# 1

# CONSERVATION LAWS AND CONTINUA

## 1.1. INTRODUCTION

The laws of conservation of mass and energy are the most important laws of environmental modeling. In this chapter, several different forms of the conservation of mass law are developed. By way of introduction, we can say that conservation of mass is a little like a no-interest bank account. When the amount of deposits made during a certain period equals the amount of withdrawals, the amount of money in the bank stays the same. Or in the terminology of this chapter, we might say the accumulation term is zero. However, if the amount of withdrawals made during the period exceeds the deposits, the money in the bank must decrease. Essentially the same principles apply to environmental systems that exchange mass (or energy) with the surrounding environment. In general, for a fixed system, the mass into the system (per unit time) will only equal the mass out of the system (per unit time) when there are no sources, losses, or accumulations of mass within the system. The conservation of mass idea usually boils down to an equation. If the equation can be solved, we may be able to make some important inferences about the state or the performance of the system. In fact, we will find that the laws of conservation of mass work themselves into almost every analysis covered in this book.

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*Transport Modeling for Environmental Engineers and Scientists,* by Mark M. Clark

## 1.2. CONSERVATION LAWS: SYSTEMS APPROACH

The law of *conservation of mass* (*or energy*) can be stated as follows: *Mass (or energy) can be neither created nor destroyed.* This law and several extensions of it can be used to solve numerous problems in environmental science and engineering. The conservation laws are often applied to *a system,* which here is a *representation of a process or a region of space*. An example of a system exchanging mass with its surroundings is shown in Figure 1.1.

In Figure 1.1, the $Q$ values are flows ($L^3/T$) going into or out of the system; the $C$ values are mass concentrations ($M/L^3$) of some component of interest; $V$ is the volume of the system, which can be variable; and $C_{\text{sys}}$ is the average concentration of the component of interest in the system. For a system with no reactions (i.e., *conservative* mass constituents), sources, or sinks, and no molecular diffusion across the boundaries (see Chapter 6), a differential equation based on the conservation of mass is

$$\frac{d}{dt}(VC_{\text{sys}}) = \sum_{i=1}^{N} Q_{\text{in},i}C_{\text{in},i} - \sum_{j=1}^{M} Q_{\text{out},j}C_{\text{out},j} \tag{1.1}$$

The subscripts "in" and "out" refer to inputs and outputs, respectively. The reader should verify that the units of this equation are mass per time ($M/T$). Equation 1.1 simply states that *the rate of change or accumulation of mass of some component within a system is equal to the difference between the rate of mass input and mass output.*

Note the number of unknowns in Eq. 1.1—$V$, $C_{\text{sys}}$, and the $Q$ and $C$ values. These unknowns may also vary in time. One common simplification is to assume a constant volume system. Equation 1.1 can then be expressed somewhat more compactly as

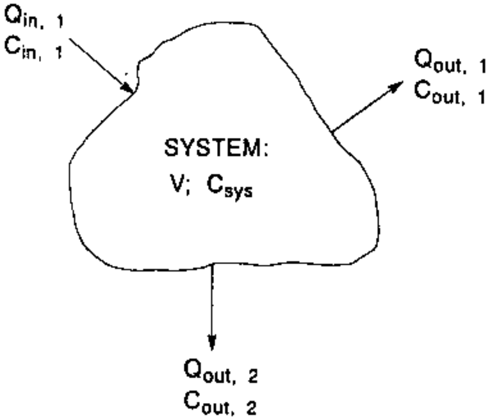


**Figure 1.1.** System with a single input, two outputs, and no reactions, sources, or sinks.

$$\frac{dC_{\text{sys}}}{dt}=\frac{1}{V}\sum_{i=1}^{N}Q_{\text{in},\,i}C_{\text{in},\,i}-\frac{1}{V}\sum_{j=1}^{M}Q_{\text{out},\,j}C_{\text{out},\,j} \tag{1.2}$$

For *steady-state* conditions, the time derivative in Eq. 1.1 is zero and all the $Q$ and $C$ values are constants. Hence, a new equation results:

$$\sum_{i=1}^{N}Q_{\text{in},i}C_{\text{in},i}=\sum_{j=1}^{M}Q_{\text{out},j}C_{\text{out},j} \tag{1.3}$$

Another important equation results if we let concentration in Eq. 1.1 actually refer to the mass concentration of fluid in the system, that is, the density, $\rho$. Then Eq. 1.1 becomes

$$V\frac{d\rho_{\text{sys}}}{dt}+\rho_{\text{sys}}\frac{dV}{dt}=\sum_{i=1}^{N}Q_{\text{in},i}\rho_{\text{in},i}-\sum_{j=1}^{M}Q_{\text{out},j}\rho_{\text{out},j} \tag{1.4}$$

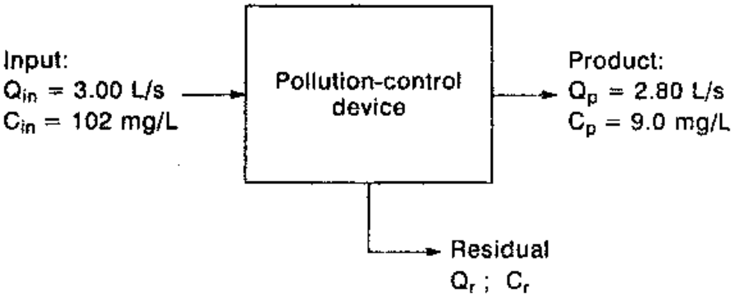
If the density is assumed to be constant (an *incompressible* fluid), Eq. 1.4 yields

$$\frac{dV}{dt}=\sum_{i=1}^{N}Q_{\text{in},i}-\sum_{j=1}^{N}Q_{\text{out},j} \tag{1.5}$$

Finally, for a constant-density *and* constant-volume system, Eq. 1.5 becomes the famous *continuity equation* of hydraulics:

$$\sum_{i=1}^{N}Q_{\text{in},i}=\sum_{j=1}^{M}Q_{\text{out},j} \tag{1.6}$$

***Example 1.1.*** A certain pollution-control device is processing a waste stream, which has a flow rate of 3.00 liters per second (L/s) and a contaminant concentration of 102 milligrams per liter (mg/L). We want to produce a treated product flow of 2.80 L/s with a contaminant concentration of 9.0 mg/L. Determine the flow and concentration of the residual stream.



**Example 1.1**

SOLUTION. Since there is no reason to believe this is not a steady-flow problem, Eq. 1.3 can be used:

$$Q_{\text{in}}C_{\text{in}} = Q_p C_p + Q_r C_r$$

There are two unknowns in the equation, $Q_r$ and $C_r$. However, if a constant-density and constant-volume system is assumed, Eq. 1.6 gives the flow of the residual stream:

$$Q_r = Q_{\text{in}} - Q_p = 3.00 - 2.80 = 0.20 \text{ L/s}$$

Therefore, from Eq. 1.3, the concentration of contaminant in the residual stream is

$$C_r = \frac{Q_{\text{in}}C_{\text{in}} - Q_p C_p}{Q_r} = \frac{3.00(102) - 2.80(9.0)}{0.20} = 1.4 \times 10^3 \text{ mg/L} \qquad \blacksquare$$

Note that a strength and weakness of the systems approach is that the system is essentially treated as a "black box." Although this approach is satisfactory for many problems, limitations become apparent when there are transformations of mass in the system and we need to forecast a system output knowing only the input. The approach in this section is then only useful if some rather heroic (but common) assumptions are made about the system. (For example, see the "box model" discussion of Section 1.6.)

## 1.3. CONSERVATION LAWS: CONTROL VOLUME APPROACH

For our purposes, a *control volume* is *a region of space corresponding to an actual physical space, in which we can describe the conditions of mass, momentum, and/or energy exchange across the surface of the control volume* (*i.e., the control surface*). Thus, we need to develop the ability to draw control volumes. Figure 1.2 shows several examples; note that control volumes are often drawn immediately inside an actual physical boundary, as in Figures 1.2*b* and 1.2*c*. We can imagine that the control volume is an infinitesimally thin boundary between the physical boundary and any internal fluid. It is also occasionally advantageous to draw control volumes outside physical boundaries.

We will develop the integral form of the equation of conservation of mass with reference to the control volume shown in Figure 1.3. Note that vector notation is used in the derivation. (A review of relevant aspects of vector algebra is provided in Appendix II.) The vector **u** is the local velocity at the infinitesimal area *dA*. The vector **n** is called the *outward unit normal vector,* which is normal (perpendicular) to the surface *dA*, points away from the

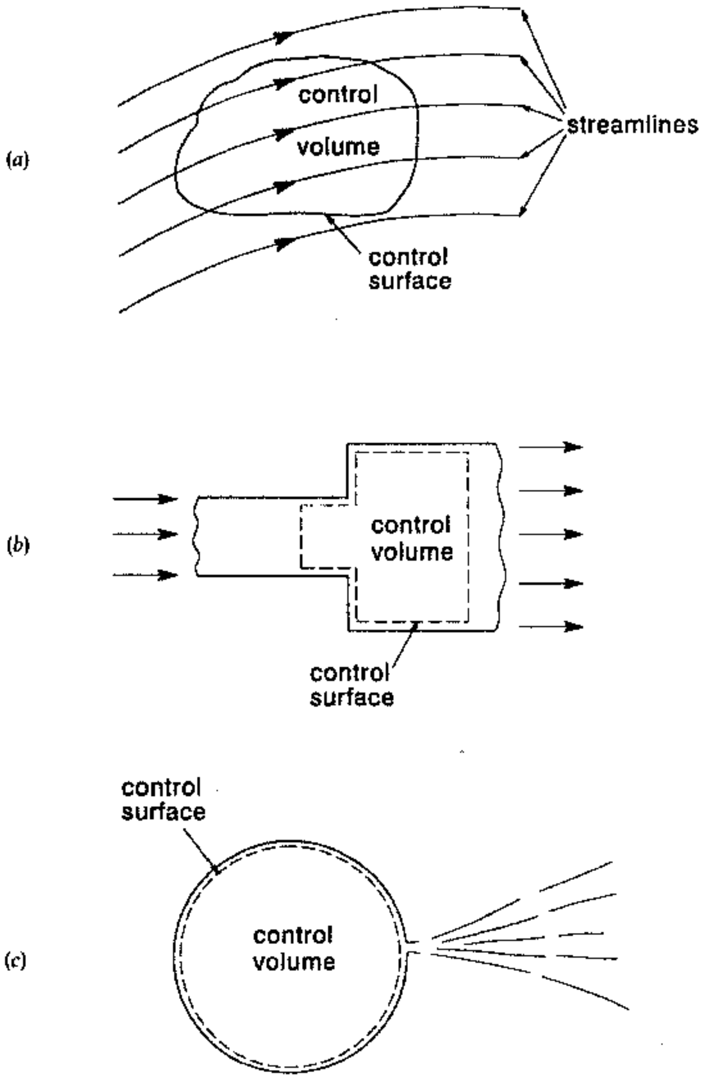


**Figure 1.2.** Examples of control volumes: (*a*) general control volume in a flowing fluid, (*b*) control volume drawn inside a pipe expansion, and (*c*) control volume for a balloon or ruptured cell.

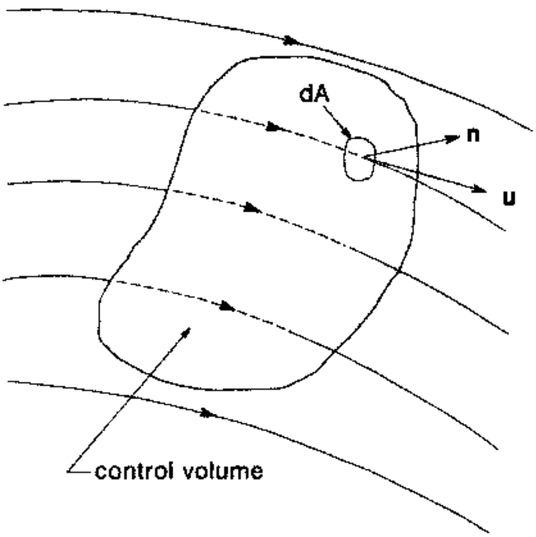


**Figure 1.3.** General control volume for derivation of integral relation for conservation of mass.

control volume, and has a magnitude of unity. Using this notation, we can derive the three terms of the equation of conservation of mass:

$$\begin{bmatrix} \text{I: rate of} \\ \text{mass inflow} \end{bmatrix} - \begin{bmatrix} \text{II: rate of} \\ \text{mass outflow} \end{bmatrix} = \begin{bmatrix} \text{III: rate of} \\ \text{accumulation of mass} \end{bmatrix} \tag{1.7}$$

Note in Figure 1.3 that the local velocity component normal (perpendicular) to the surface element $dA$ is the simple dot product, $\mathbf{n} \cdot \mathbf{u}$ $(L/T)$. The scalar *mass flux* across $dA$ is simply $\rho(\mathbf{n} \cdot \mathbf{u})$ $(M\text{-}L^{-2}\text{-}T^{-1})$. Then the rate of mass flowing out through $dA$ is

$$\begin{bmatrix} \text{rate of mass} \\ \text{outflow at } dA \end{bmatrix} = \rho(\mathbf{n}\cdot\mathbf{u})\,dA \quad (M/T) \tag{1.8}$$

We might now move the differential element around and sum all contributions to term II in Eq. 1.7; however, we find that a surface integral in Eq. 1.7 does the trick more elegantly than summations. In fact, the surface integral accounts for terms I and II in Eq. 1.7, since the dot product accounts for the sign changes in mass transport at different points on the control surface:

$$\begin{bmatrix} \text{rate of} \\ \text{mass inflow} \end{bmatrix} - \begin{bmatrix} \text{rate of} \\ \text{mass outflow} \end{bmatrix} = -\iint_{\text{control surface}} \rho(\mathbf{n}\cdot\mathbf{u})\,dA \tag{1.9}$$

The negative sign in Eq. 1.9 is added to ensure that if mass outflows are larger than mass inflows, the integral of all inflows and outflows will indeed be negative.

The rate of accumulation of mass in the control volume is equally elegant in vector notation:

$$\begin{bmatrix}\text{rate of accumulation}\\ \text{of mass}\end{bmatrix} = \frac{\partial}{\partial t}\iiint_{\text{control volume}} \rho\, dV \tag{1.10}$$

Equations 1.7, 1.9, and 1.10 can now be combined to yield the *integral form of the equation of conservation of mass*:

$$\iint_{\text{control surface}} \rho \mathbf{n}\cdot\mathbf{u}\, dA + \frac{\partial}{\partial t}\iiint_{\text{control volume}} \rho\, dV = 0 \tag{1.11}$$

It is worth noting several things about Eq. 1.11:

1. The parentheses around **n** · **u** have been dropped in the final form. Since $\rho$ and $dA$ are scalars, the form shown in Eq. 1.11 is strictly unambiguous. (The parentheses were used earlier for better visualization.)
2. The scalar density has been retained inside the double and triple integral terms, allowing for the possibility of a spatial variation in $\rho$.
3. A partial derivative with respect to time is used in the second term on the left-hand side of Eq. 1.11. This is because density can be a function of space and time.

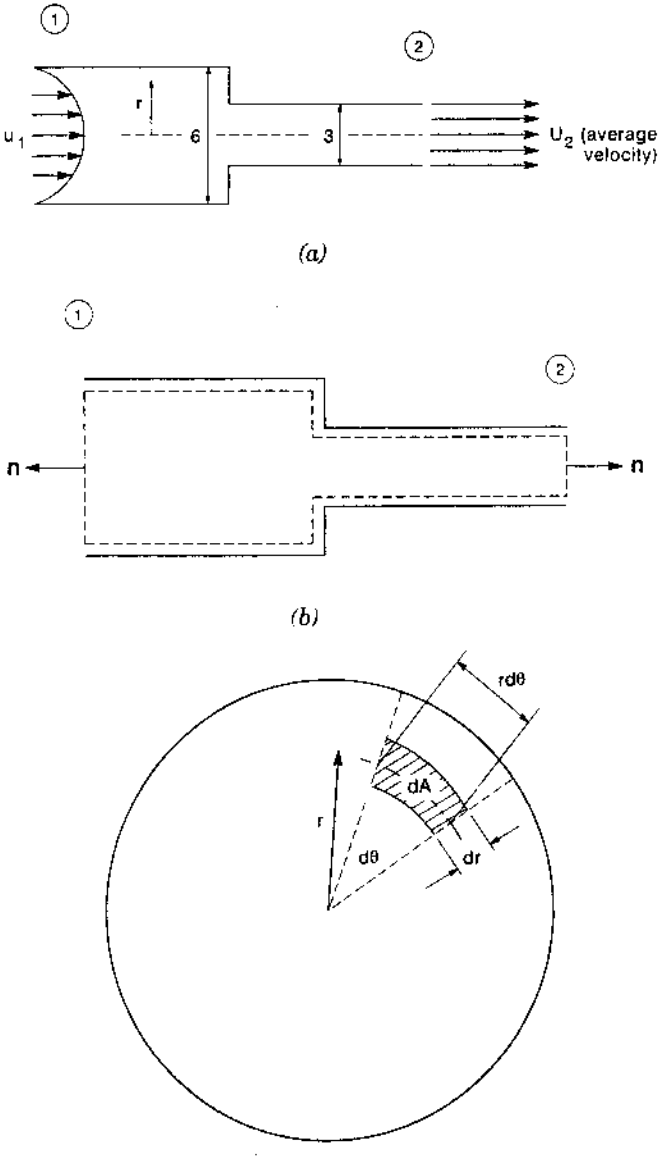
Some useful simplifications of Eq. 1.11 are noted. For *steady flows*, all time derivatives are zero; hence, Eq. 1.11 yields

$$\iint_{\text{control surface}} \rho \mathbf{n}\cdot\mathbf{u}\, dA = 0 \tag{1.12}$$

For steady flows and *incompressible fluids* (i.e., $\rho$ = constant), Eq. 1.12 simplifies to

$$\iint_{\text{control surface}} \mathbf{n}\cdot\mathbf{u}\, dA = 0 \tag{1.13}$$

***Example 1.2.*** The velocity at the inlet to the pipe constriction below has a parabolic distribution, given by $u_1 = 3(1 - r^2/9)$. Find the average velocity $U_2$ at the pipe outlet.



**Example 1.2**

SOLUTION. The first step is to draw a control volume, as shown in Example 1.2*b*. Note that with this selection of the control volume, there is mass flux into and out of the control volume at sections 1 and 2 only. Note also that at section 1, the outward unit normal vector is in a sense opposite to velocity, whereas at section 2, the outward unit normal and velocity vectors are collinear. This will cause these two contributions to the mass flux to have opposite signs. Since we have not stated otherwise, assume that this is a steady flow and an incompressible fluid; then, from Eq. 1.13,

$$\iint_{\text{control surface}} \mathbf{n}\cdot\mathbf{u}\, dA = \iint_{\text{section 1}} \mathbf{n}\cdot\mathbf{u}\, dA + \iint_{\text{section 2}} \mathbf{n}\cdot\mathbf{u}\, dA = 0$$

Realizing that the velocities must be integrated over circular end sections, we find

$$-\iint_{\text{section 1}} \mathbf{n}\cdot\mathbf{u}\, dA = \iint_{\text{section 2}} \mathbf{n}\cdot\mathbf{u}\, dA$$

The drawing in Example 1.2*c* may be of use in setting up the integral at section 1. Therefore, $dA$ is equal to $r\, d\theta\, dr$; hence,

$$\int_0^{2\pi}\int_0^3 3\left(1-\frac{r^2}{9}\right) r\, dr\, d\theta = U_2\pi(3/2)^2$$

or

$$U_2 = 6$$ ■

The idea of *mass flux* introduced in this section is one of the most powerful tools of environmental modeling, because we are so often interested in *mass transport* into or out of certain regions. Although the equations thus far concern the mass transport of the fluid medium itself, they can also describe the mass transport of any conservative mass constituent dissolved or transported with the fluid, as long as this mass constituent can be characterized by a well-defined concentration.* In other words, the approach in this section can be used to consider the conservation of mass of almost any constituent (e.g., contaminants, nutrients, or particles, in either liquid or gaseous phases). Referring to Figure 1.3 and thinking about the mass transport of some component with concentration $C$, we can write an equation analogous to Eq. 1.11:

$$\iint_{\text{control suface}} C\mathbf{n}\cdot\mathbf{u}\, dA + \frac{\partial}{\partial t}\iiint_{\text{control volume}} C\, dV = 0 \tag{1.14}$$

Note that the only difference between Eqs. 1.11 and 1.14 is that $\rho$ has been replaced by $C$, which represents the concentration of some mass component of interest. The equation says that any nonzero net mass transport across the control surface (i.e., a positive or negative value of the surface integral) results

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*As in Section 1.2, we do not allow molecular diffusion across any control surface. This is taken up in Chapter 6.

in a positive or negative accumulation of mass in the system. This is an extremely powerful tool, since it allows us, to a certain degree, to discover what is going on within a system knowing only mass transfer at the boundaries of the system or control volume (the control surface). Extension of Eq. 1.14 to sedimenting particles in still fluids is examined in Exercise 1.18 and very extensively in Chapter 2.

Calculation of the mass transport of $C$ across the control surface is accomplished with the first term on the left-hand side of Eq. 1.14. The local scalar mass flux at a point on a surface or control volume is given by the term within the surface integral:

$$C\mathbf{n}\cdot\mathbf{u} \tag{1.15}$$

From this expression, the units of mass flux are $M\text{-}L^{-2}\text{-}T^{-1}$. In other words, flux is like the amount of mass crossing a unit surface (per surface) per unit time. Integrating over the control surface eliminates the units of surface ($L^2$), resulting in *mass transport*, which in this book always has the units $M/T$ or mol/$T$. Note also from Eq. 1.15 that mass flux only involves the component of velocity *normal* (perpendicular) to the surface (i.e., the dot product of **n** and **u**). This of course makes sense since the component of velocity *parallel* to the surface cannot transport mass across the surface. So the dot product adds mathematical elegance to a simple but important idea. Mass fluxes are discussed extensively in this book.

Finally, note that the product $C\mathbf{u}$ has the same units as flux ($M\text{-}L^{-2}\text{-}T^{-1}$). This term is also a flux, but it is the *vector flux*, since the product of a scalar (concentration) and velocity (vector) is also a vector.

## 1.4. CONSERVATION LAWS: DIFFERENTIAL ELEMENT APPROACH

Our final method for deriving the conservation of mass equation requires that we imagine a differential element fixed in the flow region of interest. This is the so-called Eulerian coordinate system. Figure 1.4 shows a small-volume element with sides $\Delta x$, $\Delta y$, and $\Delta z$. As in Section 1.3, we will evaluate the terms in Eq. 1.7, but in this case, three components of terms I and II must be evaluated separately. For example, considering the $x$ direction in Figure 1.4, the mass transport through the left face of the volume element is simply $\rho u_x\ \Delta y\ \Delta z$. But how do we express the mass leaving the right face of the element? From elementary calculus, the *Taylor theorem* allows us to approximate the value of a function at one point in terms of its known value at a nearby point. The Taylor theorem states that the value of $f(x)$ at $b$ can be estimated from its values at $a$, provided $\Delta x$ is sufficiently small (Figure 1.5):

$$f(b) \cong f(a) + \frac{df(a)}{dx}(b-a) + \frac{1}{2!}\frac{d^2 f(a)}{dx^2}(b-a)^2 + \cdots \tag{1.16}$$

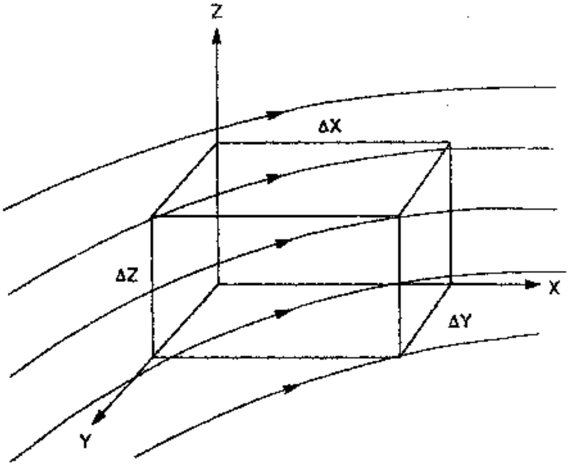


**Figure 1.4.** Volume element for derivation of the differential relation for conservation of mass.

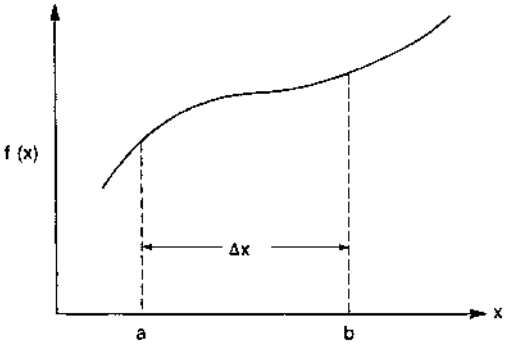


**Figure 1.5.** Function used to demonstrate a Taylor series.

Equation 1.16 can be called a *Taylor series* expansion or approximation. Using this idea, we can express the rate of mass transport out of the right-hand side of the control element as

$$\left(\rho+\frac{\partial\rho}{\partial x}\Delta x+\frac{1}{2!}\frac{\partial^2\rho}{\partial x^2}\Delta x^2+\cdots\right)\left(u_x+\frac{\partial u_x}{\partial x}\Delta x+\frac{1}{2!}\frac{\partial^2 u_x}{\partial x^2}\Delta x^2+\cdots\right)\Delta y\,\Delta z \tag{1.17}$$

Next, we observe that as $\Delta x$ becomes sufficiently close to zero, the terms of higher order in $\Delta x$ approach zero much "faster" than lower-order terms. In other words, as we let $\Delta x$ approach zero, we can cancel all the higher-order terms. This is a classic maneuver in applied math and engineering, which makes sense after studying Figure 1.5. As $\Delta x$ becomes smaller, $a$ and $b$ become closer; therefore, fewer terms should be required to estimate $f(b)$ based on

$f(a)$. Retaining only the two lowest-order terms in Eq. 1.17, the difference in mass transport between left and right faces is

$$\left[\rho u_x - \left(\rho + \frac{\partial \rho}{\partial x}\Delta x\right)\left(u_x + \frac{\partial u_x}{\partial x}\Delta x\right)\right]\Delta y\, \Delta z \tag{1.18}$$

Expanding the term in square brackets we find

$$\left(\rho u_x - \rho u_x - \rho \frac{\partial u_x}{\partial x}\Delta x - u_x \frac{\partial \rho}{\partial x}\Delta x - \frac{\partial \rho}{\partial x}\frac{\partial u_x}{\partial x}\Delta x^2\right)\Delta y\, \Delta z \tag{1.19}$$

The first terms cancel each other, while we argue that as $\Delta x$ approaches zero, the last term approaches zero faster than the previous lower-order terms; hence, Eq. 1.19 reduces to

$$-\left(\rho \frac{\partial u_x}{\partial x} + u_x \frac{\partial \rho}{\partial x}\right)\Delta x\, \Delta y\, \Delta z \tag{1.20}$$

The rate of mass accumulation in the volume element is simply

$$\frac{\partial \rho}{\partial t}\Delta x\, \Delta y\, \Delta z \tag{1.21}$$

Finally, we can write expressions similar to Eq. 1.20 for the $y$ and $z$ components of mass transport across the various faces of the volume element. These expressions and Eq. 1.21 can be substituted into Eq. 1.7, and after simplifying, the *differential form of the equation of conservation of mass* is found to be

$$\frac{\partial \rho}{\partial t} + \rho\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}\right) + u_x \frac{\partial \rho}{\partial x} + u_y \frac{\partial \rho}{\partial y} + u_z \frac{\partial \rho}{\partial z} = 0 \tag{1.22}$$

Referring to Appendix II, we recognize that some of the terms in Eq. 1.22 can be expressed in more compact vector notation:

$$\frac{\partial \rho}{\partial t} + \rho\, \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \rho = 0 \tag{1.23}$$

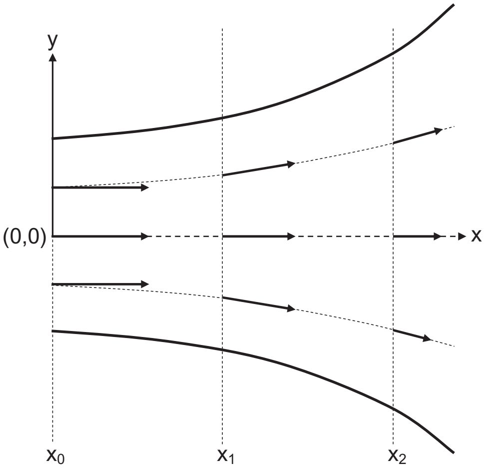
An interesting conclusion is made from Eq. 1.23 if we assume that density is constant (i.e., $\rho$ = constant—an incompressible fluid). Then the first and third terms on the left-hand side are zero and

$$\nabla \cdot \mathbf{u} = 0 \tag{1.24}$$

Equation 1.24 is another form of the *continuity equation* of fluid mechanics (cf. Eq. 1.6).

***Example 1.3.*** Is the differential continuity equation (Eq. 1.24) consistent with the (incompressible) flow observed in the two-dimensional duct expansion shown below? That is, does

$$\partial u_x/\partial x + \partial u_y/\partial y = 0?$$



**Example 1.3**

SOLUTION. Focus on the centerline of the flow, that is, $y = 0$. Moving from upstream to downstream, that is, $x = x_0$ to $x = x_1$ to $x = x_2$, we note that $\mathbf{u} = u_x$ is decreasing; hence, *$du_x/dx$ is negative* at any $x$-value along $y = 0$. Now consider moving vertically along $x = x_1$ from $y = 0$. There is no $y$-component velocity right at $y = 0$; that is, $u_y = 0$ at $y = 0$. However, moving upward from $y = 0$, $u_y$ must increase, in order for the velocity vectors to start pointing more and more upward as the upper wall of the duct is reached. Therefore, $du_y/dy$ must be *positive*. Now, from Eq. 1.24,

$$\frac{\partial u_y}{\partial y} = -\frac{\partial u_x}{\partial x}$$

Since $du_x/dx$ was found to be negative, $du_y/dy$ must be positive according to Eq. 1.24, which is indeed what we reasoned. Final question: See if Eq. 1.24 is also consistent with observation when moving downward from $y = 0$ (along $x = x_1$). ■

As in Section 1.3, an equation similar to Eq. 1.23 can be derived in terms of the mass concentration of some nonreactive ("conservative") component of local concentration $C$ as long as the component is not diffusing:

$$\frac{\partial C}{\partial t} + C\nabla\cdot\mathbf{u} + \mathbf{u}\cdot\nabla C = 0 \tag{1.25}$$

For an incompressible fluid, this equation simplifies to

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = 0 \tag{1.26}$$

The left-hand side of Eq. 1.26 appears in Chapter 7 during the development of the famous *convective-diffusion* equation.

## 1.5. CONTINUA

In the preceding sections, we imagined scalars like density and concentration and vectors like velocity to vary smoothly and continuously in space. But is this always a good assumption? This is not a trivial question, since many concepts of integral and differential calculus rely on this assumption. In particular, application of some of the previous equations would be hard to imagine in the absence of a continuum.

One way to examine this problem is to complete a thought experiment. Assume that we have an instrument that precisely measures fluid density. The instrument consists of a probe, density meter, and strip chart recorder (Figure 1.6). From the probe tip detail shown in the figure, it appears that the probe senses the local density in a region characterized by dimension $L$. We can presume that the probe senses an average value of density in the sensitive region.

Continuing the thought experiment, assume that the manufacturer will sell us probe tips of any dimension $L$ we wish, even down to molecular dimensions. The output of the meter is shown in Figure 1.7 for three choices of probe tip dimension $L$. Note that as $L$ increases relative to the spacing of the molecules of the fluid, the measured density function becomes smoother. Since we require that density have a well-defined value in a continuum, we could say that a continuum can be assumed for the following condition:

$$\frac{1}{N} <<< L^3 \tag{1.27}$$

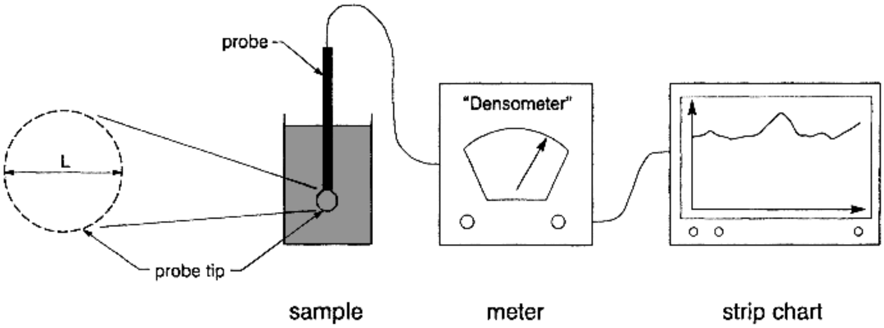


**Figure 1.6.** Imaginary density-measuring equipment.

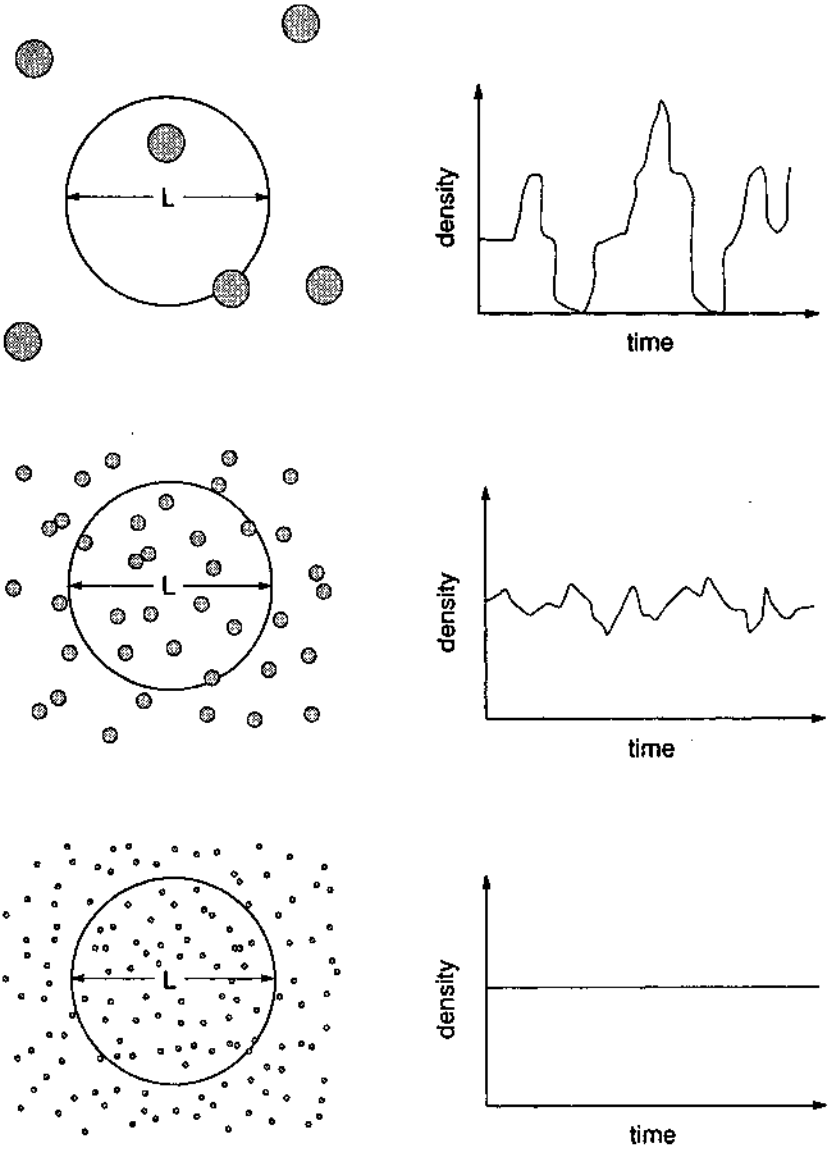


**Figure 1.7.** Density measurements for three choices of the sensor-characteristic dimension *L*.

where $N$ is the number of molecules per unit volume. Now terminating our successful thought experiment, what relevance does the experiment have to the real world? The answer is known as the *continuum hypothesis* of fluid mechanics: *A continuum is a region of space where characteristic flow scales L are large enough that properties like density and velocity can be assumed to vary smoothly and therefore have "point" values.* In water, $N$ is about $3.3 \times 10^{28}/\text{m}^3$; in air, $N$ is about $2.5 \times 10^{25}/\text{m}^3$. It is almost always safe to assume a continuum in liquids; however, gases cannot always be presumed to be continua (see also Sections 2.2, 5.9, and 6.4.3).

To see these problems more clearly, we need to know a little more about characteristic flow scales. The best way to introduce the idea of flow scales is through some examples. Figure 1.8*a* shows the classic case of fully developed laminar flow in a smooth pipe. The only characteristic flow scale is the pipe diameter, which is usually large enough that it is safe to asssume a continuum. (An important exception may be flow through some membrane pores, see Section 5.9.) Porous media flow, such as filter or groundwater flow, is somewhat more complicated (Figure 1.8*b*). We would agree that the characteristic length scale is related to the distance separating the grains of the porous media. But since the grains are arranged randomly in the media, what is the correct length scale? Here we rely on our intuition and consider that the *typical* or *characteristic* length scale of the flow is the same order of magnitude as the grains themselves. Although typical natural porous media have a variety of grain sizes, all are generally large enough to support the continuum assumption.

Another interesting case is suggested in Figure 1.8*c*. Here a particle is diffusing or sedimenting in air (the air molecules are the little circles). As long as the aerosol particle senses a continuum, the characteristic flow length is the particle diameter. But does the aerosol particle sense a continuum, or a series of discrete bombardments by the air molecules? This question arises so often in air physics and air-pollution-control engineering that scientists frequently make use of a dimensionless parameter known as the *Knudsen number:*

$$\text{Kn} = \frac{2\lambda}{d} \tag{1.28}$$

Here $d$ is the aerosol particle diameter and $\lambda$ is the *mean free path* in the fluid—the average distance a fluid molecule travels before striking another molecule. The mean free path in air is given by the following formula from Flagan and Seinfeld (1988):

$$\lambda = \frac{\mu}{0.499P\left(\dfrac{8m_a}{\pi RT}\right)^{1/2}} \tag{1.29}$$

Here $\mu$ is the fluid (gas) viscosity, $P$ is the pressure, $m_a$ is the molar mass of the gas, $R$ is the universal gas constant, and $T$ is the absolute temperature. In

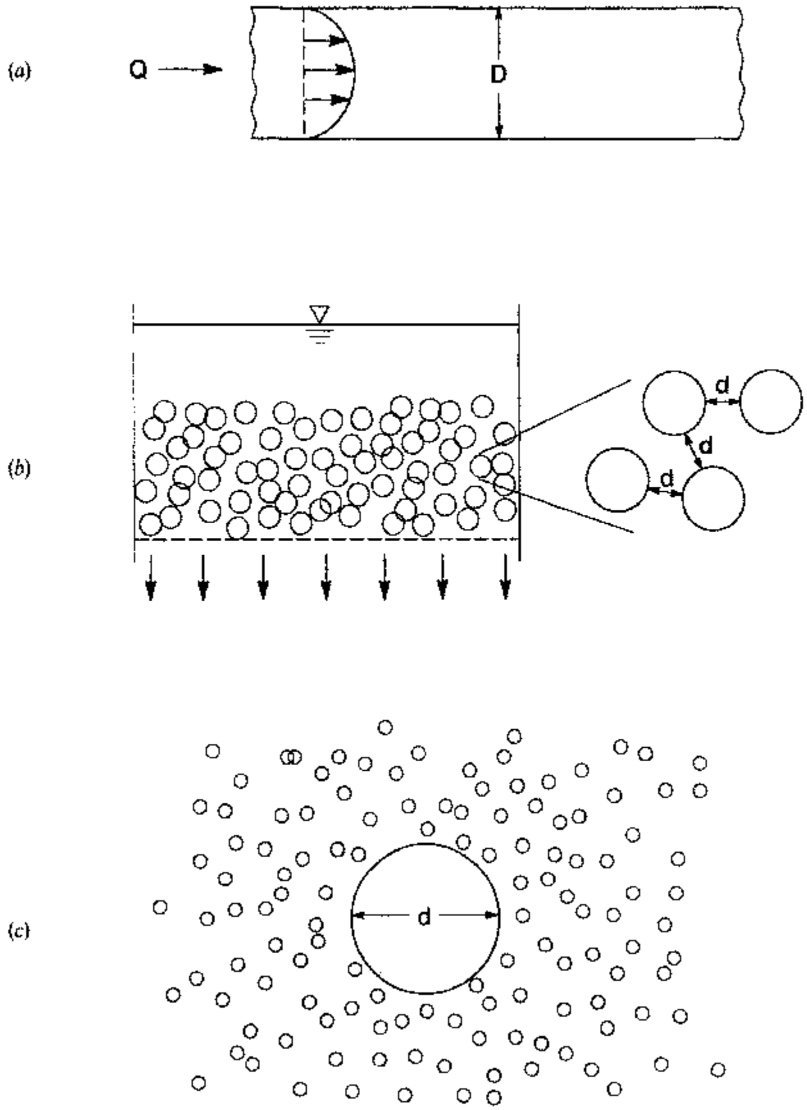


**Figure 1.8.** Examples of characteristic flow scales: (*a*) pipe diameter in laminar pipe flow, (*b*) pore “diameter” in porous media flow, and (*c*) aerosol particle diameter in diffusion or sedimentation.

air at 25 °C and 1 atm pressure, $P$ is $1.013 \times 10^5$ Pa and $\mu$ is $1.8 \times 10^{-5}$ Pa-s. Taking the molar mass of air as 0.0289 kg/mol, we find from Eq. 1.28 that the mean free path is 0.0653 $\mu$m.

When the Knudsen number is less than $10^{-2}$, a continuum can safely be assumed. The range $10^{-2} < \text{Kn} < 10^{-1}$ is called the *slip-flow* regime, where the continuum assumption begins to break down. Beyond $\text{Kn} = 10^{-1}$ the particle is considered to behave more or less like a free molecule in a gas. Even when the continuum assumption is weak, it is possible to solve problems of environmental and industrial importance (see Sections 2.2 and 5.9 for examples).

## 1.6. SOURCES, SINKS, REACTIONS, AND BOX MODELS

Note that in this chapter we have assumed that nothing "happens" to a particular species while in the system volume, control volume, or differential element. However, we know that this assumption will eventually have to be relaxed: Some of the most important problems in environmental modeling are those in which there exist chemical reactions, adsorption, sedimentation, biological degradation, volatilization, and other sources and sinks for mass constituents. Although these problems are a little more complicated, it is not difficult to see how some of the equations in this chapter must be modified. For example, a new version of Eq. 1.1 that takes into consideration reaction within the system could be

$$\frac{d}{dt}(VC_{\text{sys}}) = \sum_{i=1}^{N} Q_{\text{in},i}C_{\text{in},i} - \sum_{j=1}^{M} Q_{\text{out},j}C_{\text{out},j} + \sum_{k=1}^{L} Vr_k \tag{1.30}$$

Here $r_k$ are any reactions, sources, or sinks of material in the system volume. The units of $r_k$ are apparently $M\text{-}L^{-3}\text{-T}^{-1}$. Reactions can have either positive or negative magnitudes, depending on the reaction and constituent (reactant or product) being considered.

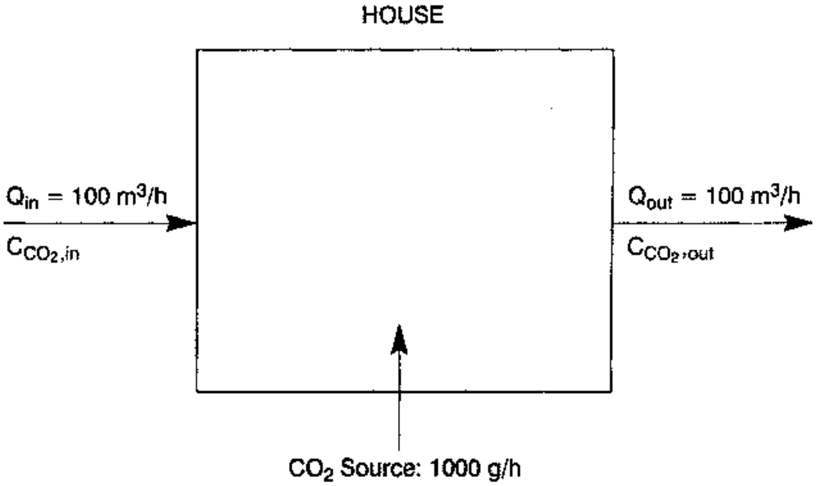
For the control volume approach, the equation corresponding to Eq. 1.14, which includes a single reaction, is

$$\iint_{\text{control surface}} C\mathbf{n}\cdot\mathbf{u}\, dA + \frac{\partial}{\partial t}\iiint_{\text{control volume}} C\, dV = \iiint_{\text{control volume}} r\, dV \tag{1.31}$$

and the equation corresponding to Eq. 1.26 for one reaction is

$$\frac{\partial C}{\partial t} + \mathbf{u}\cdot\nabla C = r \tag{1.32}$$

***Example 1.4.*** A house has a ventilation rate of 100 m$^3$/h. A kerosene heater is being used in the house, which emits 1000 g/h of $CO_2$. What is the average steady-state $CO_2$ concentration in the house? *Note*: The concentration of $CO_2$ in dry air at 20 °C and 1 atm pressure is 0.031% (by volume).



**Example 1.4**

SOLUTION. It is always a good idea to draw a picture of the physical system, as in Section 1.2. We model the input of $CO_2$ from the heater as a source of $CO_2$. (See the figure above.)

Substituting into Eq. 1.30 we find, at steady state,

$$0 = Q_{\text{in}}C_{\text{CO}_2,\text{ in}} - Q_{\text{out}}C_{\text{CO}_2,\text{out}} + Vr_{\text{CO}_2}$$

We know $Q_{\text{in}} = Q_{\text{out}} = 100\,\text{m}^3/\text{h}$. $C_{\text{CO}_2,\text{in}}$ is just the normal background concentration of $CO_2$. If the volumetric concentration of $CO_2$ in the atmosphere is 0.031%, and if 1 mol of ideal gas occupies 24.0 L at 20 °C and 1 atm pressure, the concentration of $CO_2$ in the air coming into the house is

$$C_{\text{CO}_2,\text{in}} = 0.00031\frac{1\text{ mol}}{24.0\text{ L}}\frac{44\text{ g}}{\text{mol}}\frac{1000\text{ L}}{\text{m}^3} = 0.568\frac{\text{gCO}_2}{\text{m}^3}$$

where the molar mass of carbon dioxide is 44 g. Finally, note that the source term, $Vr_{\text{CO}_2}$, must be 1000 g/h, as shown in the figure. Substituting into the equation above, we find that $C_{\text{CO}_2,\text{ out}} = 10.6\text{ g/m}^3$. The concentration at specific points in the house may be greater or less than this value, but the average concentration in the house must be 10.6 g/m³. This is about 17 times the normal background concentration of $CO_2$. ■

Example 1.4 and Eq. 1.30 are essentially the systems approach to mass conservation modified to account for reactions, sources, and sinks of mass within the system. Equation 1.30 is used so often in environmental modeling that it goes by a special name—the *box model*. This indicates that the environmental system under consideration is treated as a box (often a "black box"). Almost always, a special type of internal condition called *perfect mixing* is assumed (Chapter 10). In perfect mixing, any molecule entering the system is instantaneously mixed with all other molecules in the system. This is a convenient assumption because any internal gradients in concentration are ignored. The box model is used at several junctures in this book, as well as in several exercises at the end of this chapter. Perfect mixing is not a critical assumption for simple mass balances with sources and sinks (like Example 1.4). However, when reactions are present, the common perfect-mixing assumption of box modeling must be considered carefully. We return to box modeling at several junctures in this book, and the reader's understanding of the critical assumptions will be increased.*

## 1.7. SUMMARY

In this chapter the conservation of mass law was derived in three different forms. Some extensions and simplifications of this law were shown that result from assumptions like steady state and incompressibility, and which are useful in problem solving. The reader may wonder why three forms of the conservation equation are necessary. The simple answer is that engineering (and environmental) mass conservation problems are usually more easily cast and solved in one of the basic forms.

Box modeling techniques were introduced, and some of the power of this technique was demonstrated in a simple example. The idea of the continuum was also introduced. The continuum assumption is important in work with fluids (liquids and gases) and has particular importance in some air-pollution-control studies and in a growing number of nanotechnology and *nanofluidic* applications (Eijkel, 2007).

Completing the exercises at the end of this chapter should provide he student with more confidence in applying the laws of conservation of mass (and energy). The surprising utility of the simple concept of conservation should become evident to the reader.

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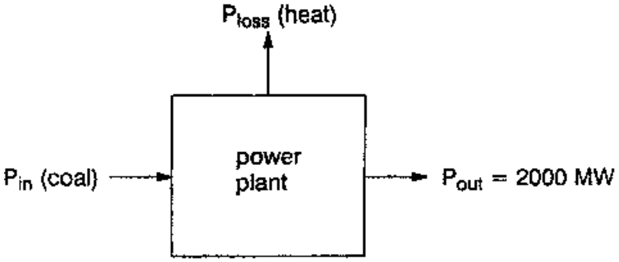
*Chapter 10 includes a thorough introduction to several ideal mixing models (e.g., perfect mixing). The reader is welcome to jump ahead to this material at any time; however, a rigorous understanding of mixing is not needed to understand the material covered in the first nine chapters of this book.

## EXERCISES

**1.1.** A power plant delivers 2000 MW of power to the distribution grid:



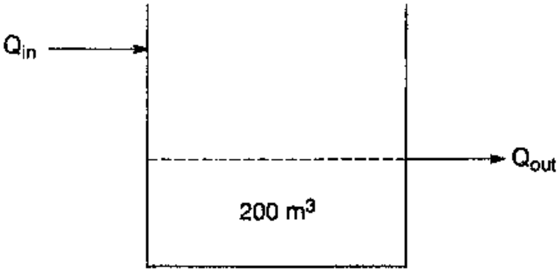
**Exercise 1.1**

If the plant is 45% efficient (i.e., $P_{\text{out}} = 0.45\,P_{\text{in}}$), what is the plant's consumption of coal if the coal has an energy content of 40 kW-h/lb? *Hint*: In analogy to Section 1.2,

$$\begin{bmatrix}\text{rate of accumulation}\\ \text{of energy}\end{bmatrix} = \begin{bmatrix}\text{rate of}\\ \text{energy input}\end{bmatrix} - \begin{bmatrix}\text{rate of}\\ \text{energy output}\end{bmatrix}$$

What is the rate of heat loss to the environment?

**1.2.** A 500-$m^3$ detention pond initially contains 200 $m^3$ of water. At the 200-$m^3$ level or below, there is no discharge from the pond, but discharge will begin for any level above 200 $m^3$.



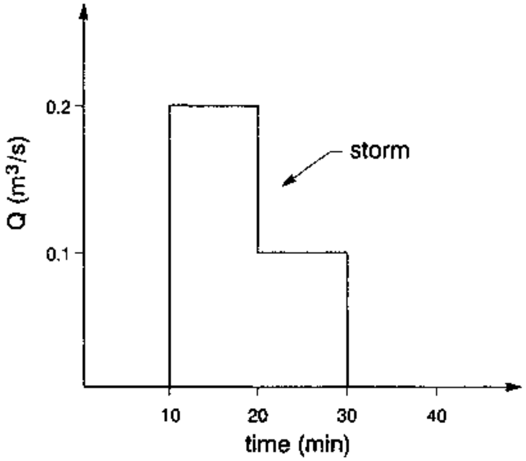
**Exercise 1.2**

An input flow of 0.2 $m^3/s$ begins, and at the same time, a valve controls the output flow according to the following expression:

$$Q_{\text{out}} = 0.001[V - 200]\left(\frac{\text{m}^3}{\text{s}}\right) \quad \text{for } V > 200\ \text{m}^3$$

In the equation, $V$ is the detention pond volume. Determine the pond volume over time, as well as the steady-state pond volume.

**1.3.** This problem uses the same detention pond described in Exercise 1.2. A thunderstorm upstream of the pond produces a short flood described in the following sketch:

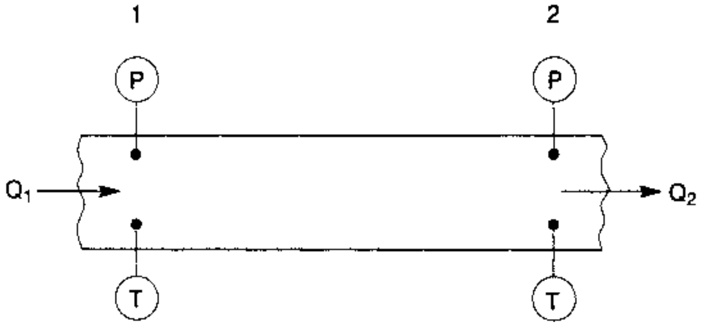


**Exercise 1.3**

Using the same outflow function of Exercise 1.2, determine the pond volume and outflow over time (include sketches of these functions). From the point of view of someone downstream of the retention pond, what effect do retention ponds have on floods? (Express answer in words.)

**1.4.** Consider a steady-state system with constant volume, a single constant inflow, and a single constant outflow, but with spatially varying fluid density within the system. Use Eq. 1.4 to derive a simple formula for $\rho_{out}$ if $Q_{in}$, $Q_{out}$, and $\rho_{in}$ are known. Why might fluid density change within a system?

**1.5.** Consider gas flow in a tube. Pressure and temperature are measured at points 1 and 2 as shown:

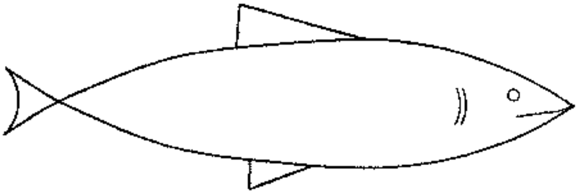


**Exercise 1.5**

**(a)** Use the ideal gas law to show how gas density is related to pressure and temperature. Recall that $PV = nRT$, where $P$ is pressure, $V$ is volume, $n$ is the number of moles of gas, $R$ is the universal gas constant, and $T$ is temperature.

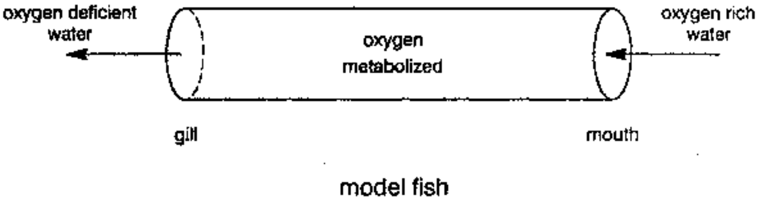
**(b)** If the gas flow is known at point 1, develop a steady-state equation to compute the gas flow at point 2 in terms of $Q_1$, $P_1$, $P_2$, $T_1$, and $T_2$. *Hint*: The results of Exercise 1.4 should be helpful. Assume steady state.

**1.6.** A fish that is exchanging mass with the surrounding water is shown below. Typically speaking, what types of mass would be exchanged between the water and the fish?



**Exercise 1.6a**

For modeling purposes, consider a cylindrical fish in which all oxygen is transferred to the fish from water which is brought into the fish through the mouth, and which leaves the fish through the gills:

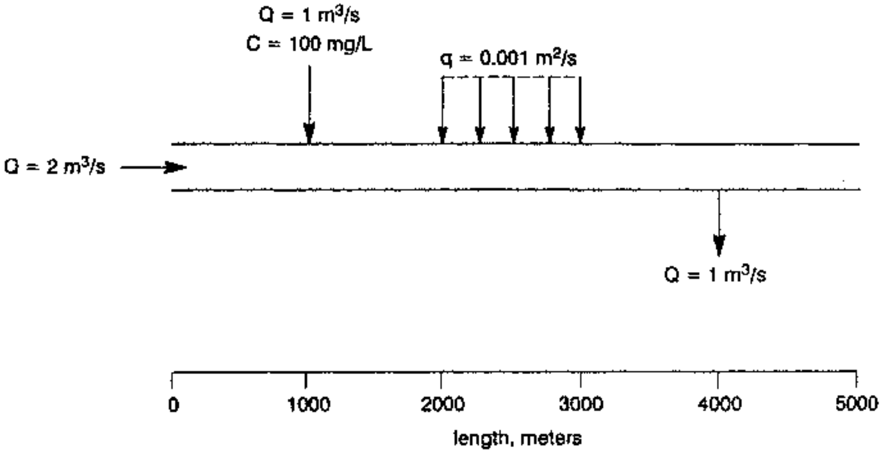


**Exercise 1.6b**

**(a)** If the oxygen content of the water is $7.5 \times 10^{-3}\,\mathrm{kg/m^3}$, and the fish is 25% efficient in transferring oxygen from the water, at what rate is oxygen metabolized by the fish if the fish processes 1 L of water every minute? Give answer in kilograms of $O_2$ per hour. *Hint*: Can the metabolism of $O_2$ in the fish be considered a sink for $O_2$ in the fish? If so, the approach in Section 1.6 may be useful.

**(b)** In the described analysis above, does it really matter what shape we have assumed for the fish?

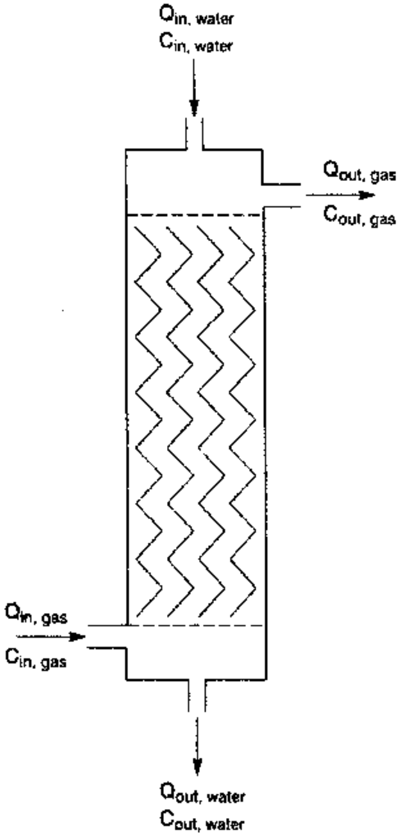
**1.7.** A 5000 m stretch of a certain river can be approximated for modeling purposes as:



Exercise 1.7

In the figure, $q$ is a distributed "nonpoint source" flow input given in units of $L^3/(L\text{-}T)$. As shown in the figure, at 1000 m, a flow enters the river with a contaminant concentration of 100 mg/L. This is a conservative contaminant, which means that it undergoes no reactions or degradation (e.g., NaCl). Plot the concentration of the contaminant along the 5000 m stretch of river. You may assume perfect mixing of the contaminant in the river cross section, but consider only transport downstream due to the average flow velocity.

**1.8.** A countercurrent gas absorption tower is shown in the figure below. It is called countercurrent because the liquid and gas phases move through the tower in opposite directions on average. The tower can be optimized to transfer dissolved gases from the liquid to the gas phase ("stripping"), or to transfer gas from the gas to the liquid phase ("scrubbing"). Using the approach in Section 1.2, write a steady-state mass balance on a gaseous contaminant that is also soluble in the water phase.



**Exercise 1.8**

*Comment*: This type of problem could be called a "multiphase mass balance."

**1.9.** The outflow and inflow to a $10^6\,m^3$ lake are $1\,m^3/s$. At a certain point in time, contamination of the inflow to the lake starts. Thereafter, the contaminant concentration in the lake inflow is 25 mg/L.

**(a)** If there is no prior contaminant in the lake inflow, determine the concentration of contaminant in the lake over time. Assume that once the contaminant enters the lake, it is efficiently mixed with the rest of the lake water; that is, in the terminology of Section 1.2, $C_{sys} = C_{out}$.

**(b)** What is the concentration in the lake effluent at a very long time after the contamination begins ($t \to \infty$)? *Hint*: This is called the steady-state concentration in the lake.

**1.10.** A retention pond with no outflow and a dry-period (starting) volume of $200\,\mathrm{m}^3$ suddenly starts receiving an inflow of $0.2\,\mathrm{m}^3/\mathrm{s}$. The inflow has a contaminant concentration of $10\,\mu\mathrm{g/L}$. There is initially $2\,\mu\mathrm{g/L}$ of contaminant in the pond.

- **(a)** Develop an equation for the pond volume as a function of time. Start with the appropriate differential equation and integrate using the appropriate initial condition.
- **(b)** Develop the governing differential equation for the contaminant concentration in the pond, assuming perfect mixing. The independent variable is time. Make all justifiable substitutions for known values and functions in the final differential equation.
- **(c)** Solve the equation from part (b) using the initial condition $C_{\mathrm{sys}} = 2$ at $t = 0$.
- **(d)** If the pond volume increases without limit, what must the concentration in the pond be as time approaches infinity?

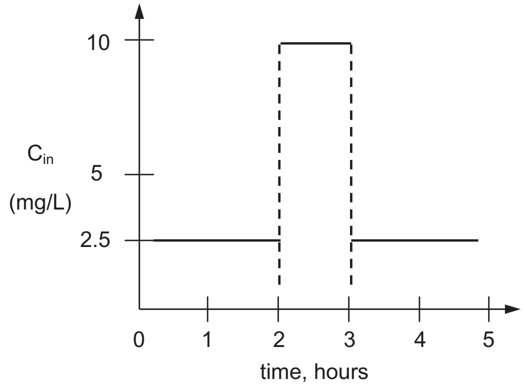
**1.11.** Your bathtub is filled with dirty water with a soap concentration of $C_0$ and you are splashing around having a good time. At $t = 0$, a special faucet opens pouring in clean water at a constant rate $Q$. The tub drain is also simultaneously opened so the tub is draining at rate $Q$ as well, that is, $V =$ constant.

- **(a)** Derive an equation to predict the soap concentration for $t > 0$.
- **(b)** What is the steady-state soap concentration in the bathtub?

**1.12.** You are washing and rinsing dishes. This problem is about rinsing the dishes. What is the more efficient method (in terms of water conservation) of rinsing a single glass: **(a)** fill the glass with water to its top, empty, fill again, empty again, and so on, until the glass is sufficiently rinsed of soap (you have special abilities to detect when this occurs), or **(b)** place it under the water tap and run water continuously until the glass is sufficiently rinsed of soap?

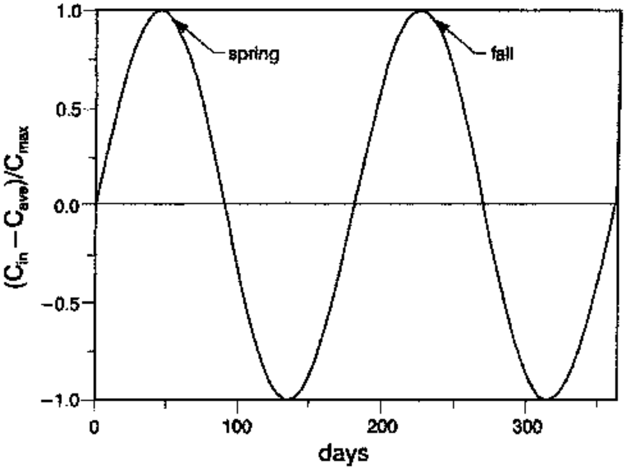
You may use the following information and assumptions: concentration of soap in the wash water = $C_0$; volume of full glass = $V_0$; volume soap film left on glass after emptying = $V_f = 0.01\,V_0$.

**1.13.** Consider a lake of $V = 10{,}000\,\mathrm{m}^3$ that is perfectly mixed. The flow into (and out of) the lake is constant, $Q = 1.0\,\mathrm{m}^3/\mathrm{s}$. There is always a background concentration of 2.5 mg/L entering the lake, but as shown, for 1 hour that concentration increases to 10 mg/L, and then goes back to the background concentration. What is the concentration leaving the lake at "3 hours"?



**Exercise 1.13**

**1.14.** A refractory organic compound (a compound not easily degraded biologically) enters a lake with a seasonally varying concentration profile that can be modeled as a sinusoidal function.



**Exercise 1.14**

The sinusoidal input can be described by the following function:

$$C_{\text{in}} = C_{\text{ave}} + C_{\max} \sin(\omega_0 t)$$

where $\omega_0$ is the frequency of the sinusoidal function:

$$\omega_0 = \frac{4\pi}{365} \frac{\text{rad}}{\text{day}}$$

**(a)** If there is no decay or other reaction of the compound in the lake (i.e., a conservative compound), use the systems approach (with the perfect-mixing assumption) to show that the appropriate differential equation describing the system is

$$\frac{dC}{dt}+\frac{1}{\bar{t}}C=\frac{1}{\bar{t}}[C_{\text{ave}}+C_{\max}\sin(\omega_0 t)]$$

where $\bar{t}$ is the mean residence time in the lake:

$$\bar{t}=\frac{V}{Q_{\text{in}}}=\frac{V}{Q_{\text{out}}}$$

**(b)** Show that for the initial condition $C = C_{\text{ave}}$ at $t = 0$, the solution to the differential equation given above is

$$C=C_{\text{ave}}+\frac{C_{\max}}{\frac{1}{\bar{t}}+\omega_0^2\bar{t}}\left[\frac{1}{\bar{t}}\sin(\omega_0 t)-\omega_0\cos(\omega_0 t)+\omega_0 e^{-t/\bar{t}}\right]$$

*Hint*: The integrating factor method of solving differential equations may be of some use.

**(c)** For lake volume $V = 10^6\,\text{m}^3$ and $Q_{\text{in}} = Q_{\text{out}} = 0.35\,\text{m}^3/\text{s}$, plot the solution on the same figure with the input function shown above.

**(d)** For $t \to \infty$ and $1/\bar{t} \gg \omega_0$, show that the solution to (b) simplifies to

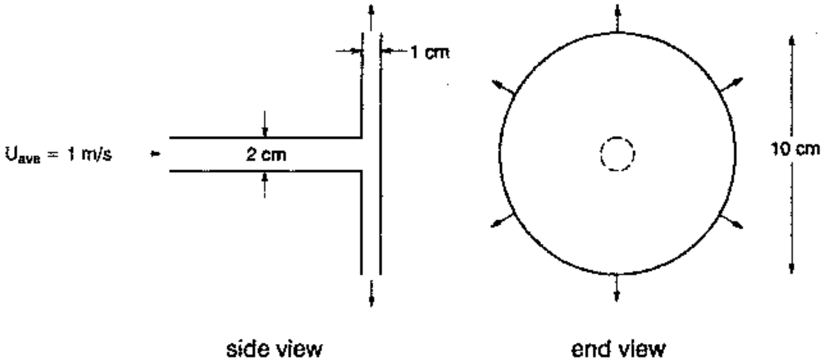
$$C=C_{\text{ave}}+C_{\max}\sin(\omega_0 t)$$

This is the same function as the input function, $C_{\text{in}}$. Next, show that for $t \to \infty$ and $1/\bar{t} \ll \omega_0$, the solution to (b) simplifies to

$$C=C_{\text{ave}}$$

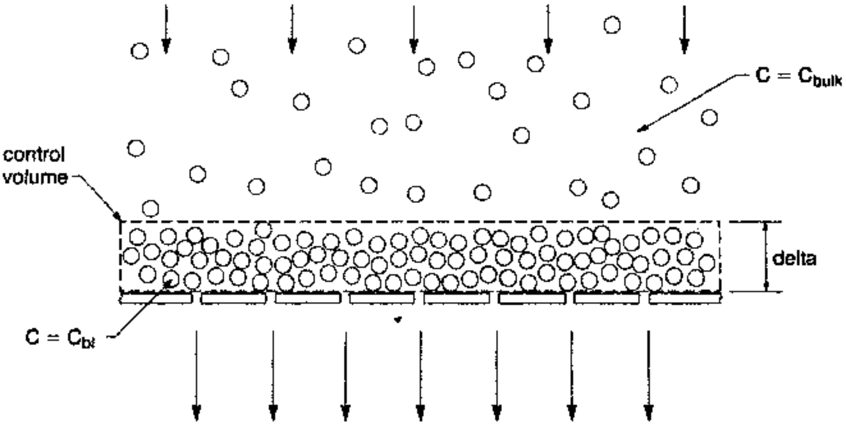
Try to explain why these two simplified solutions make sense (i.e., explain the effect of the lake on the concentration of organic matter leaving the lake).

**1.15.** An air flow enters the impaction device shown in the figure. What is the average velocity leaving the circular section? *Hint*: Use the approach in Section 1.3.



**Exercise 1.15**

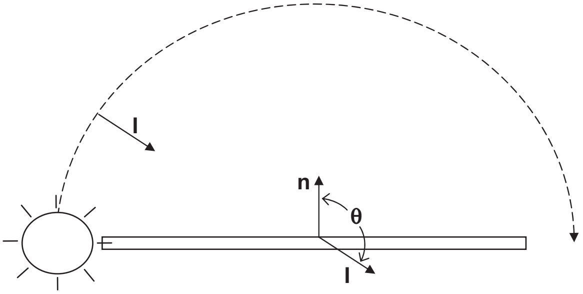
**1.16.** Ultrafiltration membranes can be used to separate macromolecules and small particles from liquid streams. If the membrane pores are much smaller than the particle or molecular diameters, the membrane is thought to pass the suspending liquid but reject or retain the particles or molecules. A section of membrane filtering particles from a liquid stream is shown below.



**Exercise 1.16**

As shown in the diagram, the thickness of a concentrated particle layer above the membrane surface increases as more fluid is filtered. Use the control volume approach discussed in Section 1.3 to calculate the thickness (delta) of the particle layer in terms of the membrane area ($A$), the volume of "permeate" passing through the membrane ($V_p$), the particle concentration in the concentrated layer ($C_{bl}$), and the particle concentration in the liquid approaching the membrane ($C_{bulk}$). *Hint*: Assume that the permeate flow is constant over time; hence, the control volume is increasing uniformly in size over time.

**1.17.** The idea of flux can also be used with radiative forms of energy. A photovoltaic cell is mounted horizontally on the ground. Assume the vector intensity of light from the sun, ***I*** (watt/m$^2$), is constant during the day and is not affected by the earth's atmosphere. Also assume that the panel happens to be located at the place on earth where the sun's intensity is greatest (a very warm climate).

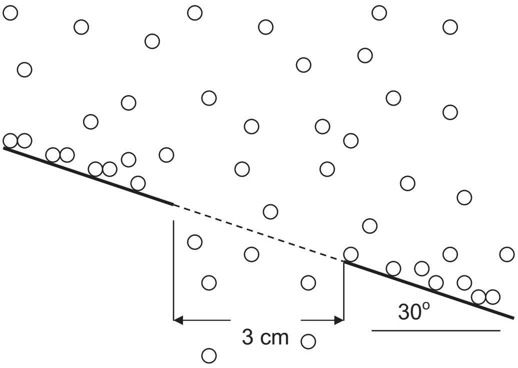


**Exercise 1.17**

**(a)** As the sun traverses the path shown in the figure, when is the panel producing the most power, that is, where is the flux of solar energy the greatest?

**(b)** Suppose the panel is mounted vertically rather than horizontally. Compare energy production with the horizontally positioned panel. *Note:* Sunlight is only collected from one side of the panel.

**1.18.** Particles of the same diameter are falling due to gravity through an otherwise still fluid. They encounter a tilted wall with a small opening. Particles that encounter the wall stick to the wall, while others pass through the opening.



**Exercise 1.18**

If the concentration of particles in the fluid is 50 mg/L, what is the steady-state mass transfer through the opening (per unit width into the page)? *Hints*: (1) Use control volume approach, (2) This is *not* about continua—assume the concentration of particles is great enough to ensure a continuum.

**1.19.** Equation 1.25 has a compact form because of vector notation. However, when practical problems are solved, a vector equation often has to be expanded into its Cartesian component form (i.e., $x$, $y$, and $z$ components). Expand Eq. 1.25 into component form.

**1.20.** A certain microbe has a spherical shape with a diameter of 1 $\mu$m. Assuming the interior of the microbe can be approximated as water, is the interior of the microbe a fluid continuum? Suppose you are told that the interior of the microbe has a pH of 7.5. How many $H^+$ atoms are expected on average to be inside the microbe? Is the interior of the microbe a continuum with respect to the $H^+$ concentration?

**1.21.** In air, are particles of 0.005, 0.05, 0.5, and 5.0 $\mu$m diameter in the continuum range?

**1.22.** Ryan et al. (1983) studied the generation of nitrous oxide ($NO_2$) by portable kerosene heaters and the effect of this pollutant on indoor air quality. The authors' model of this nonconservative compound imagines a house as a relatively closed system with an input of $NO_2$ from the heater, loss of $NO_2$ due to unspecified sink reactions, and exchange of $NO_2$ with the atmosphere outside the house due to ventilation. (Ventilation can be from an actual ventilation system and/or from leaks in walls, ceilings, and windows.)

**(a)** Using the box model approach with an assumption of perfect mixing inside the house, show that the appropriate differential equation governing the concentration of $NO_2$ is

$$\frac{dC}{dt} = R(C_e - C) - kC + S$$

where $C$ is the concentration of $NO_2$ in the house ($M/L^3$), $C_e$ is the concentration of $NO_2$ in the external atmosphere ($M/L^3$), $S$ is the $NO_2$ source ($M\text{-}L^{-3}\text{-}T^{-1}$), and $R$ is the so-called ventilation rate (which is not the same as the ventilation rate used in Example 1.4—the units are number of house volumes exchanged per unit time, $T^{-1}$). Here $k$ is the first-order decay constant for the unspecified sink, which is connected to $r$ in Eq. 1.30,

$$r = -kC$$

(First-order reactions are studied in more detail in subsequent chapters, including a fundamental definition in Section 9.2.)

**(b)** Using the initial conditions $C = C_0$ at $t = 0$, show that the equation above integrates to

$$C = \frac{S'}{R'}\left(1 - e^{-R't}\right) + C_0 e^{-R't}$$

where $R' = R + k$ and $S' = S + RC_e$.

**(c)** Plot the indoor concentration of $NO_2$ over time for $k = 0.5\,\text{h}^{-1}$, $S = 200\,\mu\text{g-m}^{-3}\text{-h}^{-1}$, and $R = 0.3$, 1.0, and $3.0\,\text{h}^{-1}$. Assume $C_0 = C_e = 0$.

**(d)** Solve the integrated equation for steady-state conditions (i.e., $t \to \infty$). Does the equation predict the same steady-state values as shown in your plot?

## REFERENCES

Eijkel, J., "Liquid Slip in Micro- and Nanofluidics: Recent Research and Its Possible Implications," *Lab Chip*, **7**, 299–301 (2007).

Flagan, R. C. and Seinfeld, J. H., *Fundamentals of Air Pollution Engineering*, Prentice Hall, Englewood Cliffs, NJ, 1988.

Ryan, B. P., Spengler, J. D., and Letz, R., "The Effects of Kerosene Heaters on Indoor Pollutant Concentrations: A Monitoring and Modeling Study," *Atmos. Environ.*, **17**, 7:1339–1345 (1983).

## BIBLIOGRAPHY

Batchelor, G. K., *An Introduction to Fluid Dynamics*, Cambridge University Press, Cambridge, UK, 1967 (available in paperback).

Felder, R. M. and Rousseau, R. W., *Elementary Principles of Chemical Processes*, Wiley, Hoboken, NJ, 1986.

Mackay, D., *Multimedia Environmental Models: The Fugacity Approach*, Lewis Publishers, Chelsea, MI, 1991.

Schnoor, J. L. and McAvoy, D. C., "Pesticide Transport and Bioconcentration Model," *J. Environ. Eng.*, **107**, EE6:1229–1246 (1981).

Sorenson, R., "Thought Experiments," *Am. Sci.*, **79**, 3:250–263 (1991).

Van den Berg, G. B. and Smolders, C. A., "Flux Decline in Ultrafiltration Processes," *Desalination*, **77**, 101–133 (1990).

Welty, J. R., Wicks, C. E., and Wilson, R. E., *Fundamentals of Momentum, Heat, and Mass Transport*, Wiley, Hoboken, NJ, 1976.

Wylie, C. R., *Advanced Engineering Mathematics*, McGraw-Hill, New York, 1975.