

CHAPTER 4.

4.1 Introduction

4.2 Mechanic Dispersion and Molecular diffusion

4.3 G. I. Taylor's analysis of shear flow dispersion

4.2 Concept of Dispersion

Consider a non-viscous fluid flowing displacing another non-viscous fluid with different color through a frictionless pipe at a steady laminar flow rate. If the pipe is perfectly uniform and straight, we will likely to observe that the interface between the two fluids moves uniformly along the pipe as piston type of displace, maintaining its shape with some smearing. After a period time, the straight interface is still maintained but is broaden (see Figure 4.1). Consequently, we may conclude that the piston-type displacement corresponds to the advection and the smearing is related to molecular diffusion, or random motion of molecules of the two fluids.

Based on our previous discussion of advection-diffusion process, one would certainly conclude that a one-dimensional advection-diffusion equation,

$$D_m \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (4.1)$$

is adequate to describe the movement of the interface and its spread. The first term on the left-hand side of equation (4.1) is the molecular diffusion term in which D_m is the molecular diffusion coefficient, accounting for random motion of the fluid molecules at the microscopic scale. The second term represents the advection term, where u denotes the bulk movement of the fluids, and C is the concentration of the displacing fluid.

While the above conjecture appears to be valid, fluids always have some viscosity and pipes are always somewhat frictional. As we conduct the fluid displacement experiments in a real-work situation, we likely observe a non-uniform velocity field with the maximal velocity at the center of the pipe and the minimal near the pipe wall. That is, an initial straight line interface between the two fluids becomes a parabolic surface, the curvature becomes greater, and the surface becomes more smeared as time progresses as illustrated in Figure 4.1. The parabolic shape is simply caused by the non-uniform velocity of the fluids due to the friction of the pipe wall and viscosity of the fluids. The smearing is merely a result of random motion of molecules. Consequently, it is logical to conclude that the concentration distribution can be quantified by using an axisymmetrical advection-diffusion equation:

$$D_m \frac{\partial^2 C}{\partial x^2} + D_m \frac{\partial^2 C}{\partial r^2} - u(r) \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (4.2)$$

where D_m is the constant molecular diffusion coefficient, x is the horizontal coordinates, r is the radial coordinates with $r=0$ at the center of the pipe; u is the velocity, which varies with r only; $C(x,r,t)$ is the point concentration in the pipe. To implement this approach to a real-world problem, it is necessary to determine the velocity along the radius of the pipe, if the roughness of the pipe is uniform everywhere. However, we generally do not measure the velocity and are not interested in the concentration at a point within the pipe. Instead, we measure the average velocity using inflow rate or outflow rate over the cross-sectional area of the pipe and collect the concentration at the end of the pipe. That is,

$$U = \frac{1}{a} \int_0^a u(r) dr \quad \text{and} \quad C(x,t) = \frac{1}{a} \int_0^a C(x,r,t) dr \quad (4.3)$$

where U is the mean or average velocity (see Figure 4.2), constant over the length of the pipe and likewise, $C(x,t)$ is the concentration average of the cross-sectional area, which is a function of x and t only. If we adopt this practical approach, we can assume that a one-dimensional advection-diffusion equation will be adequate, i.e.,

$$D \frac{\partial^2 C(x,t)}{\partial x^2} - U \frac{\partial C(x,t)}{\partial x} = \frac{\partial C(x,t)}{\partial t} \quad (4.4)$$

Nevertheless, this equation appears neglecting the effects of velocity deviation around the mean velocity and the concentration gradient in the r direction. To circumvent this problem, we will assume that the effects can be lumped into a dispersion term, D , which is the sum of molecular diffusion and the effects of the velocity variation around the mean velocity. In other words,

$$D = D_m + D_h \quad (4.5)$$

where D_h is called mechanic dispersion coefficient, representing the effect of velocity variation around its mean on the average concentration. In general, the magnitude of mechanic dispersion coefficient is much greater than the coefficient of molecular diffusion.

According to the above reasoning, it is clear that dispersion term is merely a correction term used to account for the effects of velocity variations around the mean velocity that is neglected in the advection term (the second term) in equation (4.4). Now, a logical question to ask is: is this simplified assumption valid? The next section dealing with shear flow dispersion will answer this equation.

Before we proceed into the next section, we emphasize that a three-dimensional advection-diffusion equation can reproduce tracer point concentration at any time and any point in the pipe, if we can determine the velocity at every point along the pipe. The dispersion concept arises merely from our averaging approach for practical purposes. Table 4.1 summaries the differences between molecular diffusion and the dispersion we discussed here.

Table 4.1

	Molecular Diffusion	Dispersion
Scale	molecular (microscopic scale)	macroscopic scale greater than many molecules,
Mechanism	Random motion of molecules	Velocity variations due to friction and viscosity
Rationale	Randomness of molecule velocity is too small to measure; our instrument size or scale is often much greater than the size of a molecule.	Point velocities in a pipe may be measurable but is impractical to measure (i.e., the scale of the problem is much greater than our instrument scale).

4.3 G. I. Taylor's analysis of shear flow dispersion

To study the validity of Fick's law for the dispersion, we will examine displacement of a slug of tracer in a flowing fluid in a circular pipe of a radius of R as shown in Figure 4.3. We further assume the flow is uniform and steady (independent of time) such that all flow lines are parallel to the wall of the pipe. The question we want to answer is if the spatial distribution of the tracer concentration averaged over the cross-sectional area of the pipe at different times can be described by the advection-diffusion equation that is based on Fick's law. Here, the average concentration of the cross-sectional area can be written as

$$\bar{C}(x,t) = \frac{1}{2R} \int_{-R}^R C(x,r,t) dr$$

where $C(x,r,t)$ is the point concentration at any point in the pipe at any time t . The cross-sectional average concentration is denoted by $\bar{C}(x,t)$, which is a function of x and t only. Since the flow is assumed to be steady and uniform, the point velocity variation exist only in the r direction, i.e., $u(r)$, we can express the average (or mean) velocity over the cross-sectional area as

$$\bar{u} = \frac{1}{2R} \int_{-R}^R u(r) dr \quad (4.6)$$

Notice that both average concentration and velocity are independent of the type of point concentration and velocity distributions. Subsequently, we can write the point concentration and velocity in terms of the mean and perturbations:

$$u(r) = \bar{u} + u'(r) \quad \text{and} \quad C(x,r,t) = \bar{C}(x,t) + C'(x,r,t) \quad (4.7)$$

Note that the average of the perturbation terms must be zero. That is,

$$\frac{1}{2R} \int_{-R}^R C'(x,r,t) dr = 0 \quad \text{and} \quad \frac{1}{2R} \int_{-R}^R u'(r) dr = 0 \quad (4.8)$$

Now, according to our previous discussion, it is reasonable to assume that an axis-symmetrical advection-diffusion equation (4.2) can provide a good description of the tracer displacement along the pipe. By substituting (4.7) into Equation 4.2, we have

$$D_m \frac{\partial^2 \bar{C}(x,t) + C'(x,r,t)}{\partial x^2} + D_m \frac{\partial^2 \bar{C}(x,t) + C'(x,r,t)}{\partial r^2} - (\bar{u} + u'(r)) \frac{\partial \bar{C}(x,t) + C'(x,r,t)}{\partial x} = \frac{\partial \bar{C}(x,t) + C'(x,r,t)}{\partial t} \quad (4.9)$$

in which we assume that the molecular diffusion coefficient, D_m , is a scalar and constant, implying the molecular diffusion process is isotropic: independent of directions and that Fick's law for molecular diffusion is valid at this scale.

Our aim is to investigate if the effect of velocity variation around the mean can be described by Fick's law. As a consequence, we would like to observe the effect of velocity variation on the spread of the tracer as an observer moving at the mean velocity of the fluid. To do so, a coordinate transformation is necessary. That is, we will define a convective coordinate:

$$\xi = x - \bar{u}t \quad \text{and let } \tau = t.$$

Employing the chain rule of calculus, we have

$$\frac{\partial C}{\partial x} = \frac{\partial C}{\partial \xi} \quad \text{and} \quad \frac{DC}{Dt} = \frac{\partial \xi}{\partial t} \frac{\partial C}{\partial \xi} + \frac{\partial \tau}{\partial t} \frac{\partial C}{\partial \tau} = -\bar{u} \frac{\partial C}{\partial \xi} + \frac{\partial C}{\partial \tau}$$

which is basically the substantial derivative. Equation 4.9 becomes

$$D_m \frac{\partial^2 \bar{C} + C'}{\partial \xi^2} + D_m \frac{\partial^2 C'}{\partial r^2} - u'(r) \frac{\partial \bar{C} + C'}{\partial \xi} = \frac{\partial \bar{C} + C'}{\partial t} \quad (4.10)$$

Notice that the second derivative of mean concentration in the r direction vanishes because it is constant over r . In the section 4.1, we assume that the rate of spreading along the flow direction due to the velocity variation is much greater than that caused by molecular diffusion. This will be shown to be true later. We therefore will neglect the longitudinal diffusion term in Equation (4.10) and it becomes

$$D_m \frac{\partial^2 C'}{\partial r^2} = \frac{\partial \bar{C}}{\partial \tau} + \frac{\partial C'}{\partial \tau} + u'(r) \frac{\partial C'}{\partial \xi} + u'(r) \frac{\partial \bar{C}}{\partial \xi} \quad (4.11)$$

Next step is to find a general solution for C' in Equation (4.11) if the mean concentration, velocity perturbations, and molecular diffusion coefficient are known. However, there is no analytical solution available at this moment. To avoid this difficulty, Taylor took a brave and brilliant assumption that the first three terms of the right-hand side of Equation (4.11) can be omitted at large time such that it can be reduced to

$$D_m \frac{\partial^2 C'}{\partial r^2} = u'(r) \frac{\partial \bar{C}}{\partial \xi} \text{ with boundary conditions } \frac{\partial C'}{\partial r} = 0 \quad \text{at } r = \pm R \quad (4.12)$$

Equation (4.12) has the solution

$$C'(\xi, r, \tau) = \frac{1}{D_m} \frac{\partial \bar{C}(\xi, \tau)}{\partial \xi} \int_0^r \int_0^r u'(r) dr dr + C'(0, \tau) \quad (4.13)$$

Now, you may ask why we need to solve for $C'(r)$. The reason follows. If we integrate Equation (4.11) over the cross-sectional area, $\frac{1}{2R} \int_{-R}^R () dr$, to each term of (4.11), we have

$$\frac{\partial \bar{C}}{\partial \tau} + \overline{\frac{\partial u'(r) C'(\xi, r, \tau)}{\partial \xi}} = 0, \quad (4.14)$$

where the overbar indicating a cross-sectional average of the term. Equation (4.14) is in essence an equation that allows us to describe the behavior of the cross-sectional-averaged concentration, $\bar{C}(\xi, \tau)$. As we have postulated previously, if the cross-sectional-averaged concentration can be described by Fick's law, (4.14) must have a form identical to the diffusion equation. More specifically, the cross-sectional average of the product terms of velocity and concentration perturbation must follow Fick's law. Since $u'(r)$ is known, from (4.13) we then have

$$\overline{u'(r) C'(\xi, r, \tau)} = \int_{-R}^R u'(r) C'(\xi, r, \tau) dr = \frac{1}{D_m} \frac{\partial \bar{C}(\xi, \tau)}{\partial \xi} \int_{-R}^R u'(r) \int_0^r \int_0^r u'(r) dr dr dr \quad (4.15)$$

Now we shall define $u'(y)c'(x,y)$

Consider the mass flux, relative to the moving coordinate system.

$$M = \int_0^h u'c' dy = \left[\frac{1}{D_m} \int_{-R}^R u'(r) \int_0^r u'(r) dr dr dr \right] \frac{\partial \bar{C}(\xi, \tau)}{\partial \xi}$$

While G.I. Taylor simplified the analysis, his analysis contributes significantly. The result of his analysis concludes that the total mass flux over the depth in the flow direction is proportional to the concentration gradient in the flow direction at large times. **This is exactly the same as the Fickian mechanism in the molecular diffusion.** That is, recall Fick's law for molecular diffusion

$$q = -D_m \frac{\partial c}{\partial x}$$

and compare it to the result of the shear flow analysis:

$$M = -hD_D \frac{\partial \bar{c}}{\partial x}$$

where

$$M = \left[\frac{1}{D_m} \int_{-R}^R u'(r) \int_0^r u'(r) dr dr dr \right] \frac{\partial \bar{c}}{\partial x}$$

or

$$D_D = \frac{1}{D_m} \int_{-R}^R u'(r) \int_0^r u'(r) dr dr dr$$

where D_D is called the longitudinal dispersion coefficient, which is a constant. We must remember that this analysis deals with cross-sectional area average concentration (one-dimensional solute transport analysis). Thus, the 1 - D dispersion equation in the moving coordinate system is:

$$\frac{\partial \bar{c}}{\partial \tau} = D_D \frac{\partial^2 \bar{c}}{\partial \xi^2}$$

Returning to the fixed coordinate system, we have

$$\frac{\partial \bar{c}}{\partial t} + \bar{u} \frac{\partial \bar{c}}{\partial x} = D_D \frac{\partial^2 \bar{c}}{\partial x^2}$$

This equation in essence is an advection-diffusion equation. In other words, effects of the velocity variation around the cross-sectional area averaged velocity due to fluid viscosity and roughness of the wall of pipe can be represented by Fick's law and the advection-diffusion equation can be applied to describe the cross-sectional area averaged concentration. However, we must recognize that

1) Taylor's analysis is only valid if the solute is displaced after a sufficiently long period of time. In other words, the validity of the convection-dispersion equation is unproven (i.e., it is likely a weakly approximated, or wrong model) at the early time.

2) The average concentration distribution will be a normally distributed cloud moving at the mean velocity, \bar{u} , and continuing to spread according to

$$\frac{d\sigma_x^2}{dt} = 2D_D$$

3. The longitudinal dispersion coefficient, D_D , is invariant in time and space.

How long is long enough?

The next question we must address is: how long is long enough to reach this situation?

On the interpretation of some long dispersion experiments. J. Fluid Mech., 48, Part 4, 689-709, 1971.

Chatwin (1971)

t at time after its injection t

$$t > 0.4 \frac{h^2}{D_m}$$

the variance of the dispersing cloud grows linearly with time and the cloud tends to have a normal distribution.

Taylor 1953

Dispersion of a solute in a laminar flow in a tube.

Velocity distribution $u(r) = u_0(1 - r^2/a^2)$

a the radius of the tube

u_0 the maximum velocity

$$D_D = a^2 u_0^2 / 192 D_m$$

For salt in water $D_m = 10^{-5} \text{ cm}^2/\text{sec}$

$u_0 = 1 \text{ cm/sec}$

$a = 2 \text{ mm}$

Then $D_D = 20 \text{ cm}^2/\text{sec}$

$D_D \gg \gg D_m$

The initialization time

$$0.4 \frac{4a^2}{D_m} = 1600 \text{ sec}$$

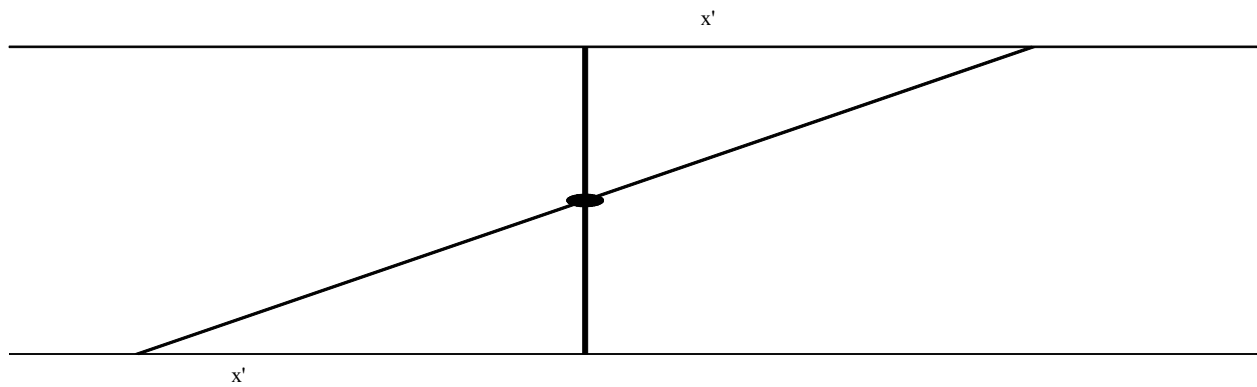
During which a slug of tracer would flow $\sim 1000 \text{ cm}$.

The dispersion during the first is not described by the 1 - D dispersion equation.

Spreading without Lateral diffusion.

$$u(y) = u_m y / h$$

$$\bar{u} = \frac{1}{h} \int u(y) dy = \frac{1}{h} \int \frac{u_m y}{h} dy = \frac{u_m}{h^2} \frac{y^2}{2} \Big|_0^h = \frac{u_m}{2}$$



$$\begin{aligned} u'(y) &= u(y) - \frac{u_m}{2} = \frac{u_m y}{h} - \frac{u_m}{2} \\ &= u_m \left[\frac{y}{h} - \frac{1}{2} \right] \end{aligned}$$

$$\text{Let } y = h \quad u' = \frac{u_m}{2}$$

$$c' = u't = \frac{u_m}{2} t$$

$$\sigma_x^2 = \left[\frac{u_m}{2} \right]^2 t^2$$

$$2D = \frac{d\sigma_x^2}{dt} = \frac{(u_m)^2}{2} t = \frac{u_m}{2} u_m t$$

The rate of spreading $= \left[\frac{u_m}{2} \right] x$ grows linearly with time.