

DISCONTINUITIES IN ChE EDUCATION

STEPHEN WHITAKER

University of California • Davis, CA 95616

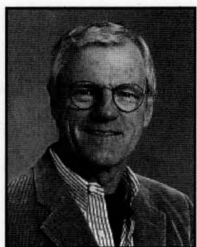
From the perspective of the first-year student, the entire four-year chemical engineering program represents an overwhelming array of courses and subject matter. One must learn about ionic strength and indefinite integrals, acoustics and hydrostatics, turbulence and chemical kinetics, organic chemistry and process dynamics, optics and quantum mechanics, stoichiometry and process synthesis, radiant energy heat transfer and partial differential equations, etc., etc. Viewed in its entirety, the typical chemical engineering program is enough to make a student change majors; but if taken *one step at a time*, the overall objective becomes quite feasible.

In the ideal chemical engineering program, one would like to develop a seamless passage from ionic strength to process synthesis. Given the size of the task, it should not be surprising that the route from A to Z contains a few "leaps of faith." The failed leap of faith within the confines of the university leads only to a lurking sense of insecurity and no real physical damage. Outside the university, however, a failed leap of faith may be a financial disaster, a physical disaster, or both. For this reason, we should avoid or minimize the leaps of faith in our educational programs or we should clearly identify them as such. A discussion of the so-called principle of lost work represents an interesting example of the latter.⁽¹⁾

THE MECHANICAL DISCONTINUITY

In the first physics course, students encounter Newton's second law for a particle written in the form

$$\frac{d}{dt}(mv) = F \quad (1)$$



Stephen Whitaker received his undergraduate degree in chemical engineering from the University of California, Berkeley, and his PhD from the University of Delaware. He is the author of two undergraduate texts, *Introduction to Fluid Mechanics* and *Fundamental Principles of Heat Transfer*, and a monograph, *The Method of Volume Averaging*. He has received a number of awards for his contributions to both undergraduate and graduate teaching.

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Here, m is the mass of the particle, \mathbf{v} is the velocity of the particle relative to an inertial frame, and \mathbf{F} is the force acting on the particle. Given the success of Eq. (1) in predicting the motion of the planets around the sun and in predicting the motion of projectiles in a physics lecture hall, students acquire a certain degree of confidence in Newton's second law. This confidence may begin to weaken when they move on to a chemical engineering study of fluid flow where they are often confronted with a dictum of the form

$$\begin{array}{ccccccc} \text{sum of forces} & & \text{rate of} & & \text{rate of} & & \text{rate of} \\ \text{acting on} & = & \text{momentum out} & - & \text{momentum into} & + & \text{accumulation of} \\ \text{the control} & & \text{of the control} & & \text{the control} & & \text{momentum in the} \\ \text{volume} & & \text{volume} & & \text{volume} & & \text{control volume} \end{array} \quad (2)$$

It is true that the concept of a *control volume* has already been presented in a course on material balances; but the distance between Eq. (1) and Eq. (2) is so great that most students view the latter with some distrust. The student's skepticism is quite justified, but the repeated use of Eq. (2) to solve real problems eventually leads to its acceptance. Such a leap of faith in the design of an oil pipeline passing underneath the city of Los Angeles would never be considered, but Eq. (2) is something that *everyone knows is true*, and many students move successfully through their programs of study with it securely locked in their tool boxes.

THE THERMODYNAMIC DISCONTINUITY

When students have made sufficient progress in their studies of fluid mechanics, they will often solve a variety of incompressible flow problems (it is important to keep in mind that there are no incompressible fluids, but there are *flows* that can be approximated as incompressible) using the Navier-Stokes equations and the continuity equation. These equations can be expressed as

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \rho \mathbf{g} + \mu \nabla^2 \mathbf{v} \quad (3)$$

$$\nabla \cdot \mathbf{v} = 0 \quad (4)$$

Equation (3) represents the governing differential equation

for the fluid velocity, \mathbf{v} , and Eq. (4) is the *constraining equation* for the vector field represented by ∇p . That is to say that the *momentum source*, ∇p , must be distributed in such a manner that the velocity determined by Eq. (3) will be solenoidal. If the pressure is specified at some point, one can use the vector field, ∇p , to calculate the pressure everywhere. The actual determination of the pressure field is discussed in some detail in Reference 2.

At the same time that students are using Eqs. (3) and (4) to determine the pressure in a course on fluid mechanics, they are also calculating the pressure in a course on thermodynamics using an equation of state. The simplest equation of state is the ideal gas law given by

$$p = \frac{n}{V} RT \quad (5)$$

This expression for the pressure would appear to have no connection with the pressure that one would determine from Eqs. (3) and (4), thus suggesting that there is a *mechanical pressure* used in the solution of certain fluid-flow problems and a *thermodynamic pressure* used in the solution of thermodynamics problems. It would be best to think of the pressure, as determined by an equation of state, as *the pressure*, and to think of the pressure determined by Eqs. (3) and (4) as a good approximation of *the pressure*. If it is not a good approximation, Eqs. (3) and (4) should not be used to solve the flow problem under consideration. The resolution of the conflict between Eqs. (3) and (4) and an equation of state, such as Eq. (5), relies on Birkhoff's plausible intuitive hypothesis that *small causes give rise to small effects*.

THE MULTIPHASE DISCONTINUITY

After having completed courses in fluid mechanics, thermodynamics, heat transfer, and mass transfer, chemical engineering students are often confronted with a course on mass transfer operations or unit operations. Since virtually all chemical engineering processes involve multiphase systems, a study of the gas-liquid contacting device illustrated in Figure 1 is a harbinger of things to come, and students approach this problem with a great deal of interest. Often they are equipped with Eqs. (3) and (4) from a course on fluid mechanics, the thermal energy equation from a course on heat transfer^[4]

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = k \nabla^2 T \quad (6)$$

and the species continuity equation from a course on mass transfer^[5]

$$\frac{\partial c_A}{\partial t} + \nabla \cdot (c_A \mathbf{v}_A) = R_A \quad A = 1, 2, \dots, N \quad (7)$$

Most students are somewhat dismayed when the process illustrated in Figure 1 takes on the form shown in Figure 2, and the rigor represented by Eq. (7) is replaced by the

suggestion that

$$\begin{array}{l} \text{mass of A entering} \\ \text{in the gas phase} \end{array} = \begin{array}{l} \text{mass of A leaving} \\ \text{in the gas phase} \end{array} + \begin{array}{l} \text{mass of A transferred} \\ \text{to the liquid phase} \end{array} \quad (8)$$

After the struggle to reach Eq. (7) via a series of challenging courses, it is disappointing to be asked to return to the concepts encountered in the course on material balances. What is worse is that the analysis of the process illustrated in Figure 1 will be heavily based on the intuition suggested by Figure 2 and most students will have no idea how reliable the final result will be. The resolution of this problem can be achieved using the method of volume averaging.^[6]

RESOLUTION OF THE MECHANICAL DISCONTINUITY

Rather than leap from Eq. (1) to Eq. (2), one can follow a sequence of steps that begins in the eighteenth century^[7] and leads to our current understanding of continuum mechanics. A central idea in continuum mechanics is that the laws of physics can be applied to any body that one imagines as being cut out of a distinct body. Truesdell^[7] attributes this idea to Euler and Cauchy and refers to it as the *cut principle*. Engineering students encounter this idea in a course on statics where it leads them to the concept of a free-body diagram. If we accept this idea, we can cut an arbitrary body from a moving, deforming fluid and state the axioms for mass and mechanics as follows:

Mass

$$\frac{d}{dt} \int_{V_m(t)} \rho dV = 0 \quad (9)$$

Linear Momentum: Euler's First Law

$$\frac{d}{dt} \int_{V_m(t)} \rho \mathbf{v} dV = \int_{V_m(t)} \rho \mathbf{b} dV + \int_{A_m(t)} \mathbf{t}_{(n)} dA \quad (10)$$

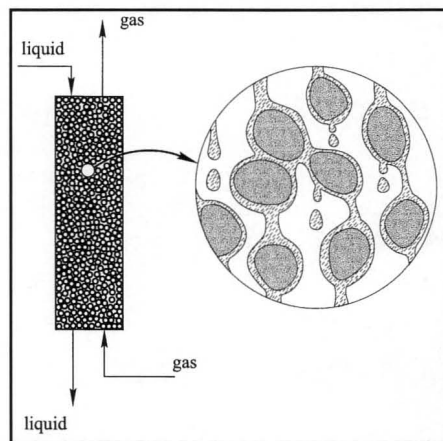


Figure 1. Gas-liquid contacting device.

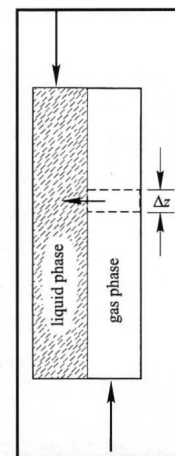


Figure 2. Model of a gas-liquid contacting device.

Angular Momentum: Euler's Second Law

$$\frac{d}{dt} \int_{\mathcal{V}_m(t)} \mathbf{r} \times \rho \mathbf{v} dV = \int_{\mathcal{V}_m(t)} \mathbf{r} \times \rho \mathbf{b} dV + \int_{\mathcal{A}_m(t)} \mathbf{r} \times \mathbf{t}_{(n)} dA \quad (11)$$

Here, $\mathcal{V}_m(t)$ represents the time-dependent region occupied by a body, ρ is the mass density, \mathbf{v} is the fluid velocity, \mathbf{b} is the body force per unit mass, $\mathbf{t}_{(n)}$ is the stress vector, and \mathbf{r} is the position vector. Both \mathbf{v} and \mathbf{r} are measured relative to some inertial frame. The representation of the angular momentum principle given by Eq. (11) assumes that all torques are the moments of forces and this ignores the existence of body torques and couple stresses that have been observed in polar fluids.^[8] The forms of these three axiomatic statements suggest the need for a study of the kinematics of volume integrals and this leads to the *general transport theorem*^[9] given by

$$\frac{d}{dt} \int_{\mathcal{V}_a(t)} \psi dV = \int_{\mathcal{V}_a(t)} \frac{\partial \psi}{\partial t} dV + \int_{\mathcal{A}_a(t)} \psi \mathbf{w} \cdot \mathbf{n} dV \quad (12)$$

Here, $\mathcal{V}_a(t)$ represents the region occupied by an arbitrary moving volume, $\mathcal{A}_a(t)$ is the bounding surface of this volume, and $\mathbf{w} \cdot \mathbf{n}$ is the speed of displacement of the bounding surface. When the arbitrary velocity, \mathbf{w} , is set equal to the fluid velocity, \mathbf{v} , we obtain the *Reynolds transport theorem* given by

$$\frac{d}{dt} \int_{\mathcal{V}_m(t)} \psi dV = \int_{\mathcal{V}_m(t)} \frac{\partial \psi}{\partial t} dV + \int_{\mathcal{A}_m(t)} \psi \mathbf{v} \cdot \mathbf{n} dV \quad (13)$$

When applied to Eq. (9), this theorem provides

$$\frac{d}{dt} \int_{\mathcal{V}_m(t)} \rho dV = \int_{\mathcal{V}_m(t)} \frac{\partial \rho}{\partial t} dV + \int_{\mathcal{A}_m(t)} \rho \mathbf{v} \cdot \mathbf{n} dV = 0 \quad (14)$$

and use of the divergence theorem leads us to

$$\int_{\mathcal{V}_m(t)} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] dV = 0 \quad (15)$$

Assuming that the integrand is continuous and noting that the limits of integration are arbitrary leads to the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (16)$$

In order to extract the governing differential equations associated with the linear and angular momentum principles, we first need to follow the work of Cauchy and prove^[7]

Cauchy's Lemma:

$$\mathbf{t}_{(n)} = -\mathbf{t}_{(-n)} \quad (17)$$

Cauchy's Fundamental Theorem:

$$\mathbf{t}_{(n)} = \mathbf{n} \cdot \mathbf{T} \quad (18)$$

The first of these is introduced as *intuitively obvious* in every statics course where it is applied to the shear stresses

acting on opposing surfaces of a beam that has been subjected to an Eulerian cut. The second result is generally avoided because of its complexity even though most students have completed a course on matrix algebra prior to their study of fluid mechanics.

The use of Eqs. (17) and (18), along with the Reynolds transport theorem, allows us to extract the following differential equations from Eqs. (10) and (11):

Cauchy's First Equation

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \rho \mathbf{g} + \nabla \cdot \mathbf{T} \quad (19)$$

Cauchy's Second Equation

$$\mathbf{T} = \mathbf{T}^T \quad (20)$$

At this point, we are in a position to derive the macroscopic momentum balance that was described in words by Eq. (2). We begin by integrating Eq. (19) over an arbitrary, moving control volume to obtain

$$\int_{\mathcal{V}_a(t)} \frac{\partial}{\partial t} (\rho \mathbf{v}) dV + \int_{\mathcal{V}_a(t)} \nabla \cdot (\rho \mathbf{v} \mathbf{v}) dV = \int_{\mathcal{V}_a(t)} \rho \mathbf{b} dV + \int_{\mathcal{A}_a(t)} \nabla \cdot \mathbf{T} dV \quad (21)$$

We now use the general transport theorem and the divergence theorem to arrange this result in a useful form given by

$$\frac{d}{dt} \int_{\mathcal{V}_a(t)} \rho \mathbf{v} dV + \int_{\mathcal{A}_a(t)} \rho \mathbf{v} (\mathbf{v} - \mathbf{w}) \cdot \mathbf{n} dA = \int_{\mathcal{V}_a(t)} \rho \mathbf{b} dV + \int_{\mathcal{A}_a(t)} \mathbf{t}_{(n)} dA \quad (22)$$

This represents a precise mathematical description of the words contained in Eq. (2), and it clearly indicates that the source of these words is Euler's first law. While the route from the axiom given by Eq. (10) to the proved theorem given by Eq. (22) consists of only a few steps, one must invest a significant amount of time in the study of kinematics and stress in order to derive this result. (At UC Davis we have two ten-week courses in fluid mechanics and time is less of a problem than in most programs.) While kinematics and stress may be confusing, we should heed the words of Pucciani and Hamel,^[10] who provide the following advice to students:

There is no learning without confusion. It is by the organization of this confusion that you will progress.

Said another way, it is better to be confused and frustrated by the concepts of kinematics and stress than to be baffled by the leap of faith from Eq. (1) to Eq. (2).

In order to follow the development from Eq. (10) to Eq. (22) in a successful manner, the faculty must be aware of what students know, what they don't know, and what they are supposed to know. For example, in the typical statics course, students make use of Euler's laws to solve problems, but the laws are never identified in a clear and concise manner. The concept of an Eulerian cut is presented as being *obvious* en route to the development of a free-body diagram,

but no mention is made of the fact that it was not obvious in the eighteenth century. Cauchy's lemma is used in the same way, *i.e.*, the shear is *up* on this side of the cut and *down* on that side of the cut. In order to unravel this mass of intuition, the faculty must be aware of the content of previous courses and must be prepared to extract some order and logic from the student's previous studies. In addition to statics, these previous studies include calculus where the definition of a derivative is presented and the projected area theorem is given.^[11] These are all that one needs to derive the general transport theorem. Previous studies also include a course on matrix algebra where the students learn that a three-by-three array can be used to transform one set of three numbers to another set of three numbers. This is the essential feature of Cauchy's fundamental theorem.

RESOLUTION OF THE THERMODYNAMIC DISCONTINUITY

In order to resolve the thermodynamic discontinuity, we begin with a reasonable description of a compressible flow process. This consists of the governing equations for the density, velocity, temperature, and pressure that can be expressed as

Governing equation for ρ

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (23)$$

Governing equation for \mathbf{v}

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \rho \mathbf{g} + \mu \nabla^2 \mathbf{v} \quad (24)$$

Governing equation for T

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = k \nabla^2 T \quad (25)$$

Governing equation for p

$$p = p(\rho, T) \quad (26)$$

The first of these equations represents a completely general form of the continuity equation, while the last represents a completely arbitrary equation of state. Equations (24) and (25) represent special forms of the equations of motions and the thermal energy equation, but they are general enough for our purposes.

The usual concept associated with an incompressible flow is that the variation of the density is *small enough* so that the dependent variable in Eq. (23) can be replaced with a constant, ρ_o . This means that one of our four dependent variables is determined by some means other than a law of physics and this, in turn, means that we must discard one of our laws of physics. Our new description of the physical process is given by

$$\nabla \cdot \mathbf{v}_m = 0 \quad (27)$$

$$\rho_o \left(\frac{\partial \mathbf{v}_m}{\partial t} + \mathbf{v}_m \cdot \nabla \mathbf{v}_m \right) = -\nabla p_m + \rho_o \mathbf{g} + \mu \nabla^2 \mathbf{v}_m \quad (28)$$

$$\rho_o c_p \left(\frac{\partial T_m}{\partial t} + \mathbf{v}_m \cdot \nabla T_m \right) = k \nabla^2 T_m \quad (29)$$

in which we have used \mathbf{v}_m , p_m , and T_m to represent the velocity, pressure, and temperature determined by Eqs. (27) through (29). These quantities differ from ρ , \mathbf{v} , p , and T that are determined by Eqs. (23) through (26), and we would like to understand the asymptotic conditions that lead to

$$\rho \rightarrow \rho_o \quad \mathbf{v} \rightarrow \mathbf{v}_m \quad p \rightarrow p_m \quad T \rightarrow T_m \quad (30)$$

When Eqs. (27) through (29) produce velocity, pressure, and temperature fields (\mathbf{v}_m , p_m , T_m) that are good approximations of the fields (\mathbf{v} , p , T) determined by Eqs. (23) through (26), we say that the flow can be approximated as incompressible. Under these circumstances, the pressure can be calculated by purely mechanical means; but it would seem best not to refer to p_m as a "mechanical pressure," but simply to say that p_m is a "good approximation" of the pressure determined by an equation of state.

The general asymptotic conditions associated with Eq. (30) are difficult to develop;^[12] we can, however, explore the first of these conditions for steady flow in the absence of any temperature effects without a great deal of effort. This requires that we consider an isothermal process described by the steady forms of Eqs. (23) through (26), and then search for conditions that lead to

$$\rho \rightarrow \rho_o \quad (31)$$

It will be in the nature of a plausible intuitive hypothesis^[3] to assume that $\mathbf{v} \rightarrow \mathbf{v}_m$ and $p \rightarrow p_m$ when the condition represented by Eq. (31) is satisfied.

For the case in which temperature effects are negligible, we can invert Eq. (26) to obtain

$$\rho = \rho(p) \quad (32)$$

and a Taylor series expansion about ρ_o leads to

$$\rho = \rho_o + (p - p_o) \left(\frac{\partial \rho}{\partial p} \right)_T + \frac{1}{2} (p - p_o)^2 \left(\frac{\partial^2 \rho}{\partial p^2} \right)_T + \dots \quad (33)$$

Here, ρ_o is the density determined by Eq. (32) at the reference pressure p_o . As an *estimate* of the density change that occurs for the process under consideration, we use the first term of the expansion to obtain

$$\rho - \rho_o = \mathbf{O} \left[\left(\frac{\partial \rho}{\partial p} \right)_T \Delta p \right] \quad (34)$$

in which Δp is representative of the maximum pressure change that occurs in the system. From a thermodynamic analysis, we know that the speed of sound is related to the derivative of the density with respect to the pressure at constant entropy. This relation is given by

$$\left(\frac{\partial p}{\partial p}\right)_s = \frac{1}{c^2} \quad (35)$$

in which c is the speed of sound. As an approximation, we use

$$\left(\frac{\partial p}{\partial p}\right)_T \sim \frac{1}{c^2} \quad (36)$$

so Eq. (34) takes the form

$$p - p_o = \mathbf{O}\left(\frac{\Delta p}{c^2}\right) \quad (37)$$

In order to obtain an estimate of the pressure change, we first make use of the steady form of Eq. (24) to estimate the gradient of the pressure as

$$\nabla p = \mathbf{O}(\rho g) + \mathbf{O}(\mu \nabla^2 \mathbf{v}) + \mathbf{O}(\rho \mathbf{v} \cdot \nabla \mathbf{v}) \quad (38)$$

The idea associated with this estimate is that ∇p may be as large as any of the other terms in Eq. (24) but not significantly larger. In addition, it is possible that ∇p may be much smaller than any of those terms, and thus Eq. (38) should be thought of as an overestimate of the pressure gradient. For example, in a laminar boundary layer created by a uniform flow past a flat plate, the pressure gradient is essentially hydrostatic

$$\begin{aligned} &\underline{\text{Laminar boundary layer flow}} \\ &\nabla p \sim \rho g \end{aligned} \quad (39)$$

while the viscous and inertial terms are essentially equal and much larger than $\nabla p - \rho g$, *i.e.*,

$$\begin{aligned} &\underline{\text{Laminar boundary layer flow}} \\ &\rho \mathbf{v} \cdot \nabla \mathbf{v} = \mathbf{O}(\mu \nabla^2 \mathbf{v}) \gg \nabla p - \rho g \end{aligned} \quad (40)$$

In this case, only the first estimate given by Eq. (38) is valid and it becomes clear that one must have some idea about the nature of the flow under consideration in order to use Eq. (38) successfully.

If u_o represents the characteristic velocity for the process, we can use order-of-magnitude analysis^[13] to obtain the estimates

$$\rho g = \mathbf{O}[(\rho g)\lambda_g] \quad (41a)$$

$$\mu \nabla^2 \mathbf{v} = \mathbf{O}\left[\left(\frac{\mu u_o}{L_\mu^2}\right)\lambda_\mu\right] \quad (41b)$$

$$\rho \mathbf{v} \cdot \nabla \mathbf{v} = \mathbf{O}\left[\left(\frac{\rho u_o^2}{L_\rho}\right)\lambda_\rho\right] \quad (41c)$$

Here, L_μ represents the viscous length, and L_ρ represents the inertial length,^[14] while $\lambda_g, \lambda_\mu, \lambda_\rho$ are unit vectors that are parallel to the gravitational term, the viscous term, and the inertial term, respectively. For the laminar boundary layer example discussed above, λ_μ and λ_ρ are parallel, and λ_g is an arbitrary unit vector.

In order to make use of Eq. (38) to estimate the pressure difference that appears in Eq. (37), we express the pressure gradient as

$$\nabla p = \mathbf{O}(\Delta p / L) \quad (42)$$

Here one must keep in mind that the pressure gradient will be influenced by all three terms represented by Eqs. (41), thus Eq. (42) represents *three separate estimates* and it is left to the reader to keep this fact in mind. Use of Eqs. (41) and (42) in Eq. (38) leads to the following estimate for the pressure change owing to gravitational, viscous, and inertial effects:

$$\Delta p = \mathbf{O}[(\rho g)L] + \mathbf{O}\left[\left(\frac{\mu u_o}{L_\mu^2}\right)L\right] + \mathbf{O}\left[\left(\frac{\rho u_o^2}{L_\rho}\right)L\right] \quad (43)$$

Substitution of this result into Eq. (37) provides the following estimate for the change in density that occurs for the process under consideration:

$$\frac{p - p_o}{\rho} = \mathbf{O}(gL / c^2) + \mathbf{O}\left(\frac{\mu u_o L}{\rho L_\mu^2 c^2}\right) + \mathbf{O}\left(\frac{u_o^2 L}{L_\rho c^2}\right) \quad (44)$$

If we define a Reynolds number and a Mach number as

$$\text{Re} = \frac{\rho u_o L_\mu}{\mu} \quad \text{M} = \frac{u_o}{c} \quad (45)$$

the estimates given by Eq. (44) take the form

$$\frac{p - p_o}{\rho} = \mathbf{O}(gL / c^2) + \mathbf{O}\left[\text{Re}^{-1} \text{M}^2 (L / L_\mu)\right] + \mathbf{O}\left[\text{M}^2 (L / L_\rho)\right] \quad (46)$$

From this result we conclude that

$$\frac{p - p_o}{\rho} \ll 1, \quad \text{or} \quad \rho \rightarrow p_o \quad (47)$$

when the following constraints are satisfied:

$$gL / c^2 \ll 1 \quad \text{M}^2 \ll \text{Re}(L_\mu / L) \quad \text{M}^2 \ll (L_\rho / L) \quad (48)$$

Here, one must remember that L has a different meaning in each one of these constraints, which are often replaced by the single condition that the Mach number squared is small compared to one. This has considerable appeal for the last constraint in Eq. (48) since L_ρ is often large compared to L ; the simplification given by $\text{M}^2 \ll 1$ has less appeal as a substitution for the second constraint, however, since L_μ is generally small compared to L . A little thought will indicate that the first constraint given by Eq. (48) is difficult to violate, and thus it is the constraints involving the Mach number that must be considered with care.

It seems plausible that when p_o is a reasonable approximation for p , we can assume that \mathbf{v}_m and p_m are reasonable approximations for \mathbf{v} and p ; but a rigorous proof would require that we identify the asymptotic conditions that allow us to simplify Eqs. (23) through (26) to the incompressible approximation represented by Eqs. (27) through (29). One should keep in mind that the analysis leading to the constraints given by Eqs. (48) was based on a steady-flow process, and that there are unsteady, low-Mach-number processes for which the flow cannot be treated as incompressible under any circumstances. An example is given in Figure 3, and for that type of process the approximation represented by

$$p - p_o = \mathbf{O}(\nabla p)L \quad (49)$$

is not at all applicable.

The *partial resolution* of the thermodynamic discontinuity required that we clearly identify the general case indicated by Eqs. (23) through (26) and that we discard a law of physics in favor of the approximation given by $\rho = \rho_0$. The

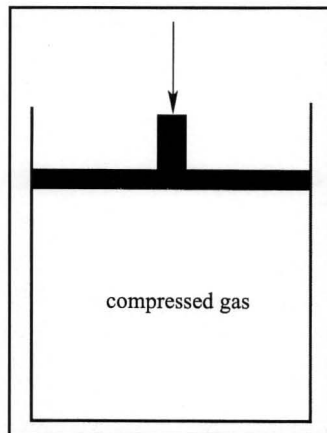


Figure 3. Compression process.

justification of this approximation was based on the equation of state that provided Eq. (37) and the order-of-magnitude analysis given by Eqs. (38) through (46). The use of order-of-magnitude analysis allows students to go beyond the assumptions based on the title of a course, the title of a text, or the title of a chapter in a text. Since these titles are not available to our students when they leave the university, we should encourage them to formulate their own assumptions

and then follow those assumptions with restrictions and constraints.^[13]

It is important to understand that the thermodynamic discontinuity cannot be resolved only by discussion in fluid mechanics courses. Faculty members who teach thermodynamics must be aware of the problem and speak to the issue. A righteous attitude about the correctness of Eq. (5), or a more general equation of state, provides no help to the student who must deal with the reality of incompressible flows. One must remember that the students take every course in the program and they do not have the luxury to choose their battleground.

RESOLUTION OF THE MULTIPHASE DISCONTINUITY

Studies of multicomponent mass transport usually include a derivation of the species continuity equation^[5], and the molar form of this result is given by

$$\frac{\partial c_A}{\partial t} + \nabla \cdot (c_A \mathbf{v}_A) = R_A \quad A = 1, 2, 3, \dots, N \quad (50)$$

Knowledge of the molar concentration, c_A , is a central issue in chemical engineering since it forms the basis for all separation and purification processes, for all reactor design calculations, and for all studies of contaminant transport in the land, air, and water. The macroscopic mole balance associated with Eq. (50) can be derived by following the steps that link Eq. (19) to Eq. (22), and the result is given by

$$\frac{d}{dt} \int_{V'_a(t)} c_A dV + \int_{A'_a(t)} c_A (\mathbf{v}_A - \mathbf{w}) \cdot \mathbf{n} dA = \int_{V'_a(t)} R_A dV \quad A = 1, 2, \dots, N \quad (51)$$

Both Eq. (50) and (51) represent powerful problem-solving tools, and most chemical engineering students acquire a certain degree of skill in the application of these results for a variety of single-phase transport problems; their application to multiphase systems, however, is problematic.

Most multiphase transport processes cannot be solved directly in terms of either Eq. (50) or Eq. (51), but require instead the local volume-averaged form of Eq. (50).^[15-18] The development of this form begins by associating an averaging volume with every point in the region under consideration. This allows one to define a volume-averaged concentration everywhere and to generate a spatially smoothed concentration field. In Figure 4 we have illustrated a two-phase system and a spherical averaging volume having the centroid located at the point identified by the position vector \mathbf{x} . For this system, we identify the point concentration of species A in the γ -phase as $c_{A\gamma}$ and we define the superficial average concentration by

$$\langle c_{A\gamma} \rangle |_{\mathbf{x}} = \frac{1}{V'_\gamma} \int_{V'_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \quad (52)$$

Here, $V'_\gamma(\mathbf{x}, t)$ represents the volume of the γ -phase contained within the averaging volume, V' , and we have clearly indicated that the

superficial average concentration is associated with the point located by the position vector \mathbf{x} . For the particular case illustrated in Figure 4, the position vector \mathbf{x} locates a point in the σ -phase where the point concentration of species A may be zero.

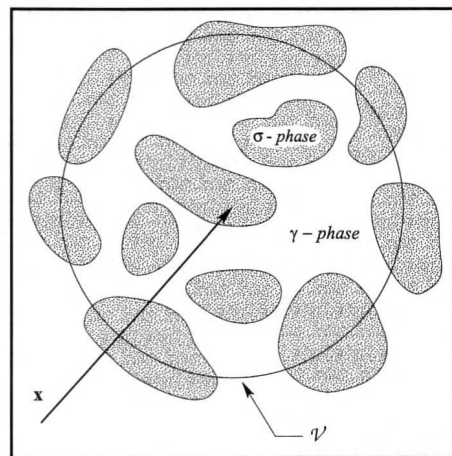


Figure 4. Two-phase system.

In general, the *intrinsic average concentration* is preferred for the analysis of multiphase transport processes, and this is defined by

$$\langle c_{A\gamma} \rangle^Y |_{\mathbf{x}} = \frac{1}{V'_\gamma(\mathbf{x}, t)} \int_{V'_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \quad (53)$$

The superficial and intrinsic average concentrations are related according to

$$\langle c_{A\gamma} \rangle = \epsilon_\gamma \langle c_{A\gamma} \rangle^Y \quad (54)$$

in which ϵ_γ is the volume fraction of the γ -phase defined explicitly by

$$\varepsilon_\gamma = V_\gamma(\mathbf{x}, t) / \mathcal{V} \quad (55)$$

In many systems, the superficial and intrinsic averages differ by a factor of three or more, and thus it is important to make use of a nomenclature that clearly identifies these two concentrations.

In Figure 5 we have shown a two-phase system for which we would like to develop the design equation for the concentration of species A. We think of the flowing fluid as the γ -phase, while the σ -phase could represent porous catalyst pellets, or droplets of a more dense fluid that is descending through the γ -phase. The governing differential equation for the concentration of species A in the γ -phase is given by

$$\frac{\partial c_{A\gamma}}{\partial t} + \nabla \cdot (c_{A\gamma} \mathbf{v}_{A\gamma}) = R_{A\gamma} \quad (56)$$

and we begin our analysis of this point equation by forming the superficial average to obtain

$$\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \frac{\partial c_{A\gamma}}{\partial t} dV + \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \nabla \cdot (c_{A\gamma} \mathbf{v}_{A\gamma}) dV = \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} R_{A\gamma} dV \quad (57)$$

In order to transform this result to something useful, we make use of two theorems that are essentially extensions of the classic one-dimensional Leibniz rule^[9, Prob. 3-5] for differentiating an integral. The first of these is the *general transport theorem*, which we used earlier in our treatment of the mechanical discontinuity. This theorem allows us to express the first term in Eq. (57) in the form

$$\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \frac{\partial c_{A\gamma}}{\partial t} dV = \frac{d}{dt} \left[\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \right] - \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} \mathbf{w} \cdot \mathbf{n}_{\gamma\sigma} dA \quad (58)$$

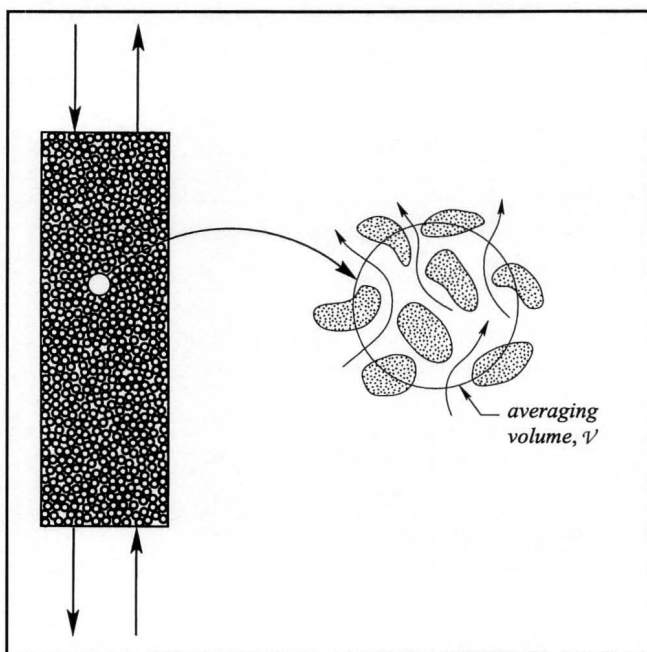


Figure 5. Mass transfer and reaction process in a two-phase system.

Here, $\mathbf{n}_{\gamma\sigma}$ represents the unit normal vector directed from the γ -phase toward the σ -phase, and $\mathbf{w} \cdot \mathbf{n}_{\gamma\sigma}$ represents the speed of displacement of the γ - σ interface. This is zero if the system under consideration is a packed-bed catalytic reactor, but would be non-zero for a fluidized-bed reactor or any fluid-fluid system. The second theorem needed for the analysis of Eq. (57) is the *spatial averaging theorem*, and the derivation of this theorem^[6,19] is analogous to the derivation of the general transport theorem. Application of the spatial averaging theorem provides

$$\begin{aligned} & \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \nabla \cdot (c_{A\gamma} \mathbf{v}_{A\gamma}) dV \\ &= \nabla \cdot \left[\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} dV \right] + \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} \cdot \mathbf{n}_{\gamma\sigma} dA \end{aligned} \quad (59)$$

and use of this result, along with Eq. (58), in Eq. (57) leads to

$$\begin{aligned} & \frac{d}{dt} \left[\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \right] + \nabla \cdot \left[\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} dV \right] \\ &+ \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} (\mathbf{v}_{A\gamma} - \mathbf{w}) \cdot \mathbf{n}_{\gamma\sigma} dA = \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} R_{A\gamma} dV \end{aligned} \quad (60)$$

One should note that this result is a superficial average transport equation, and thus each term has units of moles of species A per unit time per unit volume of the γ - σ system. Use of the nomenclature for the superficial average indicated by Eq. 52 allows us to express Eq. (60) in the more compact form given by

$$\underbrace{\frac{\partial}{\partial t} \langle c_{A\gamma} \rangle}_{\text{accumulation}} + \underbrace{\nabla \cdot \langle c_{A\gamma} \mathbf{v}_{A\gamma} \rangle}_{\text{transport}} + \underbrace{\frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} (\mathbf{v}_{A\gamma} - \mathbf{w}) \cdot \mathbf{n}_{\gamma\sigma} dA}_{\text{interfacial transport}} = \underbrace{\langle R_{A\gamma} \rangle}_{\text{homogeneous reaction}} \quad (61)$$

Here it is understood that the averaged quantities are associated with the centroid of the averaging volume identified by the position vector \mathbf{x} in Figure 4. In addition, we have expressed the accumulation in terms of the partial time derivative since $\langle c_{A\gamma} \rangle$ is associated with a point that is fixed in space.

The first and last terms in Eq. (61) can be expressed in terms of intrinsic averages by using the relation given by Eq. (54), and this leads to

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\varepsilon_\gamma \langle c_{A\gamma} \rangle^\gamma \right) + \nabla \cdot \langle c_{A\gamma} \mathbf{v}_{A\gamma} \rangle \\ &= - \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} (\mathbf{v}_{A\gamma} - \mathbf{w}) \cdot \mathbf{n}_{\gamma\sigma} dA + \varepsilon_\gamma \langle R_{A\gamma} \rangle^\gamma \end{aligned} \quad (62)$$

In order to simplify the convective transport term, one can use the averaging theorem and the divergence theorem to show that

$$\nabla \cdot \langle c_{A\gamma} \mathbf{v}_{A\gamma} \rangle = - \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} \cdot \mathbf{n}_{\gamma\sigma} dA \quad (63)$$

Discontinuities

Continued from page 25.

$\langle c_{A\gamma} \rangle^\gamma$	intrinsic volume averaged concentration of species A, mole/m ³
$\tilde{c}_{A\gamma}$	spatial deviation concentration, mole/m ³
c_p	constant pressure heat capacity, J/kgK
c	speed of sound, m/s
D	dispersion tensor, m ² /s
F	force acting on a particle, N
g	gravity vector, m/s ²
k	thermal conductivity, J/msK
L_μ	viscous length, m
L_p	inertial length, m
L	length associated with the pressure change, Δp , m
M	u_o/c , Mach number
m	mass of a particle, kg
n	number of moles
n	unit normal vector
$\mathbf{n}_{\gamma\sigma}$	unit normal vector directed from the γ – phase toward the σ – phase
p	pressure, N/m ²
p_m	pressure for an incompressible flow, N/m ²
r	position vector, m
R	gas constant, Nm/mole K
Re	$\rho u_o L_\mu / \mu$, Reynolds number
R_A	molar rate of production of species A owing to homogeneous reaction, mole/m ³ s
$R_{A\gamma}$	molar rate of production of species A in the γ – phase owing to homogeneous reaction, mole/m ³ s
T	temperature, K
T_m	temperature for an incompressible flow, K
t	time, s
$\mathbf{t}_{(n)}$	stress vector, N/m ²
T	stress tensor, N/m ²
u_o	characteristic velocity, m/s
v	mass average velocity vector, m/s
\mathbf{v}_m	velocity for an incompressible flow, m/s
\mathbf{v}_A	velocity of species A, m/s
$\mathbf{v}_{A\gamma}$	velocity of species A in the γ – phase, m/s
\mathbf{v}_γ	mass average velocity in the γ – phase, m/s
$\langle \mathbf{v}_\gamma \rangle$	superficial mass average velocity in the γ – phase, m/s
$\langle \mathbf{v}_\gamma \rangle^\gamma$	intrinsic mass average velocity in the γ – phase, m/s
$\tilde{\mathbf{v}}_\gamma$	spatial deviation velocity, m/s
V	volume, m ³
\mathcal{V}	averaging volume, m ³
$V_\gamma(\mathbf{x}, t)$	volume of the γ – phase contained in the averaging volume, m ³
w	arbitrary velocity, m/s
x	position vector locating the centroid of an averaging volume, m

Greek Letters

ε_γ	$V_\gamma(\mathbf{x}, t)/\mathcal{V}$, volume fraction of the γ – phase
λ	unit vector
μ	fluid viscosity, Ns/m ²
ρ	mass density, kg/m ³

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