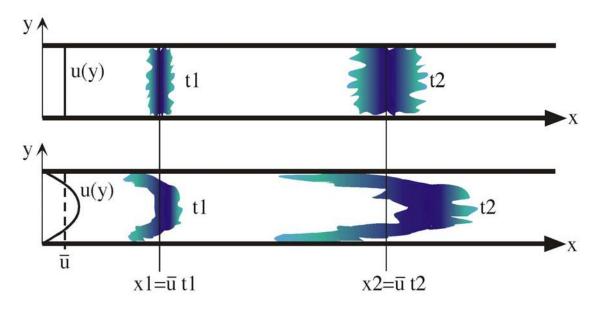
1.061 / 1.61 Transport Processes in the Environment Fall 2008

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8. Dispersion processes



This section looks at the longitudinal spreading of clouds through <u>dispersion</u>, a process distinct from diffusion. Dispersion is the spreading of a cloud by any process that causes different chemical particles to move at different velocities. The non-uniformity of particle velocity allows some particles to move quickly while others are held back, and can be caused by boundaries (which create shear in the flow), dead zones and absorption reactions (for example, to a porous medium). In environmental systems, dispersion is generally far more important than diffusion in the lengthening of chemical clouds. In this chapter, it is shown that dispersing clouds eventually reach a Fickian limit, at which point they have a Gaussian concentration profile in the longitudinal direction. It is also shown that longitudinal dispersion is maximized when lateral diffusion is small.

The example problems ask the user to make qualitative statements about the dispersion expected in various flows and to predict the shape of a dispersing cloud.

8. Shear Dispersion.

The transport models and concentration field solutions developed in previous sections assume that currents are spatially uniform, *i.e.* $u \neq f(x,y,z)$. However, spatial gradients of velocity, known as shear, must exist close to a boundary because the no-slip condition requires that the relative velocity of the fluid be zero at the boundary. When shear is present, different parts of a tracer cloud will advect at different speeds. This 'differential advection' stretches the tracer cloud, causing it to spread longitudinally more quickly than a cloud released into a uniform current (Figure 1). In addition, differential advection creates lateral gradients in concentration ($\partial C/\partial y$ in Figure 1) which, when acted upon by lateral diffusion, accelerates the dilution of the cloud.

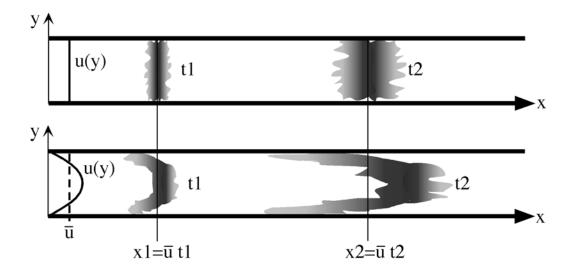


Figure 1. Top-view of two channels. In the top channel the side-wall boundary condition allows slip, and the velocity profile is uniform across y. In the bottom channel there is a no-slip condition at the side-wall boundary, creating lateral shear, $\partial u/\partial y$. Both channels have the same cross-sectional mean velocity, \overline{u} . Tracer is released at t = 0, x = 0. The spatial distribution of each cloud is shown above at time t1 and t2. Note, the center of mass for both clouds advects at speed \overline{u} . Velocity shear in the bottom channel stretches the tracer cloud, and as a result this cloud spreads longitudinally more rapidly than the cloud in the uniform channel.

The distortion observed in the bottom channel of Figure 1 can be predicted from the full transport equation,

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} D_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} D_y \frac{\partial C}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial C}{\partial z}, \qquad (1)$$

if we include the spatial variation in velocity. However, with u = f(x,y,z), it is difficult to find simple analytical solutions to (1). In many instances it is sufficient to integrate the domain over y and z, and consider only transport in the stream-wise direction. After this integration the combined impact of differential advection and lateral diffusion is

expressed as an additional process creating longitudinal spreading, which we term Shear Dispersion. It is also known as Taylor Dispersion, in honor of G. I. Taylor, who first described this process in 1953. Under limiting conditions, to be discussed shortly, Shear Dispersion behaves as a Fickian diffusion process. Thus, we represent its impact in the cross-sectionally averaged (one-dimensional) transport equation with an additional coefficient of dispersion, K_x . Integrating (1) over y and z yields the one-dimensional equation,

$$\frac{\partial \langle \mathbf{C} \rangle}{\partial t} + \langle \mathbf{u} \rangle \frac{\partial \langle \mathbf{C} \rangle}{\partial x} = D_x \frac{\partial^2 \langle \mathbf{C} \rangle}{\partial x^2} + K_x \frac{\partial^2 \langle \mathbf{C} \rangle}{\partial x^2}, \qquad (2)$$

in which brackets represent cross-sectional averages, and for simplicity we have assumed homogeneous diffusivity, $D_x \neq f(x)$. In general $D_x \ll K_x$, such that the former may be neglected, leaving us with the one-dimensional advection-dispersion equation.

$$\frac{\partial \langle \mathbf{C} \rangle}{\partial t} + \langle \mathbf{u} \rangle \frac{\partial \langle \mathbf{C} \rangle}{\partial x} = \mathbf{K}_{x} \frac{\partial^{2} \langle \mathbf{C} \rangle}{\partial x^{2}}.$$
(3)

Furthermore, in the limit of Fickian behavior, we describe the evolution of the crosssectionally averaged cloud using the same statistical description developed for diffusion in previous chapters. Specifically, the longitudinal length-scale for the cloud is σ_x , where

$$\sigma_{\rm x} = \sqrt{2 \, K_{\rm x} t} \,. \tag{4}$$

From (4) we can estimate K_x in the field by observing the evolution of variance for a tracer cloud. Specifically, observing the variance over time,

$$K_{x} = \frac{1}{2} \frac{\partial \sigma_{x}^{2}}{\partial t}.$$
(5)

We can find an analytical expression for K_x by explicitly carrying out the integration that leads to (3), utilizing scaling arguments to simplify the mathematics along the way. It is important to understand the steps of this derivation, to appreciate under what conditions the approximate equation (3) may hold. For simplicity we will consider a very wide channel for which the shear in the lateral, $\partial u/\partial y$, is so small compared to the shear in the vertical, $\partial u/\partial z$, that the lateral shear is neglected at the outset. This allows us to assume a two-dimensional channel with $\partial/\partial y = 0$. In addition, we assume that the flow is strictly in the x-direction (w = v = 0), and uniform ($\partial u/\partial x = 0$). With these assumptions, (1) reduces to

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{\partial}{\partial x} D_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial z} D_z \frac{\partial C}{\partial z}.$$
(6)

Next, we decompose u and C into depth-averaged values denoted by an over-bar, e.g. $\overline{u} = (1/h) \int_0^h u dz$. Deviations from the depth-average will be denoted by a prime.

$$u(z) = \overline{u} + u'(z)$$

$$c(x,z) = \overline{c}(x) + c'(x,z)$$
(7)

We put the decomposed variables into (6), and note that by definition $\partial c/\partial z = 0$.

$$\frac{\partial}{\partial t}(\overline{c}+c') + (\overline{u}+u')\frac{\partial(\overline{c}+c')}{\partial x} = \frac{\partial}{\partial x}D_x\frac{\partial(\overline{c}+c')}{\partial x} + \frac{\partial}{\partial z}D_z\frac{\partial(c')}{\partial z}.$$
(8)

We take the depth-average of each term, noting that by definition $\overline{c'} = 0$ and $\overline{u'} = 0$.

$$\frac{\partial \overline{c}}{\partial t} + \overline{u} \frac{\partial \overline{c}}{\partial x} + \overline{u'} \frac{\partial c'}{\partial x} = \frac{\partial}{\partial x} D_x \frac{\partial \overline{c}}{\partial x}$$
(9)

Relative to our original equation, (6), we have eliminated the vertical gradient terms by integrating over the vertical domain. In addition, a new term has appeared, $\overline{u' \partial c' / \partial x}$, that represents the flux associated with the correlation between the fluctuations in velocity, u', and concentration c', relative to their depth-averaged values. With the next few steps we will find a solution for c', so that we might evaluate this new flux term. As both (8) and (9) must both hold true, we may subtract (9) from (8) to yield.

$$\frac{\partial c'}{\partial t} + u' \frac{\partial \bar{c}}{\partial x} + u' \frac{\partial c'}{\partial x} - \overline{u' \frac{\partial c'}{\partial x}} = \frac{\partial}{\partial z} D_z \frac{\partial c'}{\partial z}$$
(10)

Now we place an important condition on the magnitude of the spatial fluctuation c'. Specifically, we assume that $c' << \overline{c}$. If this is true, then the magnitude of both the third and fourth terms in (10) must be small compared to the second term, and we may drop the small terms, reducing (10) to

$$\frac{\partial c'}{\partial t} + u' \frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial z} D_z \frac{\partial c'}{\partial z}$$
differential advection vertical diffusion
(11)

This equation describes how vertical fluctuations in concentration, c', are created by differential advection and destroyed by vertical diffusion. Initially, when $\partial \overline{c}/\partial x$ is large, differential advection dominates, creating c' faster than vertical diffusion can erase it. But, eventually, $\partial \overline{c}/\partial x$ becomes small enough that the rate at which c' is created by differential advection is balanced by the rate at which it is destroyed by vertical diffusion. When these two processes are in balance, $\partial c'/\partial t$ goes to zero and (11) becomes.

$$\mathbf{u}' \frac{\partial \mathbf{c}}{\partial \mathbf{x}} = \frac{\partial}{\partial z} \mathbf{D}_{\mathbf{z}} \frac{\partial \mathbf{c}'}{\partial z}.$$
 (12)

We can solve (12) with a no-flux boundary condition at the bed and water surface, *i.e.* $\partial c'/\partial z = 0$ at z = 0 and h. Recall that by definition, $\overline{c} \neq f(z)$. Then,

$$c'(z) = \frac{\partial \overline{c}}{\partial x} \int_{0}^{z} \frac{1}{D_z} \int_{0}^{z} u' dz dz + c'(z=0).$$
(13)

Because the diffusivity, D_z , is the sum of turbulent and molecular diffusion, it may be a function of vertical position, and so remains inside the integral.

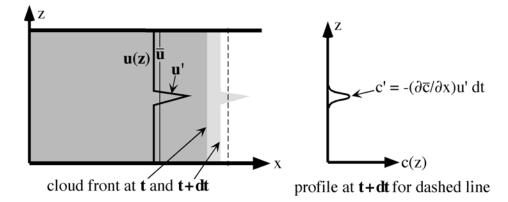


Figure 2. Consider a tracer cloud whose leading edge is uniform at time **t**. Differential advection distorts the cloud giving it a new shape by time t+dt. The spatial deviation in velocity, u', creates the concentration perturbation seen at **t** + dt. Specifically, from the first two terms in (11), c' = $-(\partial \overline{C}/\partial x)$ u' dt.

Now we return to (9) to evaluate the new term, $\overline{u' \partial c'}/\partial x$. Because we assume $u \neq f(x)$, then $u' \neq f(x)$, and we can write the new term as $\partial \overline{u'c'}/\partial x$. We evaluate the correlation $\overline{u'c'}$ with (13), noting that $\overline{u'c'(z=0)} = \overline{u'c'(z=0)} = 0$, because $\overline{u'=0}$.

$$\overline{\mathbf{u}'\mathbf{c}'} = \frac{1}{h} \int_{0}^{h} \mathbf{u}' \frac{\partial \overline{\mathbf{c}}}{\partial x} \int_{0}^{z} \frac{1}{D_{z}} \int_{0}^{z} \mathbf{u}' \, dz dz dz = \frac{1}{h} \frac{\partial \overline{\mathbf{c}}}{\partial x} \int_{0}^{h} \mathbf{u}' \int_{0}^{z} \frac{1}{D_{z}} \int_{0}^{z} \mathbf{u}' \, dz dz dz \,.$$
(14)

This correlation is the advective flux associated with spatial fluctuations in the velocity field. This flux is proportional to the concentration gradient, and so behaves as a Fickian diffusion. Thus, we choose to model this flux using a transport coefficient, just as we did for turbulent diffusion in the previous chapter. The transport coefficient is called the longitudinal dispersion coefficient, K_x . The negative sign indicates that the flux is counter-gradient.

$$\overline{\mathbf{u}'\mathbf{c}'} = -\mathbf{K}_{\mathbf{x}} \frac{\partial \overline{\mathbf{c}}}{\partial \mathbf{x}},\tag{15}$$

where

The second expression in (16) is valid when $D_z \neq f(z)$. This expression describes the contribution of vertical shear to longitudinal dispersion. A similar term describes the contribution of lateral shear.

Now we can write the new term in (9) as,

$$\overline{\mathbf{u}'\frac{\partial \mathbf{c}'}{\partial \mathbf{x}}} = \frac{\partial}{\partial \mathbf{x}}\overline{\mathbf{u}'\mathbf{c}'} = -\mathbf{K}_{\mathbf{x}}\frac{\partial^2 \bar{\mathbf{c}}}{\partial \mathbf{x}^2}$$
(17)

Using (17) in (9), we arrive at the one-dimensional equation,

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial x}D_x\frac{\partial \bar{c}}{\partial x} + K_x\frac{\partial^2 \bar{c}}{\partial x^2},$$
(18)

where D_x in (18) and D_z in (16) represent the sum of molecular and turbulent diffusion, which for practical purposes is just turbulent diffusion. Elder evaluated (16) for a logarithmic profile with $D_z = f(z)$ and found

$$K_x = 5.93u_*h.$$
 (19)

Note that (19) only accounts for velocity shear over depth $(\partial u/\partial z)$ and not for lateral velocity shear $(\partial u/\partial y)$. This is an acceptable approximation for wide, straight channels. Comparing (19) with the empirical estimate for longitudinal diffusion, $D_x = 0.45u_*h$, we see that K_x is an order of magnitude larger. Because of this, the diffusion term is often neglected in (18), and we have returned to equation (3), repeated here for convenience.

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} = K_x \frac{\partial^2 \bar{c}}{\partial x^2}$$
(20)

Solutions to this one-dimensional equation, with D_x replaced by K_x , have already been described for instantaneous and continuous point releases. These solutions can now be used for systems with shear-dispersion dominating longitudinal diffusion (as in 20). As one might expect, (16) shows that the coefficient of shear dispersion increases with the magnitude of the shear, expressed as the magnitude of the spatial deviations u'. The dependence $K_x \sim h$ is less straight-forward. However, considering that each integral is proportional to h, and that $D_z \sim h$, (16) yields $K_x \sim h$, consistent with (19). Finally, (16) indicates that K_x is inversely proportional to the cross-stream diffusivity, D_z (i.e. K_x is greatest when D_z is smallest!). To understand this somewhat unintuitive dependence, remember that shear dispersion arises because velocities on adjacent streamlines are different so particles on different streamlines advect at different speeds and thus become separated (dispersed) longitudinally. This is the differential advection component of shear dispersion. At the same time, each particle is mixed over depth (or width), experiencing the velocity of each streamline that is passes for some fraction of time. If

the cross-channel diffusion is high, the particles sample all the velocities in the profile so rapidly that they effectively travel at the mean channel velocity. If they all effectively travel at the mean velocity, they do not disperse (separate) in the longitudinal direction, and shear dispersion will be zero, even though shear is not zero. As the cross-stream diffusion is reduced, particles can accumulate more differential advection as they remain on individual streamlines for a longer period.

Now it is important to recall the assumptions that allowed us to reach the advection-dispersion equation (20). Early on we made the assumption that $c' \ll \overline{C}$. In addition, for (12) to be valid, we specifically required that the rate at which c' is created exactly balance the rate at which c' is destroyed, so that a nearly uniform concentration profile exists in the cross-stream direction. Note that a nearly uniform profile would automatically satisfy $c' \ll \overline{c}$, such that the two assumptions are closely linked. To understand when these assumptions are valid, we consider the evolution of a tracer cloud from its initial release, as shown in Figure 3. The tracer is introduced as a line distributed over the full depth at time t = 0. Differential advection, u', creates perturbations in the concentration profile, c', at the rate $\partial c'/\partial t = u' \partial \overline{c}/\partial x$. When the cloud is first introduced, the mean concentration gradients are very large, such that the creation of c' is very rapid and pronounced. This is reflected in the geometric distortion of the cloud shape (t1, Fig. 3). The concentration perturbations are dissipated by lateral diffusion, which acts at the rate, $\partial c' / \partial t = D_Z \partial^2 c' / \partial z^2$. As the cloud spreads, the longitudinal gradient of mean concentration, $\partial \bar{c} / \partial x$, decreases and the rate at which concentration perturbations are created slows. Eventually, the rate at which the perturbations are created by differential advection comes into balance with the rate at which they are destroyed by diffusion such that (12) is valid. From tracer studies, this is observed to occur at time scale

$$T_{\text{Dispersion}} = 0.4 \text{ L}_{\text{Z}}^{2}/\text{D}_{\text{Z}},$$
(21)

after the tracer is released, where L_z is the length-scale of the channel in the cross-stream direction (width or depth). For vertical shear, $L_z = h$, the water depth. After this time (e.g. **t2** in Figure 3) the concentration is close to uniform over depth, such that c' $<< \overline{C}$. The process of shear-dispersion has reached its Fickian limit and the longitudinal distribution of the depth-averaged concentration is Gaussian. Note that this time scale is inversely proportional to cross-stream diffusion, D_z . And recall from (16) that K_x is also inversely proportional to D_z . This means that the conditions (D_z) which yield the greatest K_x will also require the longest time (longest distance from source) for shear-dispersion to take hold and for (20) to apply.

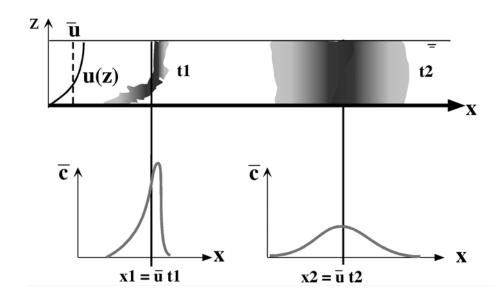


Figure 3. Evolution of tracer cloud released at t = 0 as a line distributed over depth. Initially (**t1**) differential advection dominates, visibly distorting the geometric shape of the cloud. At this time (**t1**) the longitudinal distribution of the depth-averaged concentration, \overline{C} , is skewed. Eventually differential advection and diffusion balance and the cloud approachs uniform concentration over depth. After this time (**t2**) the longitudinal distribution of the depth-averaged concentration is Gaussian and the dispersion process has reached its Fickian limit.

Other Mechanisms of Dispersion

Dispersion is a broad term used to describe all processes, except diffusion, that disperse a patch of tracer and diminish concentration. Typically dispersion coefficients reflect a combination of advection and diffusion processes that are difficult to model separately. For example, the coupled effects of differential longitudinal advection and cross-channel diffusion create shear dispersion. In flow through porous media, the existence of multiple discrete flow paths also creates differential advection that leads to dispersion. The flow paths in a porous medium are constrained to discrete, intertwining pore channels, and multiple flow paths exist between any two points. The time to traverse a given flow path depends on the geometry of the pores. Flow through narrow pores is slower than flow through wider pores. Also, some flow paths are nearly linear, and thus short, and others are very tortuous (bending) and thus long. In addition, each pore channel behaves like a small tube, with higher velocity at the center of the pore than at the grain surface. The pore-scale shear contributes to dispersion in the same manner as channel-scale shear, as described above. Together, the above processes contribute to a longitudinal spreading of tracer particles. That is, tracer particles released together will take different flow paths and get separated (dispersed) both laterally and longitudinally. This is called mechanical dispersion. This form of dispersion can reach a Fickian limit after every tracer particle has sampled a sufficient number of pore channels.

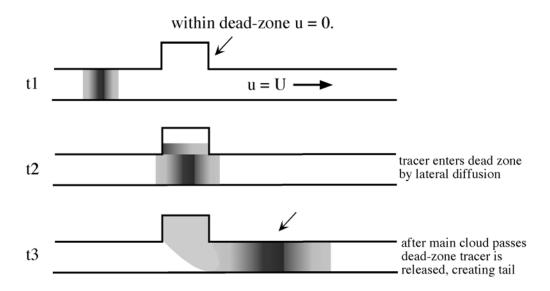


Figure 4. **Dead-zone Dispersion.** The lateral diffusion of particles into a region of zero velocity, called a dead-zone will create longitudinal dispersion. Tracer that enters the dead-zone is held back relative to the tracer that does not. When the tracer is released from the dead-zone, it is separated in space (dispersed) from the rest of the cloud.

Another form of dispersion arises when the flow field contains zones with zero velocity, called dead-zones. Tracer particles can enter these zones through turbulent or molecular diffusion. After some mean residence time, τ , within the dead-zone, the tracer is again released to the advecting zone. Any tracer that enters the dead-zone will be held back relative to the tracer that does not, so that, when the tracer is released from the deadzone, it is separated (dispersed) from the rest of the cloud. For a dead-zone to contribute to dispersion, its residence time must be long compared to the time scale of passage of the original tracer cloud. Otherwise there is no delay associated with entering the deadzone, and thus no dispersion. Possible dead-zones include pore spaces with no outlet, a side-pool in a river, and a wake behind an obstruction. If the dead-zones are distributed through out the flow field, then dead-zone dispersion can reach a Fickian limit after a sufficient number of dead-zones have been sampled by the tracer cloud. This can be the case for dead-end pores in a porous medium and for the wakes behind individual stems within a wetland. If only a few dead-zones can be experienced, e.g. a small number of pools and riffles along a river reach, then the Fickian Limit cannot be reached. The trapping and delay associated with a single or small number of dead-zones (as in Figure 4) produce non-Gaussian (non-Fickian) dispersion, and the longitudinal distribution of concentration, $\overline{C}(x)$, will be skewed, with a long tail on the upstream end associated with the tracer temporarily trapped in the dead-zone. An example of this skewed distribution is shown at t1 in Figure 3, which also represents a condition for which the Fickian limit has not been reached by the dispersion process.

A third process of dispersion can arise from chemical reaction with the stationary substrate, *e.g.* grain walls in porous media or channel boundaries. Consider the tracer depicted in Figure 5, which can adsorb to the solid boundary. When the dissolved chemical (white circles) is released into the channel, it begins to adsorb to the boundary (black circles) with reaction rate k. The chemical associated with the boundary is

stationary, and thus will be delayed relative to the dissolved phase, which continues to move downstream at speed U. Once the local dissolved concentration drops to zero, the adsorbed chemical is released back to the moving fluid (gray circles, t1 and t2, Figure 5), also at rate k. The cloud is dispersed longitudinally because some fraction of the mass is delayed by adsorption to the boundary. As with dead-zone dispersion, adsorption to the solid boundary can only result in dispersion if the time scale for the adsorption processes (1/k) is long compared to transport time-scale of the cloud, such that each adsorption under conditions for which the time-scale of the adsorption reaction is very short compared to the transport time-scales, such that the concentration in the dissolved and adsorbed phases always remain at equilibrium.

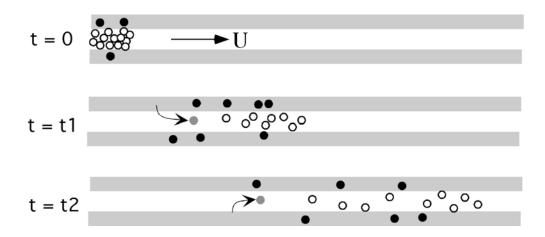


Figure 5. Some fraction of the dissolved chemical (white circles) may adsorb to the solid, stationary boundary (black circles). The adsorbed chemical is released from the boundary (gray circles) after the dissolved cloud has passed. The adsorption and desorption of chemical results in a transport delay that lengthens (disperses) the tracer cloud.