\nabla \cdot (\kappa \nabla \psi) + \lambda u \psi = 0, \quad (2.2a)$$

with

$$\kappa \mathbf{n} \cdot \nabla \psi = -\beta \psi \quad \text{on } \partial A, \quad (2.2b)$$

$$\overline{\psi^2} = 1, \quad \psi \geq 0. \quad (2.2c, d)$$

In the problems of heat transport through the cooling circuits of nuclear reactors, or more generally, in any heat exchanger circuit, the boundary condition (2.2*b*) represents the leakage of heat from the thermal (wall) conductor (Lungu & Moffatt 1982). The combined effects of diffusion and boundary adsorption are to erode the concentration variations towards this equilibrium profile $\psi(y, z)$. Note that the total contaminant in the flow is no longer a conserved quantity. The corresponding asymptotic decay rate can be written in terms of the interior and boundary values of $\psi(y, z)$:

$$\lambda = \frac{\overline{\kappa (\nabla \psi)^2} + \frac{1}{A} \oint \beta \psi^2}{u \overline{\psi^2}}, \quad (2.3)$$

where \oint denotes an integration around the flow boundary ∂A . No matter how small the value of λ , at sufficiently large time after discharge it is this decay rate that determines the total amount of contaminant remaining in the flow. In (2.3) the overbars denote the cross-sectional average values, and A is the cross-sectional areas.

As a temporary expedient, it is convenient to factor out this intrinsic decay, and the intrinsic asymptotic concentration profile, by means of a change of dependent variable

$$c = \psi(y, z) C(x, y, z, t) \exp(-\lambda x). \quad (2.4)$$

The new dependent variable $C(x, y, z, t)$ satisfies the advection-diffusion equation

$$\psi^2 \partial_t C + u \psi^2 \partial_x C - \nabla \cdot (\psi^2 \kappa \nabla C) = 0, \quad (2.5a)$$

with

$$\psi^2 \kappa \mathbf{n} \cdot \nabla C = -\psi^2 \partial_t \int_0^\infty I(\tau) C(t-\tau) d\tau \quad \text{on } \partial A. \quad (2.5b)$$

No approximations have been made. The advantage of (2.5*a, b*) over (2.1*a, b*) lies in the simplicity of the solution for $C(x, y, z, t)$ at large distances downstream.

The initial discharge distribution of $C(x, y, z)$ is not expected to affect the general conclusions (provided there is not extremely slow exchange between the main flow and the retentive layer), and therefore for simplicity it will be assumed that

$$C = \frac{\delta(x) \delta(z)}{A} \quad \text{at } t = 0. \quad (2.6)$$

3. The extension of Taylor’s (1953) method

Taylor (1953) imposed two conditions to analyse the dispersion of soluble matter in solvent flowing through a tube. These are:

(A) The changes in C due to convective transport along the tube take place in a time that is so short that the effect of molecular diffusion may be neglected.

(B) The time necessary for appreciable effects to appear, owing to convective transport, is long compared with the ‘time of decay’ during which radial variations of concentration are reduced to a fraction of their initial value through the action of molecular diffusion.

To study slow evolution of the contaminant distribution it is convenient to use axes moving at the bulk velocity \tilde{U} . In keeping with the work of Taylor (1953) and of Fischer (1967), we assume that the timescale upon which we are studying the dispersion process is sufficiently long that the contaminant is nearly uniformly distributed across the entire flow. So that, in the moving coordinate system,

$$\xi = \epsilon(x - \tilde{U}t), \tag{3.1a}$$

$$T = \epsilon^2 t, \tag{3.1b}$$

any evolution of the bulk concentration is associated with dispersion and not merely the non-uniform advection. The presence of the parameter ϵ serves to indicate that the longitudinal lengthscale ξ of the contaminant cloud is to be thought of as being much longer than the lengthscale x for mixing across the channel, with a correspondingly slow timescale T for the longitudinal dispersion.

In the (ξ, T) -coordinates, (2.5a, b) for $C(\xi, y, z, T)$ become

$$-\nabla \cdot (\psi^2 \kappa \nabla C) + \epsilon \psi^2 (u - \tilde{U}) \partial_\xi C + \epsilon^2 \psi^2 \partial_T C = 0, \tag{3.2a}$$

with

$$\psi^2 \kappa \mathbf{n} \cdot \nabla C = \psi^2 (\epsilon \tilde{U} \partial_\xi - \epsilon^2 \partial_T) \int_0^\infty I(\tau) C(\xi + \epsilon \tilde{U} \tau, y, z, T - \epsilon^2 \tau) d\tau \quad \text{on } \partial A. \tag{3.2b}$$

For small ϵ the memory term can be expanded

$$\psi^2 \kappa \mathbf{n} \cdot \nabla C = \epsilon \tilde{U} \psi^2 \int_0^\infty I(\tau) \partial_\xi C d\tau - \epsilon^2 \psi^2 \int_0^\infty I(\tau) (\partial_T C - \tilde{U}^2 \tau \partial_\xi^2 C) d\tau + \dots \tag{3.2c}$$

We again make explicit use of the fact that ϵ is small and formally expand the solution to (3.2a, b) in the form

$$C = C_0(\xi, T) + \epsilon C_1(\xi, y, z, T) + \epsilon^2 C_2(\xi, y, z, T) + \dots \tag{3.3}$$

where the C_i are all independent of ϵ . For simplicity we shall ignore possible ϵ -dependence of the transverse diffusivity tensor $\kappa(y, z)$. To leading-order terms, (3.2a, b) are satisfied trivially if C_0 is laterally well mixed. (Indeed, we can identify C_0 with the cross-sectional average concentration $\overline{\psi^2 C}$.) Also without loss of generality, we can require that the correction terms C_1, C_2, \dots give no net contribution to the concentration when ψ^2 -weighted integrated over the entire flow.

From (3.2a, b) it follows that to first approximation C_1 satisfies the equation

$$\nabla \cdot (\psi^2 \kappa \nabla C_1) = (u - \tilde{U}) \psi^2 \partial_\xi C_0, \tag{3.4a}$$

with

$$\psi^2 \kappa \mathbf{n} \cdot \nabla C_1 = \tilde{U} \partial_\xi C_0 \psi^2 \int_0^\infty I(\tau) d\tau \quad \text{on } \partial A, \quad (3.4b)$$

and

$$\overline{\psi^2 C_1} = 0. \quad (3.4c)$$

By integrating (3.4a) over the entire flow, using (3.4b), we derive the bulk velocity

$$\tilde{U} = \frac{\overline{u\psi^2}}{1 + \frac{1}{A} \oint \psi^2 \int_0^\infty I(\tau) d\tau} = \frac{\overline{u\psi^2}}{1 + \mathcal{J}_0}. \quad (3.5)$$

Note that \tilde{U} is a fraction smaller than the asymptotic advection velocity $\overline{u\psi^2}$. As the contaminant cloud moves forward the retention of contaminant at the flow boundary removes contaminant to the retentive layer at the front and unloads contaminant into the flow at the rear. The quantity \mathcal{J}_0 depends only upon the integral around the flow boundary of the product of the asymptotic concentration ψ^2 and the total volume retention

$$\int_0^\infty I(\tau) d\tau.$$

On the right-hand side of (3.4a) the $\partial_\xi C_0$ factor can be regarded as remaining constant on the x -lengthscale. This leads to a gradient formula:

$$C_1 = -G(y, z) \partial_\xi C_0, \quad (3.6)$$

where the auxiliary function $G(y, z)$ describes the balance between shear and diffusion and satisfies

$$\nabla \cdot (\psi^2 \kappa \nabla G) = -(u - \tilde{U}) \psi^2, \quad (3.7a)$$

with

$$\psi^2 \kappa \mathbf{n} \cdot \nabla G = -\tilde{U} \psi^2 \int_0^\infty I(\tau) d\tau \quad \text{on } \partial A, \quad (3.7b)$$

and

$$\overline{\psi^2 G} = 0. \quad (3.7c)$$

The normalization (3.7c) restates that C_1 does not contribute to the total average concentration. Note also that, from (3.6), $G(y, z)$ gives the shape of the longest persisting concentration profile across the entire flow, usually referred to as the shape factor.

In order to assess the role of the boundary retention effect (Purnama 1988), we decompose $G(y, z)$, into parts associated with the velocity shear $u(y, z)$ and the retention effect,

$$G(y, z) = \frac{g(y, z) + f(y, z) \mathcal{J}_0}{1 + \mathcal{J}_0}. \quad (3.8)$$

The conventional (no retention, i.e. $I(\tau) = 0$) centroid displacement function $g(y, z)$ is the solution of the diffusion equation

$$\nabla \cdot (\psi^2 \kappa \nabla g) = -(u - \overline{u\psi^2}) \psi^2, \quad (3.9a)$$

with

$$\psi^2 \kappa \mathbf{n} \cdot \nabla g = 0 \quad \text{on } \partial A, \quad (3.9b)$$

and

$$\overline{\psi^2 g} = 0. \quad (3.9c)$$

Note that $\overline{g(y, z)}$ tends to be positive where $u(y, z)$ exceeds the asymptotic advection velocity $u\overline{\psi^2}$ (see figure 4). On the other hand the term associated with the boundary retention $f(y, z)$ satisfies

$$\nabla \cdot (\psi^2 \kappa \nabla f) = -u\psi^2, \tag{3.10a}$$

with

$$\psi^2 \kappa \mathbf{n} \cdot \nabla f = Au\overline{\psi^2} \quad \text{on } \partial A, \tag{3.10b}$$

and

$$\overline{\psi^2 f} = 0. \tag{3.10c}$$

The equivalent form of (3.9a-c) and (3.10a-c) for the passive contaminant, $\psi = 1$, are given by equations (4.4a-c) and (4.8a-c) respectively of Purnama (1988).

4. Longitudinal dispersion equation

The vital contribution of Taylor (1953) to the theory of contaminant dispersion was to recognize that, without the C_1 correction term in the presentation (3.3), there is no shear dispersion, only the comparatively weak mechanism of direct longitudinal diffusion. In (2.1a, b) we have already neglected direct longitudinal diffusion. As long as there is some concentration variation across the entire flow, the different velocities in different parts of the flow provides an efficient mechanism for longitudinal dispersion. Thus the role of C_1 is highlighted when we cross-sectionally average (3.2a, b) to derive an evolution equation for C_0 :

$$(1 + \mathcal{J}_0) \partial_T C_0 + \overline{(u - \tilde{U}) \psi^2 \partial_\xi C_1} - \tilde{U} \frac{1}{A} \oint \psi^2 \int_0^\infty I(\tau) \partial_\xi C_1 d\tau - \tilde{U}^2 \partial_\xi^2 C_0 \mathcal{J}_1 = O(\epsilon). \tag{4.1a}$$

Mathematically this can be recognized as a non-secularity condition which ensures that the solution for C_2 has no systematic growth with respect to x . Here \mathcal{J}_1 denotes the first moment of $I(\tau)$, that is

$$\mathcal{J}_1 = \frac{1}{A} \oint \psi^2 \int_0^\infty \tau I(\tau) d\tau. \tag{4.1b}$$

Substituting (3.6) into (4.1a), we arrive at the longitudinal shear dispersion equation

$$(1 + \mathcal{J}_0) \partial_T C_0 - \left(\overline{(u - \tilde{U}) \psi^2 G} - \tilde{U} \frac{1}{A} \oint \psi^2 G \int_0^\infty I(\tau) d\tau + \tilde{U}^2 \mathcal{J}_1 \right) \partial_\xi^2 C_0 = 0. \tag{4.2}$$

If we multiply (3.7a) by $G(y, z)$ and integrate over the entire flow, then we can derive the identity

$$\overline{(u - \tilde{U}) \psi^2 G} - \tilde{U} \frac{1}{A} \oint \psi^2 G \int_0^\infty I(\tau) d\tau = \overline{\psi^2 \kappa (\nabla G)^2}. \tag{4.3}$$

Thus, we can rewrite (4.2) as

$$\partial_T C_0 - D \partial_\xi^2 C_0 = 0, \tag{4.4}$$

where the longitudinal shear dispersion coefficient D is given by

$$D = \frac{\overline{\psi^2 \kappa (\nabla G)^2} + \tilde{U}^2 \mathcal{J}_1}{1 + \mathcal{J}_0}. \tag{4.5}$$

This is strictly non-negative.

The extension to the work of Taylor (1953) has now been made, and this is easily checked in (4.5). For the passive contaminant, $\psi = 1$, and with no retention at the

flow boundary, $I(\tau) = 0$, it reduces to that well-known Taylor longitudinal shear dispersion coefficient. Note also that the second term in the numerator represents explicitly the contribution of the dispersion in the retentive layer. It involves only the retentive-layer properties, and is independent of the main flow velocity profile $u(y, z)$.

Alternatively, using the decomposition (3.8), we obtain

$$(1 + \mathcal{J}_0)^2 D = (u - \overline{u\psi^2}) \psi^2 g + \overline{u\psi^2} f \mathcal{J}_0 - \frac{\overline{u\psi^2} \frac{1}{A} \oint \psi^2 (g + f \mathcal{J}_0) \int_0^\infty I(\tau) d\tau}{1 + \mathcal{J}_0} + \frac{(\overline{u\psi^2})^2 \mathcal{J}_1}{1 + \mathcal{J}_0}. \tag{4.6}$$

For the open-channel flow (see §5), and from (3.9a, b) and (3.10a, b), we note that

$$\psi^2 \kappa \partial_y g = - \int_0^y (u - \overline{u\psi^2}) \psi^2 dy, \tag{4.7a}$$

and
$$\psi^2 \kappa \partial_y f = - \int_0^y u \psi^2 dy. \tag{4.7b}$$

A further integration of (4.7a, b), using the constraints (3.9c) and (3.10c), and rearranging terms, yields the solution

$$g - f = \overline{u\psi^2} \frac{1}{h} \int_{-h}^0 dy \frac{1}{\psi^2 \kappa} \left(\int_0^y \psi^2 dy' \right)^2 \quad \text{on } y = 0. \tag{4.7c}$$

It is now straightforward to obtain a formula for D , which only involves the velocity $u(y)$, diffusivity $\kappa(y)$, and asymptotic concentration $\psi(y)$ profiles:

$$\begin{aligned} (1 + \mathcal{J}_0)^2 D &= \frac{1}{h} \int_{-h}^0 dy \frac{1}{\psi^2 \kappa} \left(\int_{-h}^y \psi^2 (u - \overline{u\psi^2}) dy' \right)^2 \\ &+ \left(\frac{1}{h} \int_{-h}^0 dy \frac{1}{\psi^2 \kappa} \left(\int_0^y u \psi^2 dy' \right)^2 \right) \mathcal{J}_0 \\ &+ \frac{(\overline{u\psi^2})^2 \left(\frac{1}{h} \int_{-h}^0 dy \frac{1}{\psi^2 \kappa} \left(\int_0^y \psi^2 dy' \right)^2 \right) \mathcal{J}_0}{1 + \mathcal{J}_0} + \frac{(\overline{u\psi^2})^2 \mathcal{J}_1}{1 + \mathcal{J}_0}. \end{aligned}$$

Again, in the limit of zero retention, this reveals the crucial role of the velocity shear $u(y)$, and the strong weighting towards parts of the flow with large $\psi(y)$ or small $\kappa(y)$ (Smith 1986, equation (4.8)). Note that, in this case

$$\mathcal{J}_n = \frac{1}{h} \psi^2(-h) \int_0^\infty \tau^n I(\tau) d\tau \quad (n = 0, 1, \dots). \tag{4.9}$$

5. Turbulent open-channel flow

One of the commonest applications of the theory of longitudinal dispersion has been to turbulent open channels, rivers and canals. Here we shall consider the retentive layer to be stagnant; as shown in the Appendix this is a good approximation to the dead-zone model, which takes into account the stationary eddies trapped behind roughness of the bed in an open-channel flow.

For straight channels the turbulent diffusivities for mass and momentum scale as the product of the water depth h and the friction velocity u_* (Elder 1959; Fischer 1967). Then, the velocity and diffusivity can be modelled as (Smith 1986, equations (6.1*a-d*))

$$u = \bar{u} + \frac{u_*}{k} (1 + \ln \eta) = \frac{u_*}{k} \ln \left(\frac{\eta}{\eta_*} \right), \quad (5.1a)$$

$$\kappa = kh u_* \eta (1 - \eta), \quad (5.1b)$$

with

$$\eta = \eta_* + \left(1 + \frac{y}{h} \right) (1 - \eta), \quad u_* = \frac{k\bar{u}}{\ln \left(\frac{1}{\eta_*} \right) - 1}. \quad (5.1c, d)$$

Here \bar{u} is the discharge velocity, the von Kármán's constant k is equal to about 0.4, and η_* is a dimensionless roughness height. Typically u_* is about $\frac{1}{15}\bar{u}$, which implies that η_* is about 0.001. As pointed out by Chatwin (1970) there are severe faults with the representations (5.1*a, b*): the validity of Reynolds analogy which gives $\kappa(\eta)$ is suspect, the form of $u(\eta)$ neglects the important viscous sublayer, and turbulent flow may not have been truly two-dimensional because of the presence of the sidewalls. (The model ignores the retention at the free surface.) In spite of these remarks, dispersion in turbulent flow in a channel has been widely studied by engineers in many practical contexts using these equations.

If we ignore terms of order η_* , then the asymptotic concentration profile equation (2.2*a*) transforms to

$$\partial_\eta(\eta(1-\eta) \partial_\eta \psi) + v \left(\frac{u_*}{k\bar{u}} \right) \left(1 + \frac{u_*}{k\bar{u}} (1 + \ln \eta) \right) \psi = 0, \quad (5.2a)$$

$$\lambda = v \frac{1}{h} \left(\frac{u_*}{\bar{u}} \right)^2. \quad (5.2b)$$

In the limit of zero roughness, we can ignore the boundary condition (2.2*b*) and the solution is trivially $\psi = 1$.

To leading order the boundary condition (2.2*b*) at the bed becomes

$$\eta_* \partial_\eta \psi = B \left(\frac{u_*}{k\bar{u}} \right) \psi \quad \text{at } \eta = \eta_*, \quad (5.3a)$$

where the irreversible loss of contaminant at the bed is determined by the bed absorption coefficient (Smith 1986, equation (6.5*c*))

$$B = \frac{\beta \bar{u}}{u_*^2}. \quad (5.3b)$$

Using the fact that there is an implicit small parameter (u_*/\bar{u}) , we pose an expansion

$$\psi = 1 + \left(\frac{u_*}{k\bar{u}} \right) \phi + \dots, \quad (5.4a)$$

where the correction term ϕ satisfies

$$\partial_\eta(\eta(1-\eta) \partial_\eta \phi) + v = 0, \quad (5.4b)$$

with

$$\eta_* \partial_\eta \phi = B \quad \text{on } \eta = \eta_*. \quad (5.4c)$$

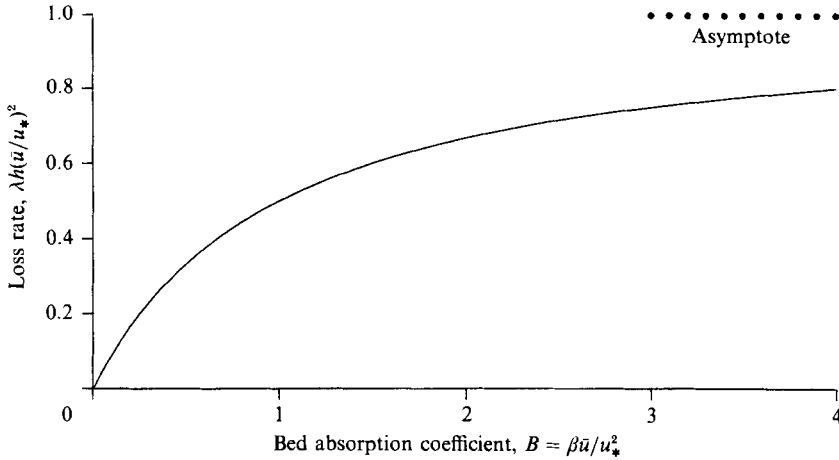


FIGURE 1. The dependence of the asymptotic loss rate λ upon the bed absorption coefficient B in turbulent open-channel flow.

Thus, without loss of generality, we take the solution to be

$$\psi(\eta) = 1 + \frac{B}{1+B} \left(\frac{u_*}{k\bar{u}} \right) (1 + \ln \eta) + \dots, \tag{5.5a}$$

with
$$v = \frac{B}{1+B}. \tag{5.5b}$$

The dots indicate neglected terms of order $(u_*/\bar{u})^2$.

The asymptotic loss rate (5.2b) is given by

$$\lambda = \frac{B}{1+B} \frac{1}{h} \left(\frac{u_*}{\bar{u}} \right)^2. \tag{5.6}$$

For large B , the finite concentration gradient limits the diffusive flux of contaminant towards the bed, hence the loss rate asymptotes to a constant (figure 1). As pointed out by Smith (1986), in the limit of total absorption ($B \rightarrow \infty$) the e-folding distance is about 225 times the water depth. The asymptotic concentration profile $\psi(\eta)$ (5.5a) is shown in figure 2 for $u_*/\bar{u} = \frac{1}{15}$ and $k = 0.4$. The main effect of the efficient removal of contaminant at the bed is, therefore, to bring the concentration close to zero at the bed. At the bed itself we have a neat result:

$$\psi = \frac{1}{1+B} \quad \text{on } \eta = \eta_*. \tag{5.7}$$

As indicated by the logarithmic term in (5.5a), the effect of the boundary absorption is predominantly local to the bed. Thus, we might expect that there is only small change to the bulk velocity \tilde{U} . If we quantify the bed retention volume in terms of a parameter δ , as

$$\int_0^\infty I(\tau) d\tau = \delta h \left(\frac{u_*}{k\bar{u}} \right), \tag{5.8a}$$

then
$$\mathcal{J}_0 = \delta \left(\frac{1}{1+B} \right)^2 \left(\frac{u_*}{k\bar{u}} \right). \tag{5.8b}$$

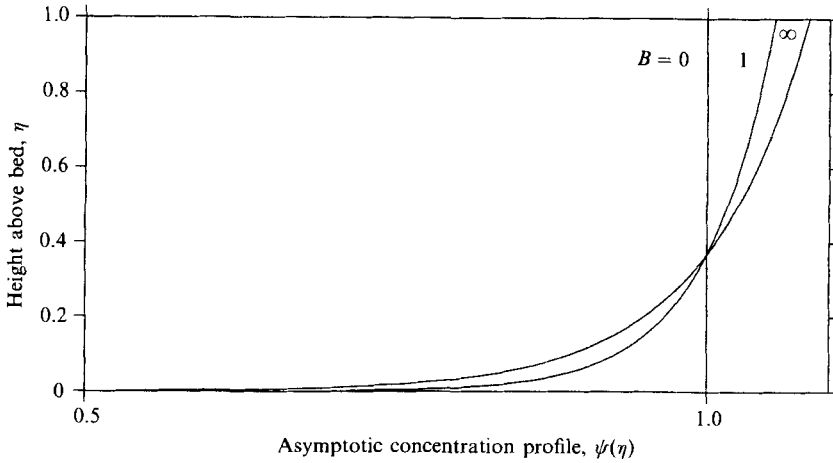


FIGURE 2. The asymptotic concentration profile across the flow when the bed absorption coefficient B has the values 0, 1 and ∞ .

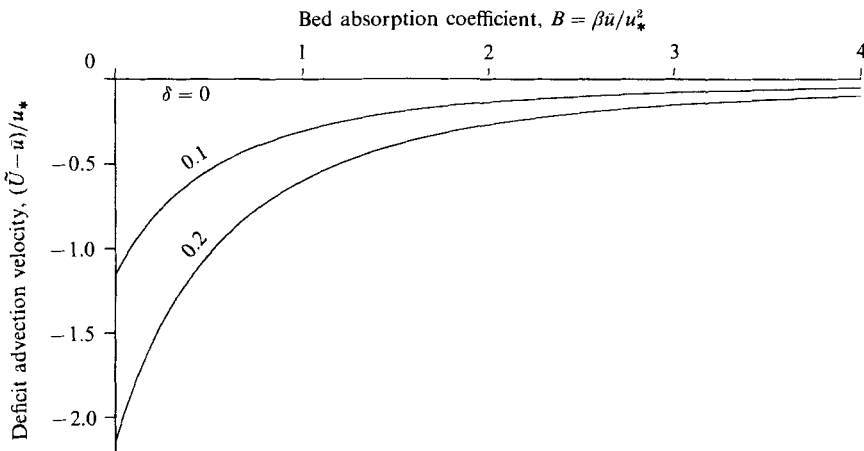


FIGURE 3. The dependence of the bulk velocity \tilde{U} upon the bed absorption coefficient B , when the bed retention layer depth has the values $\delta = 0, 0.1$ and 0.2 .

This parameter δ can also be related to the retentive stagnant layer of depth l (see Appendix):

$$\frac{l}{h} = \frac{\delta}{6}. \tag{5.8c}$$

At the leading order, we obtain

$$\tilde{U} = \frac{\bar{u}}{1 + \delta \left(\frac{1}{1+B} \right)^2 \left(\frac{u_*}{k\bar{u}} \right)}. \tag{5.8d}$$

Figure 3 shows the bulk velocity \tilde{U} as a function of the bed absorption coefficient B as the retention-layer depth increases. We observe that in the absence of bed absorption (i.e. $B = 0$), \tilde{U} decreases (because of the involvement of contaminant in the retentive layer) by an amount that increases in the retentive-layer depth. That

is, the larger the retention volume, the more time a passive contaminant spends there (Valentine & Wood 1977).

To quantify the effect of bed retention we need to evaluate the centroid displacement function $G(\eta)$. Again, we use an expansion

$$g = g^{(0)} + \left(\frac{u_\star}{k\bar{u}}\right)g^{(1)} + \dots, \tag{5.9}$$

to solve (3.9*a-c*) for $g(\eta)$. Unfortunately, it is not possible to express the conventional (no-retention) centroid displacement function $g^{(0)}(\eta)$ in closed form (Smith 1982, equation (9.7)). Following Smith (1982), if we introduce eigenfunctions $\zeta_m(\eta)$ for diffusion across the flow, then the longitudinal velocity profile has the representation

$$u = \bar{u} + \sum_{m=1}^{\infty} u_m \zeta_m(\eta), \tag{5.10}$$

with
$$\zeta_m(\eta) = (2m + 1)^{\frac{1}{2}} P_m(2\eta - 1), \tag{5.11 a}$$

$$u_m = (-1)^{m+1} \frac{(2m + 1)^{\frac{1}{2}} u_\star}{m(m + 1) k}, \tag{5.11 b}$$

where P_m denotes the Legendre polynomial of degree m . Next, at leading order, the eigenfunction expansion solution for $g^{(0)}(\eta)$ is given by

$$\begin{aligned} g^{(0)}(\eta) &= \frac{h}{k^2} \left(1 + \int_{\eta_\star}^{\eta} \left(\frac{\ln y}{1 - y} \right) dy \right) \\ &= \frac{h}{k^2} \sum_{m=1}^{\infty} (-1)^{m+1} \frac{(2m + 1)}{m^2(m + 1)^2} P_m(2\eta - 1). \end{aligned} \tag{5.12}$$

Similarly, we can infer that the term associated with the bed retention $f(\eta)$ has asymptotic expansion

$$f = f^{(0)} + \left(\frac{u_\star}{k\bar{u}}\right)f^{(1)} + \dots \tag{5.13 a}$$

From (3.10*a-c*) we find

$$f^{(0)}(\eta) = \frac{h\bar{u}}{k u_\star} (1 + \ln \eta) + \frac{(1 + 3B)}{(1 + B)} g^{(0)}(\eta). \tag{5.13 b}$$

Hence, from (3.8), at leading order, the centroid displacement function $G(\eta)$ satisfies

$$G(\eta) = g^{(0)}(\eta) + \frac{h}{k^2} \delta \left(\frac{1}{1 + B} \right)^2 (1 + \ln \eta). \tag{5.14}$$

In the limit of total absorption, i.e. as $B \rightarrow \infty$, this approaches the conventional no-retention centroid displacement $g^{(0)}(\eta)$ (see figure 4*a-c*). As we have already seen in figure 2, the contaminant almost does not ‘feel’ the presence of the bed retention. On the other hand, when $B = 0$, the development of backwards displacement close to the bed is due entirely to the retention effect at the bed.

Smith (1981) pointed out that Taylor’s (1953) Condition B can readily be adapted to apply to an open-channel flow, since the eddy diffusivity (5.1*b*) is modelled as tending to zero at both the free surface and the channel bed. Chatwin (1971) argued that the time taken to sample the whole cross-section should be greater than h/u_\star (since the lateral mixing sufficiently closed to the bed is dominated by molecular

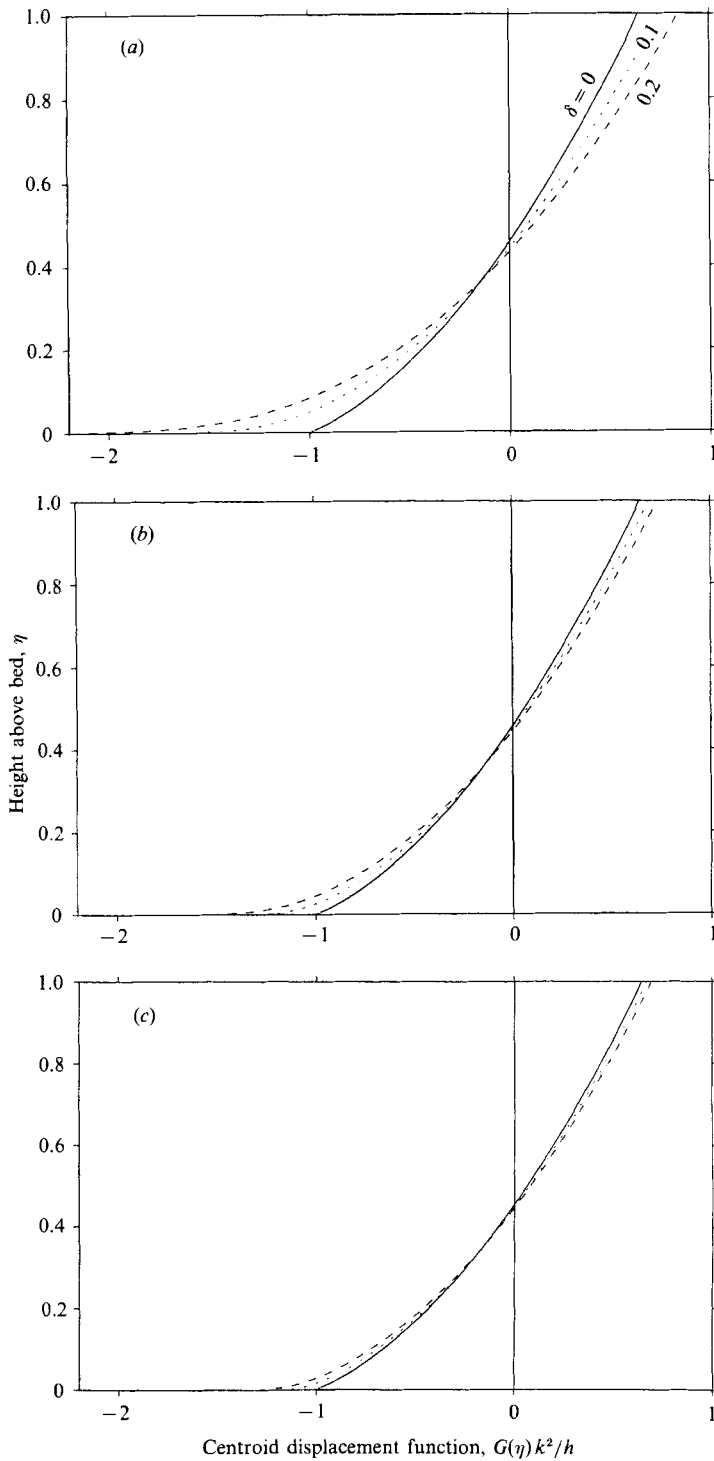


FIGURE 4. The dependence of the centroid displacement function $G(\eta)$ upon the channel depth when there is a retention at the bed: $\delta = 0$ (—); 0.1 (⋯); and 0.2 (---). The bed absorption coefficient B has the values (a) $B = 0$; (b) 0.5 ; and (c) 1 .

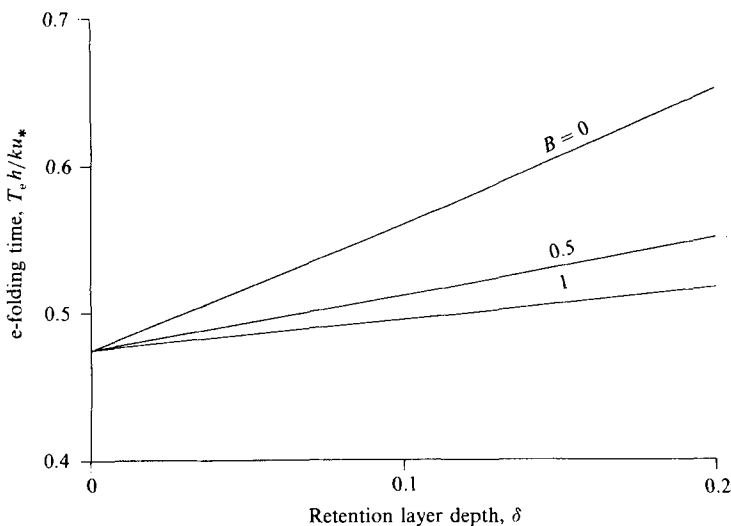


FIGURE 5. The dependence of the e-folding time T_e upon the bed retention-layer depth, when the bed absorption coefficient B has the values $B = 0, 0.5$ and 1 .

processes) by an amount that increases as the height of the viscous sublayer increases. In other words, an important role is played by the retention layer mixing time, T_l . We estimate this in the manner suggested by Valentine & Wood (1977) that T_l is the same proportion of T_e as the bed retention volume is of the total volume:

$$T_l = \frac{\mathcal{J}_0}{1 + \mathcal{J}_0} T_e, \tag{5.15a}$$

where the main flow mixing time T_e is formulated by Purnama (1988, §7):

$$(1 + \mathcal{J}_0) T_e = \frac{\overline{(g + f \mathcal{J}_0)^2 \psi^2}}{(u - \overline{u \psi^2}) \overline{\psi^2 g} + \overline{u \psi^2 f \mathcal{J}_0}}. \tag{5.15b}$$

Note that T_e is the timescale for establishment of the centroid displacement function $G(y, z)$ in (3.6). At the leading order, using the numerical results obtained by Smith (1981, equation (9.12)), we obtain

$$T_e = \frac{h}{ku_*} t_e = \frac{h}{ku_*} \left(\frac{0.4041 + \delta \left(\frac{1}{1+B} \right)^2 \left(0.8082 + \delta \left(\frac{1}{1+B} \right)^2 \right)}{0.4041 + \delta \left(\frac{1}{1+B} \right)^2} \right). \tag{5.16a}$$

This e-folding time is a monotonic increasing function of the bed retention-layer depth, as shown in figure 5. It implies (Chatwin 1971) that the retentive effect of the flow boundary delays the occurrence of the so-called ‘Taylor regime’ for which the rate of growth of the variance is linear with time. For $B = 0$, and $\delta = 0.1$ the retention layer contributes up to 20% to the non-retentive $T_e(\delta = 0)$ value. In order

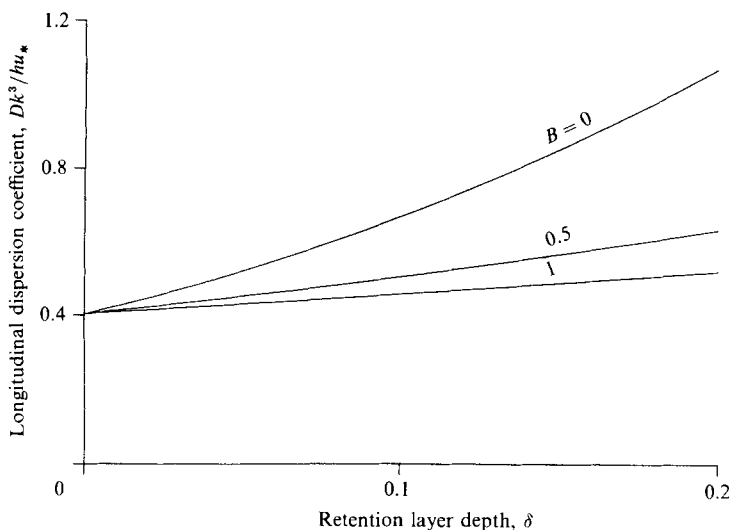


FIGURE 6. The dependence of the longitudinal dispersion coefficient D upon the bed retention layer depth, when the bed absorption coefficient B has values $B = 0, 0.5$ and 1 .

to use the Sullivan's (1971) three-stage description of the dispersion process in open channels, we note from (5.16a) that

$$\frac{t}{T_e} = \left(\frac{t_e}{k}\right) \frac{tu_*}{h}. \tag{5.16b}$$

If we take $\bar{u}/u_* = \frac{1}{15}$, $k = 0.4$, and with the value of the equivalent retentive-layer depth estimated in the Appendix, then we obtain

$$\frac{t_e}{k} \approx 1.28. \tag{5.16c}$$

Next, using (5.15a) the first moment of the kernel $I(\tau)$ can be estimated as

$$\int_0^\infty \tau I(\tau) d\tau = \frac{h^2}{k^2 \bar{u}} \delta^2 \left(\frac{1}{1+B}\right)^2 t_e \left(\frac{u_*}{ku}\right). \tag{5.17}$$

Note that this is entirely a property of the retentive layer.

From (4.6), the leading-order estimate for the longitudinal shear dispersion coefficient is given by

$$D = \overline{(u-\bar{u})g^{(0)}} + \frac{hu_*}{k^3} \delta \left(\frac{1}{1+B}\right)^2 \left[2 + \delta \left(\frac{1}{1+B}\right)^2 \left(\frac{k\bar{u}}{u_*} + t_e\right)\right]. \tag{5.18}$$

The first term on the right-hand side is the conventional (no-retention) shear-dispersion coefficient and it has been evaluated numerically by Elder (1959):

$$\overline{(u-\bar{u})g^{(0)}} = 0.4041 \frac{hu_*}{k^3}. \tag{5.19}$$

In contrast, the second term of (5.18) represents both the effects of the bed adsorption and of retention.

Again, as $B \rightarrow \infty$, (5.18) rapidly approaches the conventional no-retention shear-dispersion coefficient value (5.19) (figure 6). As was noted by Smith (1983), since the

bed is the region of lowest velocity and of strongest shear, the remaining contaminant dispersion experiences on average a reduced rate of shear dispersion. However, for a passive contaminant in which $\psi = 1$ and $B = 0$, the bed retention effect rapidly dominates the conventional no-retention shear dispersion prediction. The longitudinal dispersion coefficient D is almost double the value of (5.19) for $\delta = 0.1$. Using the equivalent retentive-layer depth estimated in the Appendix, with $u/u_* = \frac{1}{15}$ and $k = 0.4$, (5.18) gives

$$D \approx 7.93 hu_*, \quad (5.20)$$

so that, with this model, the true value of D is 26% greater than Elder's (1959) prediction (Chatwin 1971).

6. Concluding remarks

We have generalized the work of Taylor (1953) to account for dispersion of contaminant in the presence of both reactions and retention at the flow boundary; i.e. the complications caused when the contaminant is chemically active. The mass exchange across the flow boundary is represented by the kernel $I(\tau)$, which embodies the totality of motion and mixing within the retentive layer. The decomposition (4.6) of the longitudinal dispersion coefficient reveals that the shear dispersion coefficient D can be vastly increased by the presence of the boundary retention.

For turbulent flow in an open-channel, the dispersion of a passive contaminant is significantly increased by the presence of the bed retention. The conventional no-retention longitudinal dispersion-coefficient value can almost be doubled when $\delta = 0.1$, which is equivalent to a retentive layer of depth $h/60$. It is also found to be in qualitative agreement with the conclusion of Valentine & Wood (1977) that the longitudinal dispersion is delayed in reaching its full efficiency.

I wish to thank my supervisor, Dr R. Smith, who suggested the problem and provided continual advice, support and encouragement throughout the work. I should also like to thank the referees for their helpful comments. The financial support of an Overseas Research Student award is gratefully acknowledged.

Appendix. Kernel $I(\tau)$ for the stagnant-layer model

For turbulent flows in open channels, the vertical mixing within the viscous sublayer and sufficiently close to the boundary is essentially caused by molecular diffusion. In this stagnant-layer model (Purnama 1988), the equation describing the stagnant layer of depth l with concentration c_l is

$$\partial_t c_l - \kappa_l \partial_y^2 c_l = 0, \quad (A 1a)$$

$$\text{with} \quad c = c_l, \quad y = 0, \quad (A 1b)$$

$$\kappa_l \partial_y c_l = 0, \quad y = -l, \quad (A 1c)$$

and initially, at $t = 0$, $c_l = 0$. In this case of constant molecular diffusivity κ_l , by taking Laplace transform of (A 1a-c), we obtain

$$\hat{c}_l = \hat{c} \frac{\cosh q(y+l)}{\cosh ql}, \quad q^2 = \frac{p}{\kappa_l}. \quad (A 2)$$

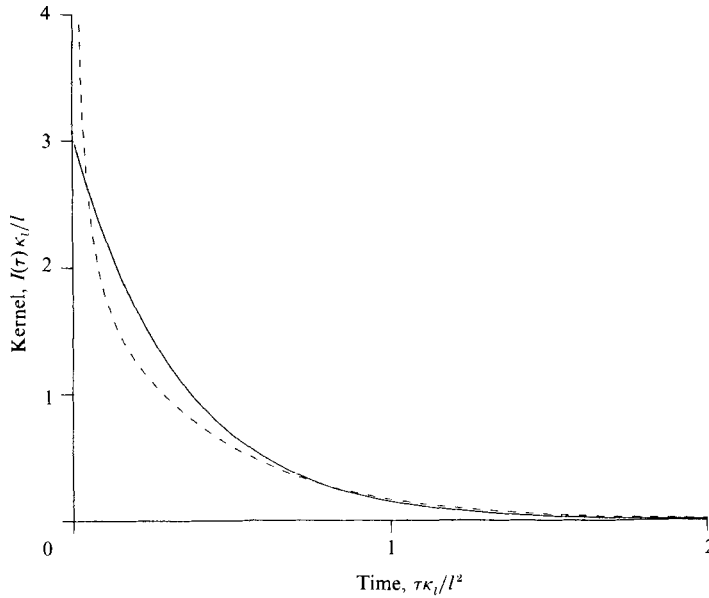


FIGURE 7. The graphs of the kernel $I(\tau)$ for the stagnant-layer model (—) and the dead-zones model (-----).

For the Davidson & Schroter (1983) model, we have to work in the cylindrical coordinates and hence, the right-hand side of (A 2) should involve the modified Bessel functions. The Laplace transform of the total flux across the stagnant layer is

$$\kappa_l \partial_y \hat{c}_l = \widehat{\partial_t c} \frac{\tanh ql}{q}. \tag{A 3}$$

Using the Inversion theorem, we have

$$I(\tau) = \frac{2\kappa_l}{l} \sum_{n=0}^{\infty} \exp\left(\frac{\kappa_l \pi^2 (2n+1)^2 \tau}{4l^2}\right). \tag{A 4}$$

In the dead-zones model, we seek to approximate $I(\tau)$ by the exponential form

$$I(\tau) = \alpha \exp(-\gamma\tau). \tag{A 5}$$

If the bulk velocity and dispersion coefficient are to be correctly reproduced, then the weighted integrals

$$\int_0^{\infty} I(\tau) d\tau \quad \text{and} \quad \int_0^{\infty} \tau I(\tau) d\tau$$

need to be correct. Substituting for $I(\tau)$ from (A 4) we arrive at the results:

$$\alpha = \frac{2\kappa_l}{l} \frac{\left(\sum_0^{\infty} \frac{1}{(2n+1)^2}\right)^2}{\sum_0^{\infty} \frac{1}{(2n+1)^4}} = \frac{3\kappa_l}{l}, \tag{A 6a}$$

$$\gamma = \frac{\pi^2 \kappa_l}{4l^2} \frac{\sum_0^{\infty} \frac{1}{(2n+1)^2}}{\sum_0^{\infty} \frac{1}{(2n+1)^4}} = \frac{3\kappa_l b}{l^2} \quad (\text{A } 6b)$$

since

$$\sum_0^{\infty} \frac{1}{(2n+1)^2} = \frac{\pi^2}{8}, \quad \sum_0^{\infty} \frac{1}{(2n+1)^4} = \frac{\pi^4}{96}.$$

Figure 7 shows that except near $\tau = 0$, the optimally chosen dead-zones model gives a good overall approximation to the stagnant-layer model. Next, from Valentine & Wood (1977), we deduce that

$$\alpha = KA'\bar{u}, \quad (\text{A } 7)$$

where the (non-dimensional) entrainment coefficient $K = 0.02$. For a man-made uniform (concrete) channel, the work of Young & Wallis (1986) suggests that the proportion of the bed covered by dead zones A' is of order of 0.15. The typical value of the molecular diffusivity for heat in water is $\kappa_l = 1.4 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$. So for the discharging of hot water into an open channel, we estimate that the equivalent retentive layer has a depth of

$$\frac{l}{h} \approx 7.54 \times 10^{-3}, \quad (\text{A } 8)$$

where we have taken (cf. Chatwin 1971, §2) $h = 6.9 \times 10^{-2} \text{ m}$ and $\bar{u} = 0.269 \text{ ms}^{-1}$.

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