Module C6.2

Miscible Dispersion

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OBJECTIVES
After completion of this module, the student
should be able to describe and discuss the effects
of convective transport and diffusive transport
on the axial dispersion of solute in a conduit.

PREREQUISITE MATHEMATICAL SKILLS
1. Elementary calculus and differential equations.
2. An introduction to partial differential equations, such as the diffusion equation. Previous exposure to the equation of conservation of mass would be helpful.

PREREQUISITE ENGINEERING AND SCIENCE SKILLS
1. Elementary modeling of transport problems, especially elementary concepts of convective and diffusive transport.

INTRODUCTION

Miscible dispersion refers to the mixing phenomena which occur when two miscible fluids are brought together either when stationary or when they are in motion. This definition is very broad, and it is not possible to do justice to the wide range of topics it covers in one module. So, attention will be confined here to the phenomenon of dispersion which takes place when a solute is introduced into fluid flowing in a conduit. Specifically, no attempt will be made to treat mixing in agitated vessels, which also would be called "dispersion."

While dispersion phenomena are fascinating to study just from the point of view of scientific interest, there are practical reasons for developing a good understanding of such phenomena. Some applications are:

1. The distribution of tracers and drugs in the bloodstream.
2. Conventional chromatography.
3. Field flow fractionation or polarization chromatography.
4. The transient behavior of tubular reactors.
5. Pollutant transport in the atmosphere.
6. Material and thermal pollution of natural streams.

The list is by no means complete. New applications will, doubtless, be found in the future. Serious study of the subject was begun only about thirty years ago by G. I. Taylor in a classic paper (52), and new developments are being made even today.

In each of these examples, it might be seen that dispersion or mixing occurs due to two basic mechanisms. These are:

1. convective or bulk transport
2. diffusive or molecular transport

Simplistic as this might sound, the interactions between these two mechanisms lead to some very interesting consequences. Before proceeding further, it is important to distinguish between two basically different types of dispersion problems which emerge from the various applications.

In the first category, called "initial distribution problems," a certain finite amount of solute is introduced into a flow and permitted to disperse. There can be no nontrivial steady state in such a situation, and all phenomena of interest are transient. Elution chromatography is a good example of this problem. In generalized dispersion theory, such problems are handled by using an infinite series solution which satisfies the appropriate initial and boundary conditions. This series will be displayed later in this module.

A second category of dispersion problems is characterized by the example of a chimney emitting pollutant continuously into the atmosphere or a chemical plant discharging effluent continuously into a nearby stream. In such problems, one might imagine the fluid medium (atmosphere or river) to be initially devoid of solute. At time zero, the appropriate source of solute is turned on at the inlet. This type of problem may be termed an "inlet distribution problem." If the discharge rate is steady, a non-trivial steady state can be established at locations close to the system inlet after a while. This steady state will propagate down the flow as time goes on, carrying in front of it a transient region. One approach for handling this class of problems is to treat the continuous source as a series of pulses, each one of which can be handled using techniques suitable for initial distribution problems. This method is known as superposition (13) and its application to inlet distribution problems has been

discussed by Gill and Sankarasubramanian* (25, 41), and Gill (26), and clarified by Subramanian (51). More recently, Smith (43–46) has used superposition innovatively to construct solutions to both classes of problems using his "delay-dispersion model."

In the rest of this module, attention is focused on "initial distribution problems" because of their relative simplicity.

THE PHYSICAL PROBLEM

The dispersion of a solute introduced into a fluid flowing into a conduit will be considered here. It is convenient to approach the complex problem in which a solute is dispersed due to the simultaneous action of convection and diffusion in the presence of a non-uniformly distributed velocity field, say in a circular tube, via simple, idealized, intermediate physical situations. These might be called "thought experiments."

Consider a slug of dilute solution, x_s units long and having a uniform concentration C_o of a suitable solute held in an infinitely long circular tube as shown in Figure 1. This slug is separated from pure solvent on either side of it by suitable impermeable barriers. The axial coordinate x and the radial coordinate r are defined as shown in the figure. All the thought experiments will be performed on this system.

Experiment 1

At time zero, imagine the barriers on either side of the slug are removed without causing any disturbance in the fluid (this is very hard to do in practice, but easy to imagine). No pressure gradient is imposed on the fluid so that it remains completely stationary.

The solute will be observed to diffuse symmetrically on either side of the original slug. The velocity resulting from this diffusion is ignored by assuming the slug to be very dilute. There is no radial or angular variation of concentration in the system, since the slug is assumed to be initially uniform in concentration everywhere. This diffusion process can be described mathematically by the one-dimensional conservation equation for the local solute concentration, $C(t, x)$. For a derivation of the conservation equation, see Bird, et al (6).

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \qquad (1)$$

Here, t is time, and D is the molecular diffusivity of the solute in the fluid. The initial and boundary conditions on $C(t, x)$ for the system are:

$$\left. \begin{array}{l} C(0, x) = C_o, \quad |x| \le \dfrac{1}{2} x_s \\[2mm] \qquad\quad = 0, \quad |x| > \dfrac{1}{2} x_s \end{array} \right\} \qquad (2)$$
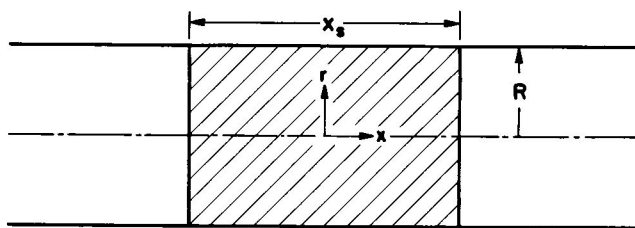

Figure 1. The system.

$$C(t, \pm \infty) = 0, \quad t \ge 0 \qquad (3)$$

Equation 2 states that initially, the solute concentration is C_o everywhere inside the slug and zero everywhere else. Equation 3 is characteristic of problems of this type, and indicates that solute never reaches axial stations infinitely far away from $x = 0$. The solution of Equations 1 to 3 for $C(t, x)$ is well-known and is given in Crank (14). Figure 2 shows the concentration distribution from this solution as a function of axial position for various values of time. In this simple thought experiment, there is no bulk (convective) transport. Figure 2 shows that symmetric axial spreading or dispersion of solute occurs due to molecular diffusion.

Experiment 2

Just as was done in the first experiment, imagine the barriers on either side of the slug are removed at time zero without causing any disturbance. However, this time, an axial pressure gradient is imposed on the fluid. This will result in bulk motion. This motion is assumed to be described by an idealized plug flow velocity profile. That is,

$$v_x = \text{constant} = v_m \qquad (4)$$

Here, v_m is the cross-sectional average velocity defined by

$$v_m = \frac{\displaystyle\int_0^R v_x r \, dr}{\displaystyle\int_0^R r \, dr} = \frac{2}{R^2} \int_0^R v_x r \, dr \qquad (5)$$
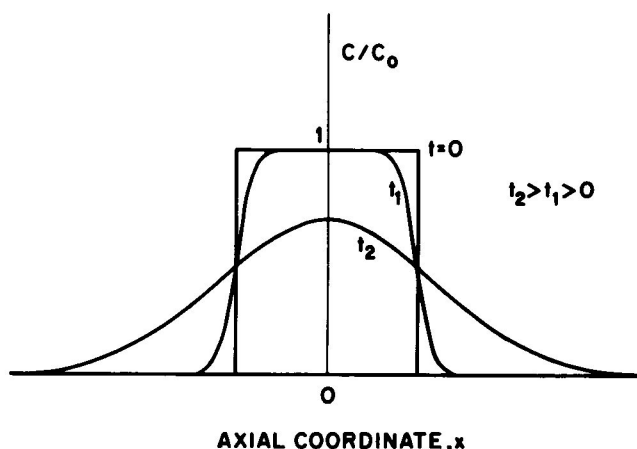
Figure 2. Concentration versus axial coordinate for the diffusion of a slug.

Since v_x is independent of position in this thought experiment, $v_m = v_x$. The fluid, and hence the solute, is moving with a constant velocity v_m everywhere. So, an observer who starts at time zero at $x = 0$, and runs along with the slug (moves axially at the same velocity v_m), should be able to "freeze" the motion of the solute. Then, the only transport seen by this observer would be molecular diffusion. That is, in a coordinate system (t, x_1) where

$$x_1 = x - v_m t \tag{6}$$

$C(t, x_1)$ would satisfy a simple diffusion equation. For this thought experiment, the concentration profiles would be identical to those in Figure 2 if the abcissa is changed from x to x_1.

The lesson to be learned from this thought experiment is that a uniform velocity field has no effect on axial spreading. The only role such bulk motion plays is to physically translate the solute slug with a velocity v_m down the tube. The center of the solute distribution is always located at $x = v_m t$ or $x_1 = 0$. Solute spreads symmetrically about this center by molecular diffusion only. For completeness, the partial differential equation satisfied by the solute concentration in the (t, x_1) system is:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x_1^2} \tag{7}$$

Note that Equation 7 is identical to the diffusion equation for C in the first thought experiment except for the fact that x_1 is measured from an origin moving at a speed v_m.

Experiment 3

This experiment is similar to Experiment 2, but the system is made more realistic by assuming laminar flow to exist instead of the idealized plug flow. That is, at time zero, the barriers are removed, and a pressure gradient is applied which causes steady, fully developed laminar flow in the tube. From the solution of the momentum conservation and total mass conservation equations for this system (6), it is known that the velocity is distributed non-uniformly across the cross-section of the tube in the shape of a parabola. That is,

$$v_x(r) = 2v_m \left(1 - \frac{r^2}{R^2} \right) \tag{8}$$

where r is the radial coordinate and R is the tube radius. v_m still represents the average velocity as can be verified from Equations 5 and 8.

From Equation 8, it may be observed that the velocity has a maximum value of $v_x = 2v_m$ at the tube center, and is zero at the tube wall. Clearly, it is impossible for an observer to "freeze" this motion by running along at any particular velocity as was done in the earlier thought experiment. The effect of the r-dependent velocity field is to cause *radial* concentration gradients in the tube even though the slug is initially radially uniform in concentration. Figure 3 shows the initial slug, and the condition of the slug after a small amount of time has elapsed.
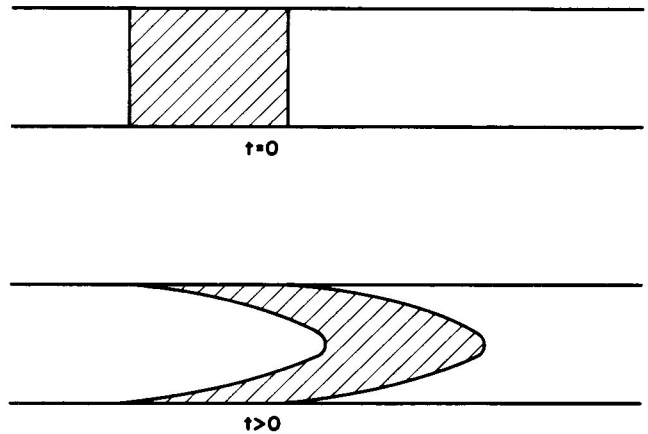

Figure 3. Axial spreading of the solute due to convection.

The front end of the slug starts out at time zero as a flat circular surface. However, due to the action of the parabolic velocity field, this surface becomes paraboloidal in shape. Similarly, the rear end of the slug becomes another paraboloidal surface. Ignoring diffusion for the time being, all the solute is located in the region between these two surfaces.

It might be noted immediately that the solute has been axially spread out just by the convection process. That is, the axial region occupied by the solute has been increased by the effect of the non-uniform velocity field. In fact, if there were no diffusional effects, this spreading process would go on distributing the solute over increasingly larger axial extents. Thus, axial dispersion is enhanced by the convective transport process in this example.

The role of diffusion in this problem is interesting and counterintuitive. One normally thinks of diffusion as a spreading mechanism. Yet, as will be seen shortly, the principal role of diffusion here is to inhibit the spreading induced by the convective transport process.

In Figure 3, the diffusive movement of solute will be normal to the surfaces which separate solute from the region devoid of solute. This diffusive flux may conveniently be broken up into an axial component (in the x-direction) and a transverse component (in the r-direction). The effects of these diffusive fluxes on the axial spreading of solute is opposite. Axial diffusion, as noted in the earlier examples, contributes to axial spreading. However, transverse diffusion inhibits axial spreading. Figure 4 illustrates why.

Shown in Figure 4 are the directions of radial solute transport due to diffusion. All over the front end of the distribution, radial diffusion moves solute from the faster central region to the slower region near the wall. Thus, the front end of the distribution cannot move ahead as rapidly as it would if there was no diffusion. At the rear
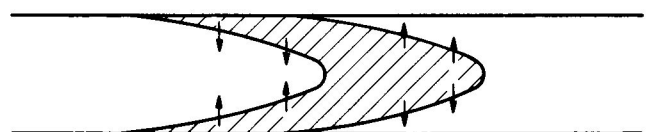

Figure 4. The role of transverse diffusion.

end, solute diffuses from the wall region to the central region, thereby helping the rear end catch up with the front. Therefore, the effect of radial diffusion is to keep the distribution compact in the axial direction, that is, to inhibit axial dispersion.

Another way of looking at this effect is to recognize that transverse diffusion ultimately permits all the solute molecules to sample all the velocities across the cross-section equally. Thus, the effects of the non-uniform velocity field in spreading the solute axially are countered by the effect of transverse diffusion which tends to equalize the average axial velocities of the solute molecules in the long run.

Interestingly, depending on the initial solute distribution, transverse diffusion may actually aid axial dispersion in the initial stages in certain situations (24). However, given time scales on the order of the diffusion time across the tube ($\sim R^2/D$), the effect of transverse diffusion is to inhibit axial spreading.

In summary, the third experiment performed under laminar flow conditions shows that convective transport in the form of a non-uniform velocity field tends to enhance axial dispersion; axial diffusion aids such axial dispersion, and transverse diffusion inhibits axial dispersion.

Unlike its predecessor, Experiment 3 can actually be set up in a laboratory. The results are fascinating when one does so. Near the beginning of this century, Griffiths (27) performed studies of the dispersion of a drop of fluorescent solution in a stream of water in laminar flow through a cylindrical capillary. *He found experimentally that the dye spreads out symmetrically about a plane which moves with the average flow velocity of the water in the tube.* This is a surprising observation since the velocity profile is asymmetric about the streamline in which the velocity is equal to the average velocity of flow. It was left to G. I. Taylor (52) to perform additional experiments and explain what Griffiths saw by means of a series of intuitive arguments. In view of the limited space available here, it is not possible to do justice to Taylor's work on this subject. However, the interested reader may consult his paper for such details. One should first recognize that when the dye concentration in a tube is visually examined, the observed average concentration is a cross-sectional average C_m. This is defined as:

$$C_m(t, x) = \frac{\int_0^R C(t, x, r) r \, dr}{\int_0^R r \, dr} = \frac{2}{R^2} \int_0^R Cr \, dr \qquad (9)$$

Recalling the second thought experiment, if an observer runs along with the mean velocity of flow v_m in Griffiths' experiments, according to Griffiths, the observer would see what *appears* to be a diffusive process as far as the average concentration is concerned. That is,

$$\frac{\partial C_m}{\partial t} = k \frac{\partial^2 C_m}{\partial x_1^2} \qquad (10)$$

where x_1 is defined in Equation 6. Note that the symbol k is used to describe this "apparent diffusivity" of C_m. k cannot be simply equal to the molecular diffusivity D

since the axial spreading of solute in Griffiths' experiments is due to the complex interaction between convective and diffusive transport, and not due to simple molecular diffusion. In fact, it is worth noting that the "apparent diffusivity" is typically several orders of magnitude larger than molecular diffusivity.

Taylor (52) performed some experiments of his own, as mentioned earlier (using potassium permanganate as the solute and water as the solvent) and confirmed Griffiths' observations. He also developed an approximate theory of the process (ignoring axial diffusion) which led to Equation 10 with the following result for the "dispersion coefficient" or the "apparent diffusivity," k.

$$k = \frac{R^2 v_m^2}{48D} \qquad (11)$$

Taylor's theoretical result is in agreement with the qualitative arguments presented in the earlier discussion of Experiment 3. The dispersion coefficient, k, which represents the axial spreading of solute in the capillary, is directly proportional to the square of the average velocity. The larger the average velocity, the greater will be the absolute velocity variations across the capillary, and therefore, the greater will be the axial spreading due to the velocity profile effect (convective spreading). Furthermore, the dispersion coefficient is inversely proportional to the molecular diffusivity D. This also is in agreement with the reasoning presented earlier which indicated that transverse diffusion should inhibit axial spreading.

Taylor's description of the dispersion process is valid only after a sufficient amount of time has elapsed since the introduction of solute into the capillary. This time scale is on the order of the diffusion time across the capillary R^2/D. Of course, several interesting transient phenomena take place before this time scale is reached in reacting systems. Also, in short conduits, the solute will leave the conduit before this time scale is reached. A generalized theory which accounts for solute behavior from time zero was developed by Gill and Sankarasubramanian (23, 24), who showed that the result for the dispersion coefficient derived by Taylor and displayed above is asymptotically valid for times $t \gtrsim 0.5 \ R^2/D$.

Taylor's result, given in Equation 11, is based on the assumption that axial molecular diffusion can be neglected. Aris (1) using a different technique (the method of moments), showed that the effect of axial molecular diffusion on the Taylor dispersion coefficient is additive. That is,

$$k = D + \frac{R^2 v_m^2}{48D} \qquad (12)$$

when one includes axial diffusion in the theory. Interestingly, the theory of Aris is indeed valid for all values of time since the introduction of the solute. However, emphasis in his work was directed at obtaining large time asymptotes consistent with Taylor's observations.

Equation 12 is known widely as the Taylor-Aris result for the dispersion coefficient in a tube.

ELEMENTS OF DISPERSION THEORY

The transport of solute in Griffiths's and Taylor's experiments may be described under suitable assumptions by the following mass conservation equation.

$$\frac{\partial C}{\partial t} + v_x(r)\frac{\partial C}{\partial x} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\,r\,\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial x^2}\right] \quad (13)$$

For an initial slug of solute of uniform concentration C_o, the following initial and boundary conditions may be written for the solute concentration $C(t, x, r)$.

$$\left.\begin{array}{ll} C(0, x, r) = C_o, & |x| \leq \frac{1}{2}x_s \\[2mm] \quad\quad\quad = 0, & |x| > \frac{1}{2}x_s \end{array}\right\} \quad (14)$$

$$C(t, \pm\infty, r) = 0 \quad (15)$$

$$C(t, x, 0) = \text{finite} \quad (16)$$

$$\left.\frac{\partial C}{\partial r}\right|_{r=R} = 0 \quad (17)$$

Equations 14 and 15 are familiar ones. Equation 16 indicates that the concentrations in the system are finite, and Equation 17 results from the fact that the tube wall is impermeable to the solute. Even though Equations 13 through 17 present a formidable problem to tackle analytically, several methods of solution are available. One may use any one of these methods to compute $C(t, x, r)$, and from this, any desired average, such as the cross-sectional average $C_m(t, x)$ or the cup-mixing or bulk average $C_b(t, x)$. However, a certain class of solution techniques permits the user to derive equations for the average concentration distribution with coefficients which may be calculated from first principles without ever computing the local concentration field. In the rest of this section, an elementary version of this method is presented, and some generalizations are pointed out. For an introduction to other approaches, the reader may consult some of the literature cited in the bibliography. Examples include the papers of Barton (2–4) Lighthill (33), Chatwin (7–12), Tseng and Besant (55, 56), Fife and Nicholes (21), and Yu (58).

Taylor's work (52) is an example where Equation 10 for $C_m(t, x)$ and Equation 11 for k permit the user to *predict* the cross-sectional average concentration field from theory without ever calculating $C(t, x, r)$. His approach was based on intuition. He recognized that for large values of time, the difference between the local concentration C and the cross-sectional average concentration C_m must be small. He also recognized that these small radial variations in C are crucial in accounting for axial dispersion, and attempted to describe them by writing, in effect,

$$C - C_m \approx g(r)\frac{\partial C_m}{\partial x} \quad (18)$$

Using Equation 18, one may determine $g(r)$ and then go on to derive the dispersion model, Equation 10 with k given by Equation 11. Equation 18 is based on the assumption that the higher axial derivatives of C_m are smaller than the first.

Later, in (54), Taylor added a correction term.

$$C \approx C_m + g_1(r)\frac{\partial C_m}{\partial x} + g_2(r)\frac{\partial^2 C_m}{\partial x^2} \quad (19)$$

This has subsequently been developed into an infinite series by Gill and Sankarasubramanian (22–24) in "generalized dispersion theory." (See Appendix.)

$$C = \sum_{k=0}^{\infty} g_k(t, r)\frac{\partial^k C_m}{\partial x^k} \quad (20)$$

An important difference between Equations 19 and 20, in addition to the infinite series generalization, is the introduction of time dependence in the functions g_k. Taylor's theory applied only for large values of time because the initial condition cannot be satisfied even with an infinite series generalization of Equation 19. As pointed out earlier, in several problems, the phenomena of interest occur before such values of time are reached. The functions $g_k(t, r)$ are time dependent precisely for accounting for such phenomena.

Another interesting feature to note is that in Equation 20, g_o can in general depend on time and radial position. In contrast, $g_o = 1$ in Taylor's work. The more general g_o is important in several practical problems where the initial solute distribution is non-uniform in r [as when a syringe and needle are used to inject a slug into a larger diameter capillary (24)]. Also, in cases where there is mass transfer at the tube wall, say due to a chemical reaction, g_o reaches steady but radially non-uniform asymptotic representations at large values of time (42). This is also the case when there is transverse flow, as shown in Doshi, et al (19), or when the solute migrates in a transverse field (31, 40).

For actual details of the development of generalized dispersion theory and its applications, the reader may refer to the series of papers by Gill and Subramanian listed in the bibliography. It may be mentioned here that, in general, Equation 20 leads to the following result:

$$\frac{\partial C_m}{\partial t} = \sum_{i=0}^{\infty} k_i(t)\frac{\partial^i C_m}{\partial x^i} \quad (21)$$

Equation 21 is a generalization of Taylor's result given in Equation 10, and is, in fact, a consequence of using Equation 20 for C instead of the approximation implied in Equation 18. The coefficients $k_i(t)$ in the generalized dispersion equation can be calculated from first principles fairly easily when $k_o = 0$, which is the case when the solute flux is zero at the tube wall. More complex cases involving reactions at the tube wall, and situations where other transverse average concentrations (such as the bulk-average) are required can be handled by the method of DeGance and Johns (15–17).

It is important to provide some physical insight into

the nature of the coefficients appearing in Equation 21. k_o may be thought of as a pseudo-homogeneous reaction rate constant accounting for disappearance of solute through possible reactions at the wall. Or as in Doshi, et al (19) where loss of fluid through the walls results in a concentration buildup within the channel, k_o accounts for this process. The quantity $-k_1$ may be thought of as the velocity of the solute cloud through the tube. It is time-dependent in general. For instance, if the solute is injected only into the central regions of the tube in Experiment 3, initially the solute cloud will move rapidly. However, as the solute diffuses across the cross-section, asymptotically, in that experiment, the solute will move with the average speed of the flow. Thus, as $t \to \infty$, $k_1 \to -v_m$.

The dispersion coefficient, $k_2(t)$, in Equation 21, is inherently time-dependent. It starts out at time zero being exactly equal to the molecular diffusivity, D. k_2 increases with time, and asymptotically approaches the Taylor-Aris value given in Equation 12 (23, 24). In a short tube, this asymptotic condition will never be reached, and the small-time behavior of the dispersion coefficient can be very important. A case in point is the study of Ultman and Blatman (57), who examined the dispersion of solutes in models of the human lung. Here, relatively short segments of tube bifurcate into new tubes, and the phenomena of interest in each tube occur over a time scale that is short compared to the diffusion time scale across the tube.

The higher–order coefficients $k_i(t)$ for $i \geq 3$ in Equation 21 are small, and the result is usually truncated after the term involving k_2, to give the classical Taylor dispersion equation. However, at small values of time, the higher–order terms can be important.

An interesting new development in dispersion theory has been presented over the last few years by R. Smith in a series of papers (43–46). He introduces a solution form, different from Equation 20, which is in a natural way able to accommodate continuous discharges of solute, as well as instantaneous ones. The approach, described by Smith as a delay-diffusion model, holds much promise. In particular, it is known from numerical calculations that the axial distributions of the cross-sectional average concentration are actually skewed in the initial stages of thought Experiment 3. Thus, a dispersion model of the type in Equation 10 cannot predict such distributions due to its inherent spatial symmetry. Smith's delay-diffusion model does very well in predicting such distributions properly.

The ideas presented in conjunction with the generalized dispersion Equation 21 can be connected logically to the development of Aris (1), who derived results for the spatial moments of the average solute concentration. In particular, the time dependences of the speed of the solute cloud and the dispersion coefficient are anticipated by Aris in the results displayed by him for the moments. The connection among the coefficients $k_i(t)$ and axial moments of the solute distribution is given by Subramanian (47).

The nature and properties of the series in the right-hand side of Equation 20 are not obvious. While it is clearly a generalization of Taylor's result in Equation 19,

it is not at all clear whether the series actually represents the left-hand side at least in some asymptotic sense. The question of the accuracy of truncated versions of Equation 20 among other things has been addressed by DeGance and Johns (15). The origin of Equation 20 becomes more clear if one examines the problem after taking Fourier transforms in the axial coordinate. This point is addressed briefly in the appendix.

As seen here, dispersion theory involves averaging the concentration over the cross-section and examining the behavior of this average as a function of the remaining variables. One might think of this as a general methodology wherein a function is averaged over "local" variables and the behavior of this average as a function of the remaining "global" variables is studied. This general point of view is put forth by Brenner (5), and is applicable to a wide variety of problems which superficially appear very different from the ones treated here. An example considered by Brenner in (5), as well as in several other papers which he has published recently, is that of the settling of a collection of non-spherical particles. Here, averaging is done over the various possible orientations the particles can assume, just as the concentration is averaged over the cross-section in the problem considered in this module.

Finally, a note of caution. The reader who goes to Taylor's classic paper (52) will find that Taylor used an intuitive procedure, not always rigorous, in arriving at the result for the dispersion coefficient k. He was successful in capturing the essence of this problem, as he had a knack of doing, because of his phenomenal insight. In particular, the axial derivatives of the average concentration are asymptotically small at large values of time. This permitted Taylor to make certain approximations, and correctly estimate the radial concentration variations which are crucial to the calculation of the asymptotic dispersion coefficient. Imitation of Taylor's procedure in a new setting without regard to rigor can easily lead the user to incorrect and indefensible predictions, a trap one must avoid.

CONCLUDING REMARKS

As demonstrated in this module, a simple experiment in the laboratory on the unsteady transport of a solute through a capillary can lead to interesting models. There are several areas which were left unaddressed in this module. The reader is encouraged to go directly to the published literature for more information. An excellent review article on the subject of dispersion authored by Nunge and Gill (34) appeared in 1969. This reference presents a state-of-the-art review of the area at that time and covers subjects such as dispersion in turbulent flow and in various flow geometries, and the effects of buoyancy on dispersion.

The bibliography provided at the end of this module not only lists the articles cited here, but also includes several pertinent articles which have appeared in the literature since the appearance of the Nunge-Gill review. While it is by no means an exhaustive list, it should direct the reader to the relevant literature for further enlightenment on this subject.

APPENDIX

The purpose of this Appendix is to briefly address the question of the origin of the generalized dispersion solution given in Equation 20 of the module. The method of Fourier transforms is used for this purpose. This material is relegated to an Appendix since it is not necessary to be familiar with it in order to understand the contents of the module; yet, it may help in appreciating the material a little better.

The Fourier transform of $f(x)$ may be defined as follows (28).

$$\bar{f}(\beta) = \int_{-\infty}^{\infty} f(x)e^{-i\beta x} \, dx \tag{A-1}$$

Then, the inverse is given by

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{f}(\beta)e^{i\beta x} \, d\beta \tag{A-2}$$

By taking Fourier transforms of both sides of Equation 20 in the module and rearranging the result, one gets

$$\frac{\bar{C}(t, r; \beta)}{\bar{C}_m(t; \beta)} \sim \sum_{k=0}^{\infty} g_k(t, r) \, (i\beta)^{k*} \tag{A-3}$$

Thus, Equation 20 results from an attempt to expand the ratio of the Fourier transforms of the local and average concentrations in a power series in β. The properties of such series can be investigated conveniently by transforming the equations for $C(t, x, r)$ to Fourier space.

ACKNOWLEDGMENT

NOMENCLATURE

C = concentration of solute
C_m = cross-sectional average concentration (see Equation 9)
C_o = initial concentration in solute slug
D = molecular diffusivity
g_k = functions appearing in Equation 20
k = dispersion coefficient
k_i = coefficients appearing in Equation 21
r = radial coordinate
R = tube radius
t = time
v_x = axial velocity of fluid
v_m = average axial velocity
x = axial coordinate
x_1 = transformed coordinate (see Equation 6)
x_s = length of solute slug

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*The symbol ~ means that the right-hand side represents left-hand side in the sense of an asymptotic expansion.

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STUDY PROBLEMS

1. How is miscible dispersion different from molecular diffusion?

2. Why does a uniform velocity field cause no axial dispersion?

3. Does the velocity profile have to be parabolic to cause axial dispersion? For instance, would you see axial dispersion with a linear velocity profile which occurs in simple Couette flow?

4. What was Taylor's principal contribution in his 1953 paper?

5. What is the difference between the Taylor dispersion coefficient and the Taylor-Aris dispersion coefficient?

6. Does diffusion help or hinder axial dispersion in flow systems?

HOMEWORK PROBLEMS

1. A capillary has a diameter of 4 mm and has water flowing through it at an average velocity of 50 mm/s. What would be the Taylor dispersion coefficient k for potassium permanganate in this system? The diffusivity of permanganate at room temperature is $D \approx 1.5 \times 10^{-9}$ m^2/s. Compare the value of k to that of the molecular diffusivity. Is the correction for axial molecular diffusion significant in this case?

2. Taylor's dispersion equation also is often written in the following form:

$$\frac{\partial C_m}{\partial t} + v_m \frac{\partial C_m}{\partial x} = k \frac{\partial^2 C_m}{\partial x^2} \qquad (H-1)$$

Show that Equations H-1 and 10 (in the module) are equivalent by carrying out the transformation from the (t, x) system to the (t, x_1) system, using Equation 6 in the module.

3. Try to satisfy the initial condition in Equation 14 by using Equation 18—do you encounter any difficulty? How would you satisfy Equation 14 if $g = g(t, r)$ in Equation 18?

4. Two identical slugs of dilute potassium dichromate solution are introduced at the same instant into water flowing through two identical tubes of inside diameter 50 mm. The only difference between the systems is that in tube 1, the average velocity of the water $v_{m_1} = 40$ mm/s, whereas in tube 2, the average velocity $v_{m_2} = 80$ mm/s. A strange result is observed! The solute distribution in tube 2 moves down the tube twice as fast as that in tube 1, as expected, but it disperses in the axial direction to a *much smaller extent than in tube 1*. Explain this observation on the basis of the physical mechanisms influencing dispersion.

5. A circular tube has its inside wall coated with a thin layer of catalyst. A dilute mixture of two solutes is introduced as a slug at the inlet at time zero. Both the solutes travel down the tube and undergo dispersion in laminar flow, but only one of them reacts at the catalytic wall. Will the reacting solute travel at a different average velocity from the non-reacting one? Will it disperse more or less in the axial direction? Why?