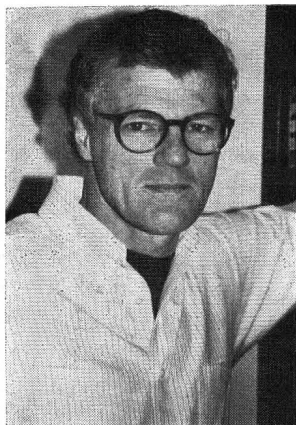


A SIMPLE GEOMETRICAL DERIVATION OF THE SPATIAL AVERAGING THEOREM

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THE CHEMICAL ENGINEERING approach to transport phenomena usually begins with the study of fluid mechanics, moves on to heat transfer, and completes the introductory sequence with a study of diffusion and mass transfer. This sequence is normally restricted to single phase transport phenomena, or situations in which the influence of the second phase is represented only in terms of a boundary condition. The beginning sequence is often treated with great care as the Navier-Stokes equations slowly evolve [17, Chap. 5], the thermal energy equation rises from the morass of Cartesian tensor analysis [10, Sec. 10-1], and the complexities of multicomponent transport phenomena [3, Sec. 18.3] complete the initial foray into the world of partial differential equations. What follows is



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crucial to chemical engineering: *multiphase transport phenomena*. However, the disparity between the precise analysis encountered in *single phase* transport phenomena and the qualitative treatment of *multiphase* transport phenomena often causes our students to question the efficacy of engineering science and encourages faculty members to adopt the position that it simply is not worth the trouble. Clearly, the transition from axioms and well-posed problems to applications and ill-posed problems deserves our attention.

The connection between single phase transport phenomena and multiphase transport phenomena is easily accomplished by means of the spatial averaging theorem. This approach was originally developed by Anderson and Jackson [1] who derived the equations of motion for a fluidized bed, by Slattery [15] who studied the problem of viscoelastic flow in porous media, and by the author [18] who used the method to derive a dispersion equation for mass transport in porous media and, more importantly, to outline a method of closure. The key mathematical theorem used in these three studies is known as the *spatial averaging theorem*, and it was presented independently by the above workers in 1967. In each study a different route to the averaging theorem was used, and since 1967 there have been numerous other treatments of this mathematical problem [2, 8, 11, 19]. The process is not yet terminated, for in recent papers Cushman [6, 7] has raised the issue of the need for time and space-dependent averaging volumes, and Veverka [16] has commented on possible limitations of the averaging theorem. Howes and

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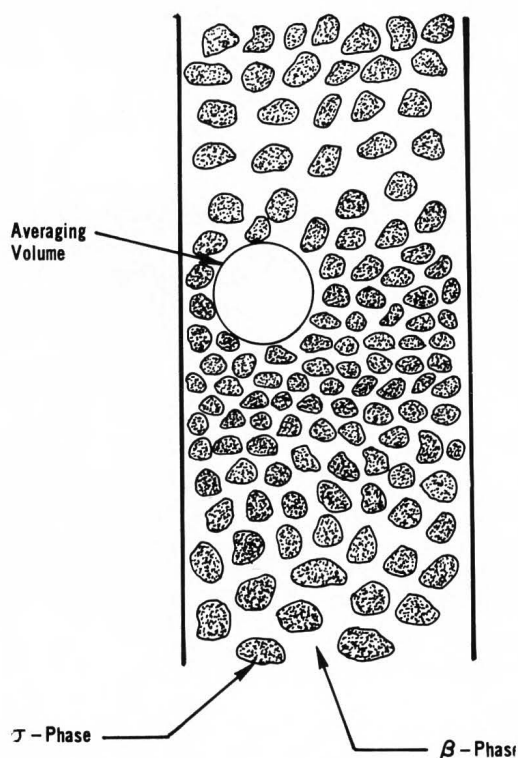


FIGURE 1. A two-phase system

Whitaker [13] have examined the questions raised by Veverka and find them to be unimportant for cases of practical interest. The objective of this paper is not to produce a new result, but merely to provide a route to the averaging theorem that can be used in our undergraduate classes.

PHYSICAL PROBLEM

In Fig. 1 a two-phase system is illustrated with the continuous phase identified as the β -phase and the discontinuous phase identified as the σ -phase. One could think of this system as a bubble column or as a fixed bed reactor. We direct our attention to the β -phase and note that the species continuity equation can be expressed as

$$\frac{\partial c_A}{\partial t} + \nabla \cdot \mathbf{N}_A = R_A \quad (1)$$

Here c_A represents the molar concentration of species A, the molar flux is given explicitly by

$$\mathbf{N}_A = c_A \mathbf{V}_A \quad (2)$$

and the molar rate of production per unit volume of species A owing to homogeneous chemical reaction is represented by R_A . It should be clear that we are thinking of the β -phase as a fluid and the

σ -phase can be either a non-porous solid, a porous solid, a liquid, or a gas. It will be sufficient for our purposes to consider only the mass transfer process in the β -phase.

Obviously we are unable to determine the details of the concentration field in the β -phase and some type of averaging procedure is in order. The method of volume averaging is based on the assumption that a *local* average concentration and a *local* average rate of reaction will suffice for design purposes. To this end, we associate with every point in space an averaging volume such as the sphere illustrated in Fig. 1. We designate the averaging volume by v and average values computed on the basis of this volume are assigned to the centroid of the volume. Since there is an averaging volume associated with every point in space, i.e. in both the β and the σ -phases, we can generate a field of average values of the concentration, temperature, etc.

In the method of volume averaging there are numerous types of averages. This is perhaps best illustrated in a recent paper dealing with diffusion and reaction in a micropore-macropore model of a porous medium [22, 23]. In that work one finds four different volume averages and eleven different concentrations for a single species. In general, there are two averages that one needs and the first of these is referred to as the *phase average* which is defined by

$$\langle c_A \rangle = \frac{1}{V} \int_{V_\beta(t)} c_A \, dV \quad (3)$$

Here $V_\beta(t)$ represents the volume of the β -phase contained within the averaging volume which can be expressed as

$$v = V_\beta(t) + V_\sigma(t) \quad (4)$$

Note that while the individual volumes, $V_\beta(t)$ and $V_\sigma(t)$, may be functions of time and space, the averaging volume is not.

When the point concentration of species A is constant, we see from Eq. 3 that the phase average

concentration is not equal to that constant value. Because of this, we usually prefer to work with the *intrinsic phase average* concentration which is defined by

$$\langle c_A \rangle^\beta = \frac{1}{V_\beta(t)} \int_{V_\beta(t)} c_A \, dV \quad (5)$$

These two average concentrations are related by

$$\langle c_A \rangle = \epsilon_\beta \langle c_A \rangle^\beta \quad (6)$$

in which ϵ_β is the volume fraction of the β -phase given by

$$\epsilon_\beta = V_\beta(t)/V \quad (7)$$

The averaging procedure is best initiated in terms of the phase average, and thus we integrate

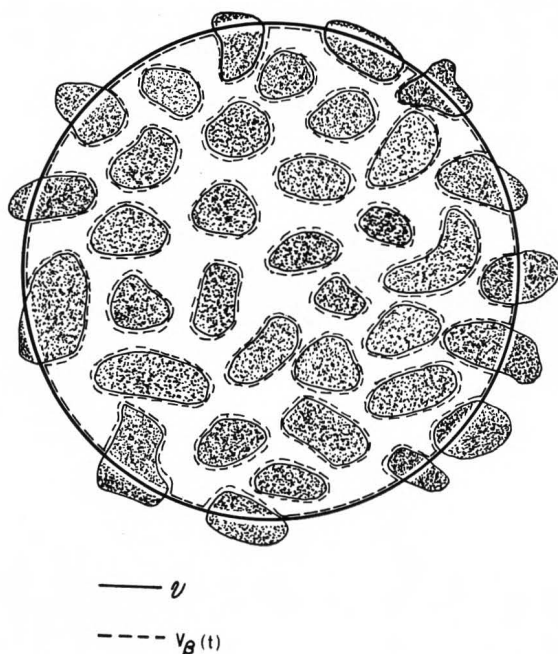


FIGURE 2. Averaging volume for a two-phase system

Eq. 1 over the volume $V_\beta(t)$ and divide by v to obtain

$$\frac{1}{V} \int_{V_\beta(t)} \frac{\partial c_A}{\partial t} \, dV + \frac{1}{V} \int_{V_\beta(t)} \nabla \cdot \mathbf{N}_A \, dV = \frac{1}{V} \int_{V_\beta(t)} R_A \, dV \quad (8)$$

Use of the traditional nomenclature illustrated by Eq. 3 leads to the form

$$\left\langle \frac{\partial c_A}{\partial t} \right\rangle + \langle \nabla \cdot \mathbf{N}_A \rangle = \langle R_A \rangle \quad (9)$$

Here it is clear that we must be able to interchange differentiation with respect to both time and space with time-dependent spatial integration if we are to obtain a governing differential equation for the average concentration. The general transport theorem [17, Sec. 3.4] will allow us to treat the first term in Eq. 9 in a precise manner, and what is needed here is a rule for interchanging spatial integration with spatial differentiation. Clearly we seek a three-dimensional form of the Leibnitz rule using the same simple approach currently available in the derivation of the general transport theorem.

MATHEMATICAL PROBLEM

In general we require an averaging volume to contain many "pores" or "particles" of both phases in order to obtain smooth and representative values [5, 19]. Such an averaging volume is illustrated in Fig. 2 in which we have clearly identified v and $V_\beta(t)$. The volume of the β -phase is bounded by two surfaces that we identify as

$A_{\beta\sigma}(t)$	interfacial area
$A_{\beta e}(t)$	area of entrances and exits

and for the purposes of our derivation it is sufficient to consider the simple system shown in Fig. 3. There we have illustrated two averaging volumes with the centroids separated by a distance Δs along a straight line, the orientation of which is designed by the unit vector λ .

The objective here is to derive the three-dimensional Leibnitz rule which can be expressed as

$$\frac{\partial}{\partial t} \int_{V_\beta(t)} c_A \, dV = \int_{V_\beta(t)} \nabla \cdot c_A \, dV - \int_{A_{\beta\sigma}(t)} n_{\beta\sigma} c_A \, dA \quad (10)$$

Rather than deal directly with the gradient, it is more convenient to begin with the directional derivative [17, Sec. 7.4] and use the definition of the derivative to write

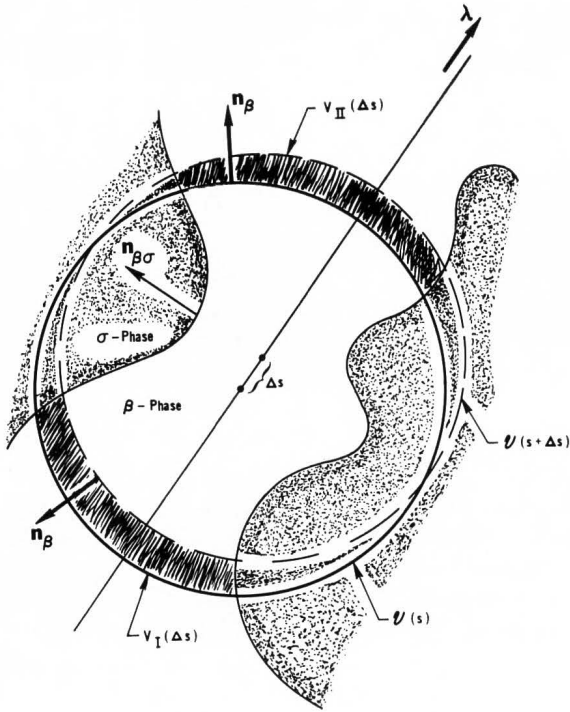


FIGURE 3. A uniform translation

of the general transport theorem [17, Sec. 3.4] in order to evaluate the integrals on the right hand side of Eq. 12. Each point on the surface of the averaging volume $v(s)$ is translated a distance Δs in the λ -direction in order to construct the volumes $V_I(\Delta s, t)$ and $V_{II}(\Delta s, t)$, and the details of the geometry are illustrated in Fig. 4. Our next step in this analysis requires that we represent the volume integrals over $V_I(\Delta s, t)$ and $V_{II}(\Delta s, t)$ in terms of the surface areas A_I and A_{II} . These two areas are identified by the unit outwardly directed normal vector \mathbf{n}_β shown in Fig. 3, and as $\Delta s \rightarrow 0$ these two areas will be coincident with the area of entrances and exits, $A_{\beta e}(t)$. When the averaging volume undergoes a displacement Δs , an element of the surface will generate a cylinder as illustrated in Fig. 4. The differential volume elements illustrated in Fig. 4 can be expressed as

$$dV_{II} = \Delta s \, dA_{CS} \quad (13)$$

where dA_{CS} represents the cross-sectional area of the cylinder under consideration. The *cross-sectional area* is related to the *surface area* element by

$$\begin{aligned} \lambda \cdot \nabla \int_{V_\beta(s,t)} c_A \, dV &= \frac{d}{ds} \int_{V_\beta(s,t)} c_A \, dV \\ &= \lim_{\Delta s \rightarrow 0} \left(\frac{\int_{V_\beta(s+\Delta s,t)} c_A \, dV - \int_{V_\beta(s,t)} c_A \, dV}{\Delta s} \right) \end{aligned} \quad (11)$$

$$dA_{CS} = \lambda \cdot \mathbf{n}_\beta \, dA_{II} \quad \text{over } A_{II} \quad (14a)$$

$$dA_{CS} = -\lambda \cdot \mathbf{n}_\beta \, dA_I \quad \text{over } A_I \quad (14b)$$

These relations allow us to express the volume
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Clearly the intersection of the two integrals will cancel in Eq. 11 so that we obtain

$$\frac{d}{ds} \int_{V_\beta(s,t)} c_A \, dV = \lim_{\Delta s \rightarrow 0} \left(\frac{\int_{V_{II}(\Delta s,t)} c_A \, dV - \int_{V_I(\Delta s,t)} c_A \, dV}{\Delta s} \right) \quad (12)$$

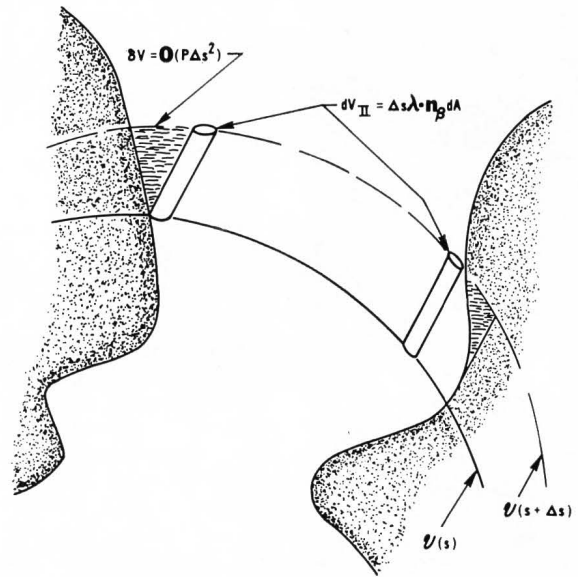


FIGURE 4

Since the two volumes, $V_I(\Delta s, t)$ and $V_{II}(\Delta s, t)$, tend to zero as $\Delta s \rightarrow 0$, we can use the simple geometrical arguments presented in the derivation

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to find others. The teacher acts as a resource and an adviser while retaining some assessing and monitoring roles. This strategy is generally used for design projects, and can be used to extend the more gifted students.

CONCLUSIONS

Successfully carrying out this major program of modernization will require

- A commitment by the departmental staff to the new concept
- The willingness of departmental staff to make short-term sacrifices
- The diversion of financial resources to fund the scheme.

Discussion within the department during 1983 has resulted in enthusiastic support from the staff and a commitment by the staff to the concept. As part of the plan each staff member will be relieved in turn of normal duties to be retrained in CAL and video techniques and to prepare new resources. The total financial resources required, including cost for staff retraining, is estimated to be in excess of half a million dollars.

While each element in the proposed mode of operation is not novel, the implementation of the integrated package on a departmental basis in chemical engineering is both new and challenging. This is the beginning. □

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integrals in Eq. 14 in terms of area integrals according to

$$dV_I = -\Delta s \lambda \cdot n_\beta dA_I \quad (15a)$$

$$dV_{II} = +\Delta s \lambda \cdot n_\beta dA_{II} \quad (15b)$$

There is a minor problem in the use of these relations at the contact point between the surface of the averaging volume and the β - σ interface. As indicated in Fig. 4 the error is on the order of $P\Delta s^2$ where P is the length of the contact line between the surface of the averaging volume and the β - σ interface. Use of Eq. 15 in Eq. 12 along with the estimate of the error

$$\delta V = Q(P\Delta s^2) \quad (16)$$

leads to

$$\frac{d}{ds} \int_{V_\beta(s,t)} c_A dV = \lim_{\Delta s \rightarrow 0} \left[\frac{\int_{A_{II}(s,t)} c_A \Delta s \lambda \cdot n_\beta dA_{II} + \int_{A_I(s,t)} c_A \Delta s \lambda \cdot n_\beta dA_I + Q(c_A P \Delta s^2)}{\Delta s} \right] \quad (17)$$

Since Δs and λ are independent of position, they can be removed from the integrals and in the limit as $\Delta s \rightarrow 0$ we obtain

$$\frac{d}{ds} \int_{V_\beta(s,t)} c_A dV = \lambda \cdot \int_{A_{\beta e}(s,t)} n_\beta c_A dA \quad (18)$$

Here we have used

$$A_{\beta e}(s,t) = \lim_{\Delta s \rightarrow 0} \left(A_I(s,t) + A_{II}(s,t) \right) \quad (19)$$

and expressing the derivative with respect to s in the form

$$\frac{d}{ds} = \lambda \cdot \nabla \quad (20)$$

quite obviously leads to

$$\nabla \int_{V_\beta(t)} c_A dV = \int_{A_{\beta e}(t)} n_\beta c_A dA \quad (21)$$

since λ is arbitrary. This is Eq. 7 of Slattery's derivation [15] and in terms of the nomenclature indicated in Eq. 3 we obtain

$$\nabla \cdot \langle c_A \rangle = \frac{1}{V} \int_{A_{\beta e}(t)} n_{\beta} c_A dA \quad (22)$$

while the vector form of this result is obviously given by

$$\nabla \cdot \langle N_A \rangle = \frac{1}{V} \int_{A_{\beta e}(t)} n_{\beta} \cdot N_A dA \quad (23)$$

The spatial averaging theorem can be obtained by use of the divergence theorem

$$\frac{1}{V} \int_{V_{\beta}(t)} \nabla c_A dV = \frac{1}{V} \int_{A_{\beta e}(t)} n_{\beta} c_A dA + \frac{1}{V} \int_{A_{\beta \sigma}(t)} n_{\beta \sigma} c_A dA \quad (24)$$

along with Eq. 22 to arrive at the result

$$\langle \nabla c_A \rangle = \nabla \cdot \langle c_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} n_{\beta \sigma} c_A dA \quad (25)$$

The analogous form for a vector is given by

$$\langle \nabla \cdot N_A \rangle = \nabla \cdot \langle N_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} n_{\beta \sigma} \cdot N_A dA \quad (26)$$

We are now in a position to continue our analysis of Eq. 9 using the general transport theorem and the spatial averaging theorem to interchange differentiation and integration.

CLOSURE

The general transport equation provides the relation

$$\frac{d}{dt} \int_{V_{\beta}(t)} c_A dV = \int_{V_{\beta}(t)} \frac{\partial c_A}{\partial t} dV + \int_{A_{\beta \sigma}(t)} c_A w \cdot n_{\beta \sigma} dA \quad (27)$$

in which we have used $w \cdot n_{\beta \sigma}$ to represent the normal component of the velocity of the β - σ interface, and we have made use of the fact that the normal component of velocity of the surface $A_{\beta e}(t)$ is zero. Use of this result allows us to express Eq. 9 in the form

$$\frac{d}{dt} \left(\frac{1}{V} \int_{V_{\beta}(t)} c_A dV \right) - \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A w \cdot n_{\beta \sigma} dA + \langle \nabla \cdot N_A \rangle = \langle R_A \rangle \quad (28)$$

and the spatial averaging theorem given by Eq. 26 can be used to obtain

$$\frac{\partial \langle c_A \rangle}{\partial t} + \nabla \cdot \langle c_A v_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A (v_A - w) \cdot n_{\beta \sigma} dA = \langle R_A \rangle \quad (29)$$

Since the phase average concentration is associated with a fixed point in space we have used the partial time derivative in writing Eq. 29, and we have used Eq. 2 to express N_A in terms of the concentration and the species velocity. From Eq. 23 we see that $\nabla \cdot \langle c_A v_A \rangle$ represents the flux at entrances and exits and under most circumstances [21, Sec. 7.4] diffusion is negligible compared to convection at entrances and exits and Eq. 29 can be written as

$$\frac{\partial \langle c_A \rangle}{\partial t} + \nabla \cdot \langle c_A v_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A (v_A - w) \cdot n_{\beta \sigma} dA = \langle R_A \rangle \quad (30)$$

Because the intrinsic phase average concentration is preferred, we can use the representation given by Eq. 6 to write

$$\begin{aligned} \frac{\partial}{\partial t} \left[\epsilon_{\beta} \langle c_A \rangle^{\beta} \right] + \nabla \cdot \left[\epsilon_{\beta} \langle c_A v_A \rangle^{\beta} \right] \\ + \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A (v_A - w) \cdot n_{\beta \sigma} dA = \epsilon_{\beta} \langle R_A \rangle^{\beta} \quad (31) \end{aligned}$$

At this point we follow the procedure used in the time averaging of turbulent transport processes and make use of Gray's [12] spatial decomposition to write

