# TAYLOR-ARIS DISPERSION

## *An Explicit Example for Understanding Multiscale Analysis via Volume Averaging*

Brian D. Wood
*Oregon State University • Corvallis, OR 97330*

The idea that the representation of a transport process is dependent upon the length-scale of observation is a perspective that has become widely adopted in chemical engineering education in recent decades; a graphical presentation of a system in which multiscale transport is important appears as Figure 1. Perhaps the clearest indication of this evolution in perspective can be found in the recent publication of the second edition of *Transport Phenomena* by Bird, Stewart and Lightfoot.[2] A new focus in this second edition, as distinct from the first edition of 1960,[3] is the multiscale structure of transport phenomena. This perspective appears throughout that text, and in particular is emphasized by the addition of a "Chapter 0" in which the connections among the molecular, microscopic, and macroscopic scales are discussed in the context of transport phenomena. It is becoming standard practice to refer to the smaller and more fundamental of the two scales involved as the "microscale" and the larger as the "macroscale" regardless of the actual dimensions that define the two scales, and this terminology will be used throughout the remainder of this discussion.

The concept of upscaling transport phenomena in complex, multiphase systems has been developed in the chemical engineering discipline extensively over the last 40 years. Although in principle this perspective is more fundamental in the sense that phenomena at different characteristic length scales are formally connected, the mathematical machinery required to understand and apply the theory has tended to keep it somewhat abstracted from applications.

New interest in the connection of transport phenomena among scales has developed in chemical engineering, however, (as evidenced, for example, by the second edition of Bird, Stewart, and Lightfoot,[2] discussed above), driven partly by the need to understand multiscale systems and partly by evolving advances in experimental methods that allow measurements at small scales with unprecedented resolution. In particular, developments in nano- and micro-technology have made it clear that a thorough understanding of the micro-macro connection in transport phenomena is essential for understanding—and ultimately engineering—systems that involve nano- and micro-scale processes.

Upscaling is possible and appropriate for systems that have a significant amount of "redundant" information. Although the concept of redundant information has a concrete definition in the context of information theory (*e.g.*, Reference 4), from a pedagogical perspective we can think of redundant information as information that can be removed without affecting

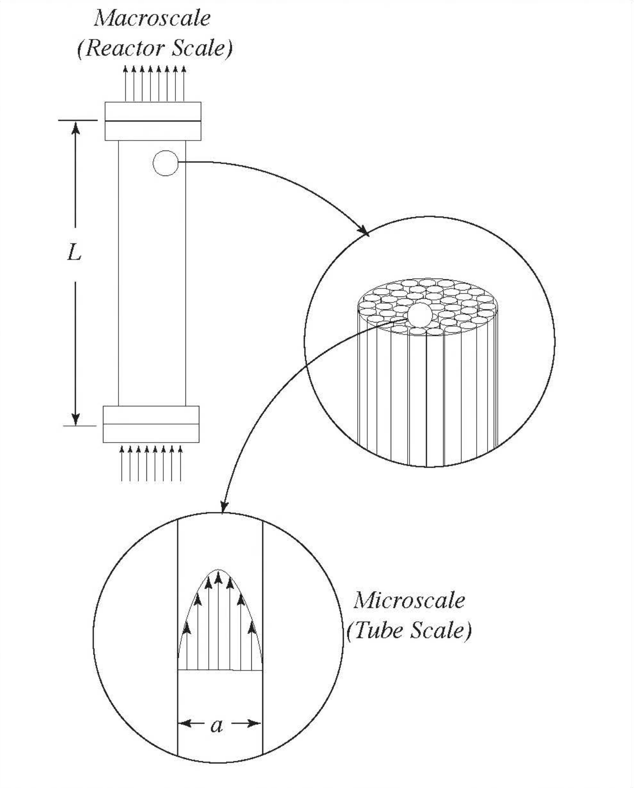

**Figure 1.** *An example of a multiscale hierarchical system.*

***Brian Wood** received his Ph.D. in environmental engineering at the University of California, Davis. He is an associate professor in the School of Chemical, Biological, and Environmental Engineering at Oregon State University in Corvallis, Ore., where he teaches environmental engineering and maintains his research program. His research interests include mass, momentum, and energy transport; transport in biological systems; upscaling in multiphase, multiscale systems; stochastic methods; and applied mathematics.*

the interpretabilily of the physical system. An example that I frequently use to communicate the ideas behind upscaling is that of the ideal gas. Viewed as a classical mechanical system, a mole of an ideal gas has an enormous number of degrees of freedom ($6.02 \times 10^{23}$ molecules times 3 position and 3 momentum coordinates gives something like $5 \times 10^{24}$ degrees of freedom!).

If, however, our goal is to predict the pressure of an ideal gas in a fixed volume, then this constitutes a large amount of redundant information. Essentially, because of the extremely large numbers involved, the momentum and coordinates of any particular molecule of gas are not important for determining the pressure of the gas. Rather, the momentum coordinates can be grouped as a distribution, and we can take a statistical approach to computing the pressure of the gas. One can, in fact, show (*e.g.*, as explained by Feynman, et al.[5]) that the system of roughly $5 \times 10^{24}$ equations of motion (Newton's laws) for the ideal gas can be "upscaled" via averaging to the well-known result PV=knT, where k is the Boltzmann constant, n is the number of molecules involved, and T is the temperature. For this result to be obtained one also has to make a number of assumptions about the behavior of the system, and for the purposes of this paper I will refer to such assumptions as "scaling laws." In the case of the ideal gas, one must adopt the scaling laws of (1) a Maxwellian distribution of speeds applies to the population of molecules, and (2) the statistics do not depend on spatial location (*i.e.*, they are spatially homogenous). Under these conditions, averaging appropriately yields the ideal gas law, and the original $5 \times 10^{24}$ degrees of freedom are replaced by a single degree of freedom—the temperature T (which is actually a proxy for the mean kinetic energy of the gas).

In Figure 2, a graphical summary of the upscaling process is presented. The essential features of upscaling are represented here as follows. Complete information for the system of interest (*e.g.*, the location and momentum of all molecules in the ideal gas example) is represented at the top of the figure, which we might think of as having, say, the number N degrees of freedom. We are always at liberty to separate such a system into two components: a mean and a deviation from the mean. Note that here there are still N degrees of freedom; given one of these fields, the other can be obtained by subtracting from the microscale (complete information) representation. At this juncture, if redundant information can be identified, it can be eliminated by upscaling (this requires identifying a scaling law, which is nothing more than a statement about the assumed form of the redundant information). In the example of the ideal gas, we found that the redundant information was the list of velocity components and locations. All that was really needed from this information (at least for the purposes of deriving the ideal gas law) was the two assumptions of velocity statistics that follow a Maxwell distribution and spatial stationarity. The third row shows the results of the upscaled model; a reduction in the number of

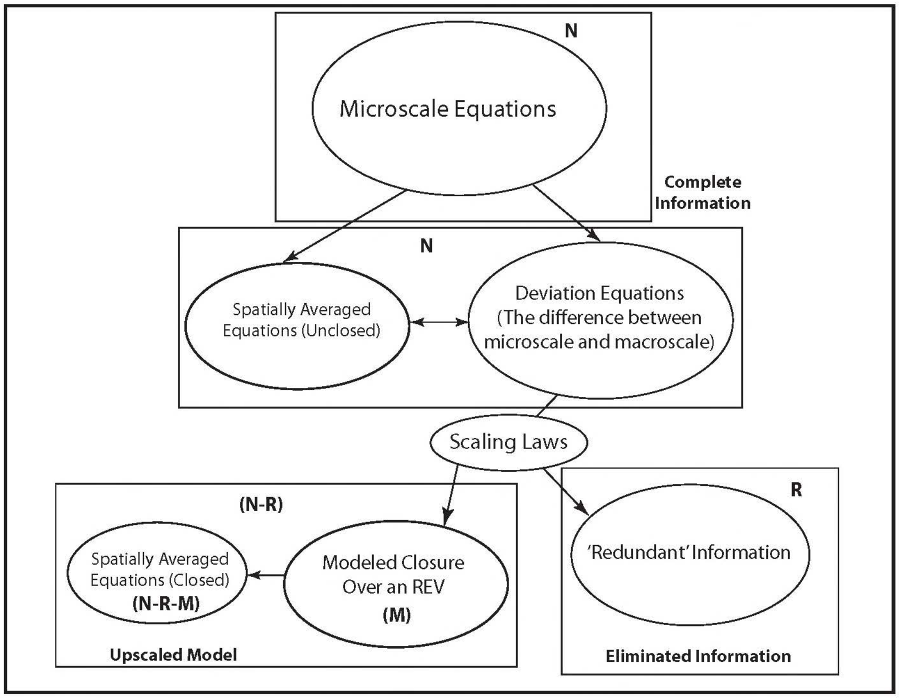

***Figure 2.** A graphical representation of information flow during the process of upscaling.*

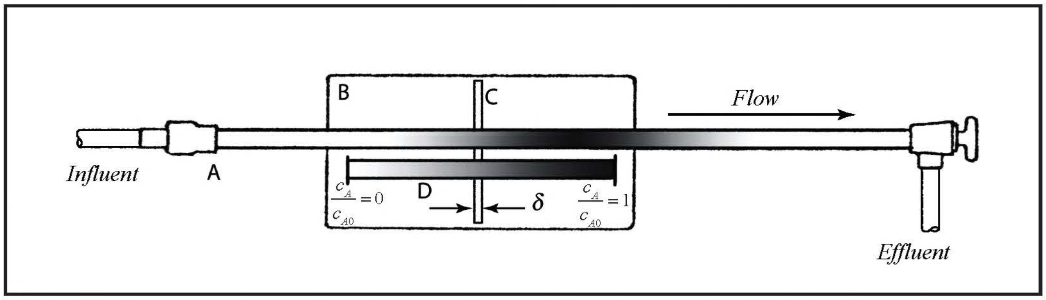

***Figure 3.** An experimental device used for examining dispersion of a visible dye in a tube, after Taylor.[1] (A) The capillary tube. (B) A ground glass plate illuminated from behind. (C) The sampling window. (D) A tube containing dye at known concentrations for comparison to the experimentally observed values.*

degrees of freedom has been accomplished by the elimination of the redundant information.

The purpose of this paper is to provide an example of upscaling a multiscale system that has particular pedagogical value. Most students of chemical engineering become familiar with the concept of dispersion, and some will even study the specific example of Taylor-Aris dispersion in detail. The methods used to perform upscaling, in contrast, tend to be presented almost solely in advanced graduate-level courses, and even then there are generally few concrete examples in which students can test the upscaling methods themselves in a familiar context. The case of Taylor-Aris dispersion is an example that is both familiar and one in which a closed-form analytical solution for the effective dispersion coefficient can be developed without having to resort to the solution of a complex, multidimensional partial differential equation. The development also provides an opportunity to review the concept of moving coordinate systems, which are always problematic for students. The objective of this paper is to present a concrete example of upscaling in a manner that is suitable for undergraduate and graduate students alike, with a particular emphasis on generating an analysis where the assumptions and constraints are explicitly identified.

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## MICROSCALE FORMULATION OF THE PROBLEM

### Background

Taylor-Aris dispersion has been studied for more than 50 years since the seminal works of Taylor[1, 6] and Aris,[7] in the mid 1950s, and it continues to remain an archetypical example for development of new dispersion theory. Partly because it has been studied so extensively using a variety of mathematical approaches, it also represents an example that has been fraught with misunderstanding, even by established experts in the field (*e.g.*, see the exchange of Beard[8, 9] and Dorfman and Brenner[10]). In principle, the concept of Taylor-Aris dispersion is straightforward. Because the fluid velocity profile in a capillary tube is parabolic (Figure 1), the fluid at the center of the tube moves faster than that near the tube walls. This causes an initially uniform pulse of solute to spread longitudinally due to fluid convection, which forms strong concentration gradients in the radial direction and allows radial diffusion to transport solute across convective streamlines; as time progresses, this tends to create a uniform concentration on planes perpendicular to flow. The question addressed by Sir Geoffrey Taylor (and amended later by Rutherford Aris[7]) was essentially this: If one observes the average concentration in a capillary tube (using, for example, light transmission of a visible tracer) then is it possible, through knowledge of the microscale transport phenomena, to predict the effective longitudinal dispersion coefficient that would be observed for this averaged concentration? The answer to this question is ultimately yes, and the analyses by Taylor[1, 6] and Aris[7] provide examples of those rare cases where a very satisfying, compact result is possible. Taylor investigated this problem both theoretically and experimentally; an illustration of Taylor's experimental device is given in Figure 3.

### Microscale Description

To begin the multiscale analysis, one first poses the microscale mass balance equations describing solute transport in a capillary tube. It is useful to recognize at this point that the microscale equations can be, in principle, formally derived by upscaling the molecular scale transport phenomena. At the smallest length scale that we attempt to pursue, however, we must ultimately adopt the laws governing the balance of mass as axiomatic. That is, we must assume that the governing laws are true (*e.g.*, in the case of a classical molecular description, that Hamiltonian dynamics are valid[11]) but are fundamentally unprovable. This feature is true of all upscaling efforts—they relate information among scales provided that one first has axiomatically defined the transport phenomena at a more fundamental scale (*i.e.*, the microscale).

For the case of transport in a capillary tube, we can pose the following microscale boundary-initial value problem for the solute [see Reference 7, Eqs. (3)-(6)]. A simplified version of Taylor's experimental system is presented in Figure 4, and the mathematical description of solute transport at the microscale is specified as follows.

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \left(\mathbf{v} c_A\right) + \nabla \cdot \left(\mathscr{D}_A \cdot \nabla c_A\right), \text{in the fluid phase} \quad (1)$$

$$-\mathbf{n} \cdot \left(\mathscr{D}_A \cdot \nabla c_A\right) = 0 \text{ on the tube walls} \quad (2)$$

$$c_A\left(x, t=0\right) = \mathscr{F}\left(x\right), \text{ initial condition} \quad (3)$$

Here, $c_A$ is the concentration of chemical species A, $\mathscr{D}_A$ is the (isotropic) molecular diffusion coefficient, and v is the fluid velocity vector. Fick's law has been adopted here for describing the diffusive flux, and this necessarily requires that the mole fraction of species A, $x_A$, be small enough such that $x_A << 1$. For the capillary tube, the velocity field is given by the well-known expression

$$v\left(r, x\right) = 2U\left(1 - \frac{r^2}{a^2}\right) \quad (4)$$

where U is the average velocity (to be defined later), and r and x are the radial and longitudinal coordinates illustrated in Figure 4.

### Moving Coordinates

For the purposes of this analysis, it is convenient to put this problem in an inertial coordinate system that moves uniformly in the x-direction with the average velocity, U. In other words, the relationship between the nonmoving longitudinal coordinate z, and the moving longitudinal coordinate x(t) is given by

$$\underbrace{x(t)}_{\substack{\text{current}\\ \text{location}}} = \underbrace{z\Big|_{t=0}}_{\substack{\text{initial}\\ \text{location}}} + \underbrace{Ut}_{\substack{\text{amount of}\\ \text{movement}}} \tag{5}$$

Moving coordinate systems frequently confuse students, and this is not without good reason. The presentation of moving coordinate systems is frequently conducted by observation rather than by showing the detailed conversion from one frame of reference to another. For that reason, it is worth spending some time on this concept in class. To start, one can explain that Eq. (5) is the relationship between a point fixed in the fluid at the initial time (t = 0) and where that point would be located later if it were to flow with the fluid at the velocity U; it is, essentially, the equation that describes a streamline for the mean velocity field. Sometimes it is easier to think about this in the reverse. In the moving coordinate system (Figure 4), any point x(t) is related to the point that it originally came from (at the time t = 0), *i.e.*,

$$z\Big|_{t=0} = x(t) - Ut \tag{6}$$

The velocity in the new frame of reference can be determined with reference to Figure 5. Here, Z(t) represents the vector following a fluid parcel in the original (fixed) frame of reference. We can think of this vector as being broken up into two parts: the vector that traces the distance to the new coordinate system, and the vector that gives the displacement relative to the new coordinate system. In mathematical terms

$$Z(t) = X(t) + x(t) \tag{7}$$

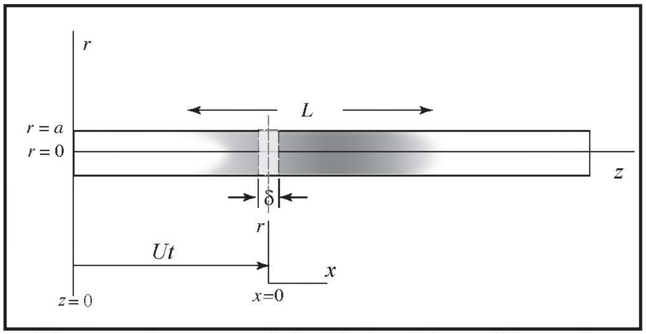

***Figure 4.** Geometry of the Taylor-Aris capillary tube.*

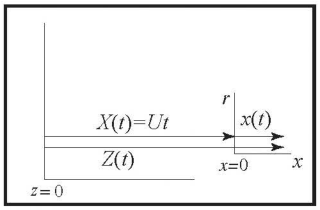

***Figure 5.** Relationship among coordinate systems.*

Taking the derivative of both sides of Eq. (7) and rearranging terms gives the following relationship

$$\frac{dx(t)}{dt} = \frac{dZ(t)}{dt} - \frac{dX(t)}{dt} \tag{8}$$

or, substituting in the definitions for velocities

$$v(x,r,t) = v(z,r,t) - U \tag{9}$$

For the particular case of interest, we are interested in steady flow. Referring to Eq. (4), we can put the function describing the velocity in the new frame of reference in the form

$$\begin{aligned} v(x,r) &= 2U\left(1-\frac{r^2}{a^2}\right) - U \\ &= U\left(1-\frac{2r^2}{a^2}\right) \end{aligned} \tag{10}$$

### Simplifications

From these general balance equations, we can make some substantial simplifications by making the following reasonable assumptions: (1) the capillary tube is cylindrical, (2) the fluid is incompressible, (3) the fluid pressure on the cross-sectional area of the two ends of the tube is uniform (which leads to a cylindrically symmetric fluid velocity field), (4) the initial condition for the solute is cylindrically symmetric so that $\partial c_A/\partial\theta=0$, and (5) there is no diffusive flux discontinuity at the center of the tube, so that $\partial c_A/\partial r=0$ at r=0. Under these conditions, we can rewrite Eqs. (1)-(3) in term of a cylindrical (but nonmoving) coordinate system (Figure 4) as follows

$$\frac{\partial c_A}{\partial t} = -2U\left(1-\frac{r^2}{a^2}\right)\frac{\partial c_A}{\partial x} + \mathscr{D}_A\left[\frac{1}{r}\frac{\partial c_A}{\partial r} + \frac{\partial^2 c_A}{\partial r^2} + \frac{\partial^2 c_A}{\partial x^2}\right], \quad \text{in the fluid phase} \tag{11}$$

$$-\mathscr{D}_A\frac{\partial c_A}{\partial r} = 0, \quad \text{at } r=0 \text{ and } r=a \tag{12}$$

$$c_A(r,x,t=0) = \mathscr{F}(r,x), \quad \text{initial condition} \tag{13}$$

As a final step, we need to put these equations in the moving frame of reference. To do this, we start by noting from Eq. (10)

$$2U\left(1-\frac{r^2}{a^2}\right) = U\left(1-\frac{2r^2}{a^2}\right) + U \tag{14}$$

Substituting this into Eq. (11) and rearranging gives us

$$\frac{\partial c_A}{\partial t} + U\frac{\partial c_A}{\partial x} = -U\left(1-\frac{2r^2}{a^2}\right)\frac{\partial c_A}{\partial x} + \mathscr{D}_A\left[\frac{1}{r}\frac{\partial c_A}{\partial r} + \frac{\partial^2 c_A}{\partial r^2} + \frac{\partial^2 c_A}{\partial x^2}\right], \quad \text{in the fluid phase} \tag{15}$$

As a final step, we note that by the definition of the total derivative we have

$$\frac{dc_A}{dt} = \frac{\partial c_A}{\partial t} + \frac{\partial c_A}{\partial x}\frac{dx}{dt} \tag{16}$$

which, by Eq (5), gives

$$\frac{dc_A}{dt} = \frac{\partial c_A}{\partial t} + U\frac{\partial c_A}{\partial x} \tag{17}$$

Substituting this result into Eq. (15) yields the form of the transport problem in the moving frame of reference

$$\underbrace{\frac{dc_A}{dt}}_{\substack{\text{Total Derivative}\\ \text{(Moving Frame}\\ \text{of reference)}}} = \underbrace{-U\left(1-\frac{2r^2}{a^2}\right)\frac{\partial c_A}{\partial x}}_{\substack{\text{Convection Term}\\ \text{with Moving Frame}\\ \text{of Reference Velocity}}} + \underbrace{\mathscr{D}_A\left[\frac{1}{r}\frac{\partial c_A}{\partial r}+\frac{\partial^2 c_A}{\partial r^2}+\frac{\partial^2 c_A}{\partial x^2}\right]}_{\substack{\text{Diffusion Term in}\\ \text{Moving Frame of Reference}\\ \text{Remains Unchanged}}}$$

$$\text{in the fluid phase} \tag{18}$$

$$-\mathscr{D}_A\frac{\partial c_A}{\partial r} = 0, \quad \text{at } r = 0 \text{ and } r = a \tag{19}$$

$$c_A\left(r,x,t=0\right) = \mathscr{F}\left(r,x\right), \text{ initial condition} \tag{20}$$

Note that this should be a familiar operation—this is exactly what happens when one transforms a system into material coordinates in the study of fluid mechanics. The derivative in this case is a total derivative that is very similar to the material derivative that is used routinely in fluid mechanics; in our case, however, the velocity is the average velocity rather than the velocity of a material body, and therefore only the average velocity is incorporated into the total derivative.

## AVERAGING

Averaging arises naturally in our experimental observations about systems, but we do not as often think about the relationship to our theoretical representation of the system. As an example, few would argue that Eqs. (18)-(20) represent a reasonable model for describing solute transport in a capillary tube. When we consider what is measurable for such a system, however, the answer is generally not "the microscale concentration, $c_A$." Although with substantial effort it may, in fact, be possible to measure the microscale concentration directly, generally we would measure some macroscale property of the system, such as the flux-averaged concentration coming out of the capillary in the effluent, or possibly the spatially averaged concentration resident within the tube at a particular time and with a particular spatial resolution that depends on the instrument used. Although we frequently measure averaged or otherwise "filtered" properties in experimental systems, we rarely think about them as such. The problem of Taylor dispersion in a capillary tube is a cogent, specific example where this micro-macro duality is explicitly recognized, and a full analysis of the interrelationship among scales is possible.

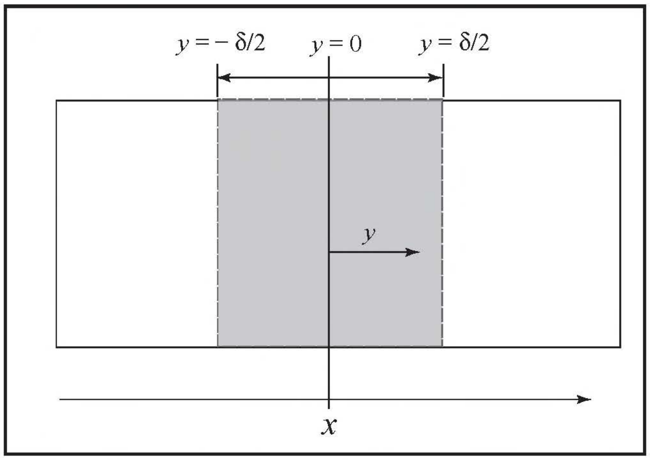

***Figure 6.*** *Integration domain for the averaging. Note that the average is still a function of the location, x. A volume average is well defined for each such location.*

Ideally, then, we would like to develop a mass balance equation where the dependent variable is related to the quantity that we can actually measure. To this end, we can consider averaging the microscale mass balance equations using a weighting function that represents the influence of our instrument used for observation (*e.g.*, Reference 12). At first, this may seem like a curious perspective, but upon reflection one can recognize that this is actually more in line with our interpretation of laboratory results than is the set of microscale equations given by Eqs. (18)-(20).

### Definition of the Average

To begin, we define an appropriate average. In the most general context, averages can be taken over any kind of weighting function that represents an instrument response. In applications of the volume averaging method in particular, however, the weighting function is usually taken to be a step function that is defined as being one inside an averaging volume, and zero outside. For our capillary system, the appropriate average is defined by

$$\left\langle c_A\right\rangle\Big|_x = \frac{1}{\pi a^2}\int_{r=0}^{r=a}\left(\frac{1}{\delta}\int_{y=-\delta/2}^{y=\delta/2} c_A\Big|_y\, dy\right)2\pi r\, dr \tag{21}$$

where y is a variable of integration. An illustration of the integration domain is given in Figure 6.

A little discussion is warranted here. Note that this is different from the area average that is conventionally used in the Taylor-Aris analysis. In part, this is due to the idea that we are attempting to generate an upscaled theory for a measurable property of the system, for example, the light transmitted through a small volume of the capillary tube (as a proxy for a dye tracer concentration) as Taylor did in his original experiments (Figure 3). The area average is not the measurable property, rather the average over some small observation window is (*e.g.*, as illustrated in Figure 3). We can, however, imagine that when the concentration field does not have large gradients, and the thickness, δ, of the averaging volume is small we may be able to neglect the changes in the concentration, $c_A$, over the interval δ. This essentially converts our observation over a small volumetric window to one that is equivalent to the area average. More formally, we can do this by expanding the concentration in a Taylor series $c_A\big|_y$ around the point

$$c_A\Big|_{x+y} + c_A\Big|_x + y\frac{\partial c_A}{\partial x}\bigg|_x + \frac{1}{2}y^2\frac{\partial^2 c_A}{\partial x^2}\bigg|_x + \ldots \tag{22}$$

Substituting into the integral given by Eq (21)

$$\langle c_A\rangle\Big|_x = \frac{1}{\delta}\frac{1}{\pi a^2}\int_{r=0}^{r=a}\left(\int_{y=-\delta/2}^{y=\delta/2} dy\, c_A\Big|_x + \int_{y=-\delta/2}^{y=\delta/2} y\,dy\frac{\partial c_A}{\partial x}\bigg|_x + \int_{y=-\delta/2}^{y=\delta/2}\frac{1}{2}y^2 dy\frac{\partial^2 c_A}{\partial x^2}\bigg|_x + \ldots\right)2\pi r\, dr$$

Note that the second integral in this expansion is identically zero. The third and higher terms can be neglected under the conditions that the concentration change over the distance δ is small compared to the distance L. To see this, we can pose the following *restriction* (see Reference 13)

$$\int_{y=-\delta/2}^{y=\delta/2} dy\, c_A\Big|_x >> \int_{y=-\delta/2}^{y=\delta/2}\frac{1}{2}y^2 dy\frac{\partial^2 c_A}{\partial x^2}\bigg|_x \tag{24}$$

We can then make the following estimates

$$\int_{y=-\delta/2}^{y=\delta/2} dy = O(\delta) \tag{25}$$

$$\int_{y=-\delta/2}^{y=\delta/2}\frac{1}{2}y^2 dy = O(\delta^3) \tag{26}$$

$$\frac{\partial^2 c_A}{\partial x^2}\bigg|_x = O\left(\frac{c_A}{L^2}\right) \tag{27}$$

Combining these yields with the restriction given in Eq (24) yields the constraint [See Reference (13)]

$$\frac{\delta}{L} << 1 \tag{28}$$

If the concentration field meets this condition, we expect the first term in Eg. (23) to provide a good estimate of the entire expansion. Under these conditions, the conventional area average concentration can be recovered.

$$\langle c_A\rangle = \frac{1}{\pi a^2}\int_{r=0}^{r=a} c_A(2\pi r)dr \tag{29}$$

The practical result of this is that, for the purposes of the upscaling effort, the conventionally adopted area average is an acceptable average to use, and should be equivalent to the concentrations found by observations of experimental systems provided that the constraint given by Eq. (28) is met.

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### Upscaling

In the process of upscaling, simplifications are *necessarily* introduced if a useful theory is to be developed. This is because a useful macroscale representation is only possible if there is an underlying structure to the physics of the problem that allows one to reduce the number of degrees of freedom in the system without eliminating essential information. Approximations that allow a reduction in the number of degrees of freedom are called *scaling laws.* In the case of the Taylor dispersion problem, one scaling law that we are assuming is that the constraint given by Eq. (28) is valid. In other words, we require that the concentration field be *smooth enough* so that there are no large fluctuations on a length scale of δ; if this condition is not met, the method may not work.

With the definition of the average identified, we can apply the averaging operator to both sides of Eq. (18) (essentially, this is done by multiplying both sides of the equation by 2πr, and then integrating with respect to r from r = 0 to r = a). The result is

$$\left\langle\frac{dc_A}{dt}\right\rangle = -U\left\langle\left(1-\frac{2r^2}{a^2}\right)\frac{\partial c_A}{\partial x}\right\rangle + \mathscr{D}_A\left[\left\langle\frac{1}{r}\frac{\partial c_A}{\partial r}\right\rangle + \left\langle\frac{\partial^2 c_A}{\partial r^2}\right\rangle + \left\langle\frac{\partial^2 c_A}{\partial x^2}\right\rangle\right] \tag{30}$$

Noting that the averaging operator does not depend on x or t, we can exchange averaging and differentiation with respect to x and t.

For the second term on the right-hand side of Eq. (30), we can use integration by parts along with the two boundary conditions to show

$$\left\langle \frac{\partial^2 c_A}{\partial r^2} \right\rangle = \frac{1}{\pi a^2} \int_{r=0}^{r=a} \frac{\partial^2 c_A}{\partial r^2} (2\pi r) dr$$

$$= \frac{1}{\pi a^2} \left[ \frac{\partial c_A}{\partial r} (2\pi r) \Big|_{r=0}^{r=a} - \int_{r=0}^{r=a} \frac{\partial c_A}{\partial r} (2\pi) dr \right]$$

$$= \frac{1}{\pi a^2} \left[ - \int_{r=0}^{r=a} \frac{1}{r} \frac{\partial c_A}{\partial r} (2\pi r) dr \right]$$

$$= - \left\langle \frac{1}{r} \frac{\partial c_A}{\partial r} \right\rangle \tag{31}$$

Combining these results gives a macroscale equation of the form

$$\frac{d\langle c_A \rangle}{dt} = -U \frac{\partial \langle c_A \rangle}{\partial x} + \mathscr{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial c_A}{\partial x} \right\rangle \tag{32}$$

Except for the last term on the right-hand side, this expression is a macroscale balance equation for the average concentration, $\langle c_A \rangle$. We can't simplify the last term as it stands because of the presence of the multiplier $r^2$ inside the averaging operator. To proceed further, we have to propose some method for expressing $\langle r^2 \partial c_A / \partial x \rangle$ in terms of the average concentration $\langle c_A \rangle$ rather than the microscale concentration, $c_A$. To do this, we define a *concentration decomposition* that relates the average and microscale concentrations as follows

$$c_A(r,x) = \langle c_A \rangle\big|_x + \tilde{c}_A(r,x) \tag{33}$$

where the quantity $\tilde{c}_A$ is called the concentration deviation (from here on we will drop the explicit reference to the coordinates for all concentrations unless explicitly required). Using this in Eq. (32) gives

$$\frac{d\langle c_A \rangle}{dt} = -U \frac{\partial \langle c_A \rangle}{\partial x} + \mathscr{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \langle r^2 \rangle \frac{\partial \langle c_A \rangle}{\partial x} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle \tag{34}$$

Finally, note that the average of $r^2$ can be readily computed as follows

$$\langle r^2 \rangle = \frac{1}{\pi a^2} \int_{r=0}^{r=a} r^2 (2\pi r) dr$$

$$= \frac{2r^4}{4a^2} \Big|_{r=0}^{r=a} = \frac{a^2}{2} \tag{35}$$

Combining this result with Eq (34) gives the simple-looking expression

$$\frac{d\langle c_A \rangle}{dt} = \mathscr{D}_A \frac{\partial^2 \langle c_A \rangle}{\partial x^2} + \frac{2U}{a^2} \left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x} \right\rangle \tag{36}$$

Eq. (36) is starting to look like the spatially averaged equation that we are seeking. Recall that we put this analysis in a coordinate system that moves with the average velocity; for this reason no convection term arises here. Our remaining goal, then, is to determine how we can obtain an expression of the form

$$\frac{d\langle c_A \rangle}{dt} = D_{A,\mathrm{eff}} \frac{\partial^2 \langle c_A \rangle}{\partial x^2} \tag{37}$$

where $D_{A,\mathrm{eff}}$ defines the effective dispersion coefficient. To accomplish this, we must find a way of *closing* the problem so that terms involving only the average concentration, $\langle c_A \rangle$, appear.

## CLOSURE

To complete the analysis, we need to find some method of predicting the concentration deviation, $\tilde{c}_A$, in terms of the average concentration, $\langle c_A \rangle$. At first, this may seem like a tall order: it is not clear at this point that there is any reason to expect that we could express $\tilde{c}_A$ as some function involving $\langle c_A \rangle$. We will see, however, that this is a tractable task. To start, we need to develop a balance equation for the concentration deviations.

The decomposition given by Eq. (33) suggests a relationship between the concentrations of the form

$$\tilde{c}_A = c_A - \langle c_A \rangle \tag{38}$$

and this suggests that a balance equation for $\tilde{c}_A$ can be obtained by subtracting the balance equation for $\langle c_A \rangle$ from the balance equation for $c_A$. This is a straightforward operation,

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***To start, one can explain that Eq. (5) is the relationship between a point fixed in the fluid at the initial time (t = 0) and where that point would be located later if it were to flow with the fluid at the velocity U; it is, essentially, the equation that describes a streamline for the mean velocity field. Sometimes it is easier to think about this in the reverse.***

and the result is

$$\begin{array}{l}\dfrac{dc_A}{dt} = \mathscr{D}_A \dfrac{\partial^2 c_A}{\partial x^2} - U\left(1-\dfrac{2r^2}{a^2}\right)\dfrac{\partial c_A}{\partial x} + \mathscr{D}_A \dfrac{1}{r}\dfrac{\partial c_A}{\partial r} + \mathscr{D}_A \dfrac{\partial^2 c_A}{\partial r^2} \\ \qquad -\left[\dfrac{d\langle c_A\rangle}{dt} = \mathscr{D}_A \dfrac{\partial^2 \langle c_A\rangle}{\partial x^2} + \dfrac{2U}{a^2}\left\langle r^2 \dfrac{\partial \tilde{c}_A}{\partial x}\right\rangle\right] \\ \hline \dfrac{d\tilde{c}_A}{dt} = -\mathscr{D}_A \dfrac{\partial^2 \tilde{c}_A}{\partial x^2} - U\left(1-\dfrac{2r^2}{a^2}\right)\dfrac{\partial c_A}{\partial x} + \mathscr{D}_A \dfrac{1}{r}\dfrac{\partial c_A}{\partial r} + \mathscr{D}_A \dfrac{\partial^2 c_A}{\partial r^2} - \dfrac{2U}{a^2}\left\langle r^2 \dfrac{\partial \tilde{c}_A}{\partial x}\right\rangle \end{array} \tag{39}$$

For the closure problem, we want a balance equation that involves only deviations and averages. Using the decomposition given by Eq. (33) to eliminate the microscale concentration in Eq. (39) and the boundary condition given by Eq. (2), we find a complete description of the closure problem that predicts the deviation concentration $\tilde{c}_A$ is given by

$$\begin{array}{l}\dfrac{d\tilde{c}_A}{dt} = -U\left(1-\dfrac{2r^2}{a^2}\right)\dfrac{\partial \tilde{c}_A}{\partial x} - \mathscr{D}_A \dfrac{\partial^2 \tilde{c}_A}{\partial x^2} + \dfrac{\mathscr{D}_A}{r}\dfrac{\partial}{\partial r}\left(r\dfrac{\partial \tilde{c}_A}{\partial r}\right) \\ \qquad \underbrace{-\dfrac{2U}{a^2}\left\langle r^2 \dfrac{\partial \tilde{c}_A}{\partial x}\right\rangle}_{\text{Nonlocal term}} \underbrace{- U\left(1-\dfrac{2r^2}{a^2}\right)\dfrac{\partial \langle c_A\rangle}{\partial x}}_{\text{Source}} \end{array} \tag{40}$$

$$-\mathscr{D}_A \frac{\partial \tilde{c}_A}{\partial r} = 0, \quad \text{at } r = 0 \text{ and } r = a \tag{41}$$

$$\tilde{c}_A(r,x,t=0) = \mathscr{G}(r,x), \quad \text{initial condition} \tag{42}$$

Note that in the development of this equation we have used the fact that $\partial\langle c_A\rangle/\partial r=0$ (*i.e.*, the average concentration depends only upon x). In principle, this equation can be solved (using, for example, Fourier transform methods) provided that the initial condition is known. This would then provide us with an expression that describes the time evolution of the deviation concentration.

From a practical perspective, it is useful to consider examining the "long time" solution to Eqs. (40)-(42), where the effective dispersion coefficient is essentially a constant. To begin the analysis of this approximation, suppose that the source term has a characteristic time scale of $T^*$. This implies that the dominant time scale for $\partial \tilde{c}_A/\partial t$ is also of order $T^*$. We can make the following estimates

$$\frac{d\tilde{c}_A}{dt} = O\left(\frac{\Delta\tilde{c}_A}{T^*}\right) \tag{43}$$

$$\frac{\mathscr{D}_A}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \tilde{c}_A}{\partial r}\right) = O\left(\frac{\mathscr{D}_A \Delta\tilde{c}_A}{a^2}\right) \tag{44}$$

$$U\left(1-\frac{2r^2}{a^2}\right)\frac{\partial \tilde{c}_A}{\partial x} = O\left(U\frac{\Delta\tilde{c}_A}{L}\right) \tag{45}$$

***The key ideas of the Taylor-Aris analysis provide a structure for understanding upscaling in many other kinds of multiscale systems.***

$$\frac{2U}{a^2}\left\langle r^2 \frac{\partial \tilde{c}_A}{\partial x}\right\rangle = O\left(U\frac{\Delta\tilde{c}_A}{L}\right) \tag{46}$$

$$\mathscr{D}_A \frac{\partial^2 \tilde{c}_A}{\partial x^2} = O\left(\mathscr{D}_A \frac{\Delta\tilde{c}_A}{L^2}\right) \tag{47}$$

Note that the estimates in Eqs. (45) and (46) are identical.

We begin simplification by imposing the restriction

$$\frac{d\tilde{c}_A}{dt} << \frac{\mathscr{D}_A}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \tilde{c}_A}{\partial r}\right) \tag{48}$$

and using our estimates, this translates into a constraint of the form

$$\frac{a^2}{\mathscr{D}_A} << T^* \tag{49}$$

We can think of the term on the left-hand side of this expression as the relaxation time of $\tilde{c}_A$ due to diffusion, whereas the right-hand side indicates the timescale for changes in the source term. This restriction indicates that diffusion must relax any radial gradients relatively "quickly" compared with changes in $\langle c_A\rangle$. Generally, this kind of relationship is known as a *quasi-steady* condition, and it is used frequently in engineering analysis.

We can make two additional restrictions to simplify the problem. Early on, we indicated that we expected radial diffusion to be "fast" relative to longitudinal convection. In the closure problem, we can formalize this by the restriction

$$U\left(1-\frac{2r^2}{a^2}\right)\frac{\partial \tilde{c}_A}{\partial x} << \frac{\mathscr{D}_A}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \tilde{c}_A}{\partial r}\right) \tag{50}$$

and making order-of-magnitude estimates as we did above, this yields a Péclet number constraint

$$\frac{Ua}{\mathscr{D}_A}\frac{a}{L} << 1 \tag{51}$$

Note that this same constraint also allows us to drop the nonlocal term on the right-hand side of Eq. (40) since it is of the same order of magnitude as the convection term that we just dropped.

Finally, we expect radial diffusion to dominate over longitudinal diffusion

$$\mathscr{D}_A \frac{\partial^2 \tilde{c}_A}{\partial x^2} << \frac{\mathscr{D}_A}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \tilde{c}_A}{\partial r}\right) \tag{52}$$

Again using the estimates above, the associated constraint is

$$\frac{a}{L} << 1 \tag{53}$$

When these three constraints are met, we can describe the closure problem by

$$\frac{\mathscr{D}_A}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \tilde{c}_A}{\partial r}\right) = \underbrace{U\left(1-\frac{2r^2}{a^2}\right)\frac{\partial\langle c_A\rangle}{\partial x}}_{\text{source}} \tag{54}$$

$$-\mathscr{D}_A\frac{\partial \tilde{c}_A}{\partial r} = 0, \quad \text{at } r = 0 \text{ and } r = a \tag{55}$$

$$\langle \tilde{c}_A\rangle = 0 \tag{56}$$

In Eq. (56), we have replaced the initial condition present in the original problem with the constraint that the average of the deviations must be identically zero. This is necessary because when we adopt the quasi-steady form the initial condition no longer enters the problem. Without some additional constraint, however, there is no longer enough information to solve the problem. The constraint that the average of the deviations is zero is consistent with the original initial condition, and allows the constants of integration in the solution to be explicitly identified.

We have made substantial simplifications here, but the benefits to these simplifications are (1) they were done in a manner in which explicit constraints were developed that indicate their domain of validity, and (2) the resulting balance still captures the essential physics of the problem, but is now significantly simpler to solve than the original problem. The solution to this problem is straightforward, and two integrations give the result

$$\tilde{c}_A = \frac{Ua^2}{4\mathscr{D}_A}\frac{\partial\langle c_A\rangle}{\partial x}\left(\frac{r^2}{a^2}-\frac{1}{2}\frac{r^4}{a^4}\right)+K \tag{57}$$

To determine the constant of integration, K, we use the constraint imposed on the problem [Eq (56)]. Taking the average of both sides of Eq (57) and using Eq (56) we find

$$K = -\frac{1}{3}\frac{Ua^2}{4\mathscr{D}_A}\frac{\partial\langle c_A\rangle}{\partial x} \tag{58}$$

so that the final solution is

$$\tilde{c}_A = \frac{Ua^2}{4\mathscr{D}_A}\frac{\partial\langle c_A\rangle}{\partial x}\left(\frac{r^2}{a^2}-\frac{1}{2}\frac{r^4}{a^4}-\frac{1}{3}\right) \tag{59}$$

## The Macroscale Dispersion Coefficient

Recall that the unclosed macroscale transport equation that we developed took the form

$$\frac{d\langle c_A\rangle}{dt} = \mathscr{D}_A\frac{\partial^2\langle c_A\rangle}{\partial x^2}+\frac{2U}{a^2}\left\langle r^2\frac{\partial \tilde{c}_A}{\partial x}\right\rangle \tag{59A}$$

where the second term on the right-hand side represented the influence of mechanical dispersion due to the nonuniform flow field. Because we have determined the concentration deviation field by Eq. (59), we are in a position to close the macroscale equation. To do this, note that we will need the derivative of the concentration deviation field

$$\frac{\partial \tilde{c}_A}{\partial x} = \frac{Ua^2}{4\mathscr{D}_A}\left(\frac{r^2}{a^2}-\frac{1}{2}\frac{r^4}{a^4}-\frac{1}{3}\right)\frac{\partial^2\langle c_A\rangle}{\partial x^2} \tag{60}$$

Substituting this into the macroscale transport equation above and regrouping terms yields

$$\frac{d\langle c_A\rangle}{dt} = \left(\mathscr{D}_A+\frac{U^2}{\mathscr{D}_A}\left\langle r^2\left(\frac{r^2}{2a^2}-\frac{1}{4}\frac{r^4}{a^4}-\frac{1}{6}\right)\right\rangle\right)\frac{\partial^2\langle c_A\rangle}{\partial x^2} \tag{61}$$

Note that this now takes the form of a dispersion equation, where the term multiplying the derivative on the right-hand side is the dispersion coefficient. It is straightforward to work out the term in the angled brackets explicitly using the definition of the average given by Eq (29). This result is

$$\left\langle r^2\left(\frac{r^2}{2a^2}-\frac{1}{4}\frac{r^4}{a^4}-\frac{1}{6}\right)\right\rangle = \frac{a^2}{48} \tag{62}$$

Finally, substituting this result into Eq (61) yields the classical Taylor-Aris result

$$\frac{d\langle c_A\rangle}{dt} = D_{A,\text{eff}}\frac{\partial^2\langle c_A\rangle}{\partial x^2} \tag{63}$$

where

$$D_{A,\text{eff}} = \left(\mathscr{D}_A+\frac{U^2a^2}{48\,\mathscr{D}_A}\right) \tag{64}$$

As a final step, we can put this equation back into a fixed frame of reference rather than one that moves with the mean flow. Doing this essentially adds back the (mean) convection term that we initially removed, and the final transport equation takes the form of the convection-dispersion equation. Using Eq. (17) we can easily convert our final expression back to the fixed frame of reference, yielding a macroscale convection-dispersion equation of the form

$$\frac{\partial \langle c_A \rangle}{\partial t} = -U \frac{\partial \langle c_A \rangle}{\partial x} + D_{A,\text{eff}} \frac{\partial^2 \langle c_A \rangle}{\partial x^2} \qquad (65)$$

Note that the interpretation of this new equation, unlike the microscale equation that we started with, is that it describes the concentration averaged over the cross section of the tube. The microscale structure (geometry and flowfield) are represented in this equation, but only indirectly through the effective dispersion coefficient.

## PERSPECTIVE

The essential ideas of the micro-macro duality of multiscale systems can be communicated to undergraduate and graduate students alike through the example of Taylor-Aris dispersion. Because of the simple geometry involved, this problem has a macroscale transport equation that is intuitively appealing, and the effective dispersion coefficient can be predicted in a simple, closed form from an analysis of the microscale flow and transport processes. The key ideas of the Taylor-Aris analysis provide a structure for understanding upscaling in many other kinds of multiscale systems. These key ideas can be summarized as follows.

1. *Many systems have a complex, multiscale structure that would be infeasible or impossible to fully resolve at the smallest scale of interest (the* microscale*).*
2. *For such systems, a* macroscale *description of the phenomena of interest is sought that applies at a scale that is much larger than the microscale. Such a description seeks to represent the unresolved microscale processes in the system by a model. In this way, the net effect of the microscale processes are captured, even if they are not explicitly resolved.*
3. *Upscaling is a method of formally averaging the complete microscale description of a system in order to develop a valid macroscale representation. The goal in upscaling efforts is to make a connection between the microscale and the macroscale that allows one to predict the effective parameters that are developed for the macroscale transport equations. This is accomplished by breaking the problem into two separate systems of transport equations: (1) equations describing the transport of the average of the quantities of interest, and (2) equations describing the transport of the deviations from this average.*
4. *If we use the concept of numbers of degrees of freedom of a system, then upscaling is the process by which the number of degrees of freedom of the system is reduced by eliminating redundant information. For upscaling to be effective, there must be some identifiable structure or regularity of the deviation quantities in the system that leads to information that can be considered redundant.*

> A scaling law *is a statement about the structure of the deviations in the system that allows one to accomplish this reduction in degrees of freedom. A few examples of scaling laws include (1) smoothness conditions (such as in the case of Taylor dispersion), (2) periodic geometric structure (such as is done in many analyses of porous media systems), and (3) statistically homogenous structure (as is done in turbulence).*

Often, when upscaling concepts are presented to students who are unfamiliar with them, a "big picture" perspective is missing. If this can be first communicated, and then followed by a tractable example like the case of Taylor-Aris dispersion, the concepts underlying upscaling become significantly more tangible and much easier for students to understand.

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