

Chapter 2

Fundamental Concepts in Biotransport

2.1 Introduction

Biotransport is concerned with understanding the movement of mass, momentum, energy, and electrical charge in living systems and devices with biological or medical applications. It is often subdivided into four disciplines: biofluid mechanics, bioheat transfer, biomass transfer, and bioelectricity. These topics are often taught together because of the great similarities in the principles that govern the transport of mass, heat, and momentum of charged and uncharged species.

Many different types of problems may be encountered in the study of biotransport processes. However, we believe that a standard approach, as introduced in Chap. 1, can be exercised to formulate a solution strategy for all biotransport problems. The formalism of the approach is straightforward, but the details will vary depending on the nature of the problem of interest and the extent to which the problem description leads directly to limiting assumptions and identification of constraints on how system and process are understood and modeled.

In this text at the introductory level, we will take a standard approach in defining systems for evaluation and in developing solution methods. Thus, the knowledge organization and presentation aspect of much of this text will resemble the very large number of preceding texts that have been written for transport. In some cases, we will introduce more advanced topics describing methods for handling the unique features of biosystems. The reader should beware that in many practical applications it will be necessary to address these features, and that special and more difficult modeling and solution methods will be required.

This chapter provides a brief introduction to a unified understanding of biotransport processes and how they can be modeled for analysis. First we will discuss some of the physical mechanisms that give rise to transport processes in a single material. Next we will address transport properties that can provide quantitative measures of a material's ability to participate in specific types of transport. Finally, we will consider transport across the interface between two different materials.

2.2 The System and Its Environment

The starting point for analyzing transport processes and problems is to define and understand the system of interest. In the most general sense, a system is identified as that portion of the universe that is involved directly in a particular process. The remainder of the universe is called the environment. The system interacts with the environment across its boundary. These interactions are directly responsible for changes that occur to the state of the system. The boundary surface provides a locus at which interactions can be identified (Fig. 2.1). Knowledge of these interactions can be used to predict resulting changes that will occur to the system.

There are two different approaches to identifying the boundary of a system. In one case the system is determined by a fixed mass. The system includes this specified mass and nothing else. As this mass moves or changes its shape, so does the boundary. Although the system may change over time in many different ways, a key feature is that the mass remains constant. Thus, this type of system is called a *closed system* since no mass can be added or removed (Fig. 2.2).

Alternatively, a system may be identified in terms of a boundary surface specified in three-dimensional space. This type of system is called an *open system* since mass may be exchanged across the boundary with the environment (Fig. 2.3).

The state of a system is described in terms of an independent set of measurable characteristics called properties. These properties can be either extensive (extrinsic) or intensive (intrinsic). *Intensive properties* are independent of the size of the system and include familiar properties, such as pressure, temperature, and density.

Fig. 2.1 A system is separated from the environment by a surface called the boundary. Interactions between a system and its environment are identified as they occur across the boundary

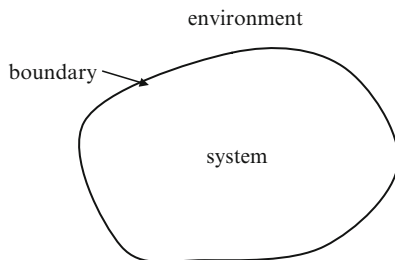


Fig. 2.2 A *closed system* is defined by a fixed mass which may change in position and shape as well as other properties. However, there is no movement of mass across the boundary. Thus, $mass_1$ is the same as $mass_2$

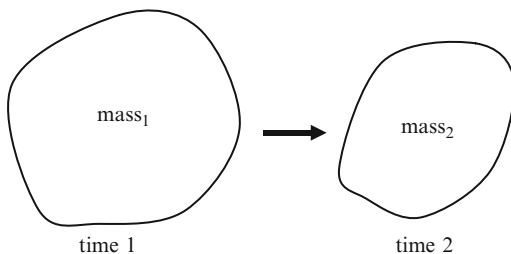
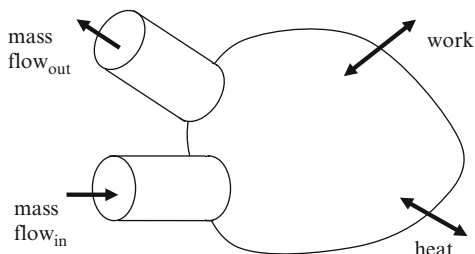


Fig. 2.3 An *open* system is defined by a boundary in space across which a system and the environment interact. The interactions may include mass exchange as well as work and heat



In addition, transport properties such as viscosity, diffusivity, and thermal conductivity are intensive properties. *Extensive properties* depend on the size of the system and include the transport properties mass, volume, heat, momentum, and electrical charge. Intensive properties can vary spatially or temporally within a system, but they do not flow into or out of the system. Extensive properties, however, can move across the system boundaries, and prediction of their movement is one of the primary objectives of this text.

2.3 Transport Scales in Time and Space

We can think of the transport of momentum, energy, mass, and charge to occur at three fundamental levels or scales, as illustrated by blood flow through the left ventricle in Fig. 2.4. Random molecular interactions can be associated with the transfer of all transport variables as shown on the right. As molecules collide, mass, energy, momentum, and electrical charge can be transferred from one molecule to another. If one considers a nanoscale open system consisting of a spherical volume with diameter of perhaps ten solvent molecules, the mass of the system will be proportional to the number of molecules in the sphere. As molecules enter and leave the boundaries of the spherical volume, the mass, energy, momentum, and charge within the system change. Changes can also occur as different species react, transfer electrons, or dissociate within the system. If molecules are treated as particles, one can write conservation equations for energy, mass, momentum, and charge for each species and add (integrate) the contributions from all molecules to produce the total for each transport variable within the system. Because of the large number of molecules per unit volume, this approach is only practical when we are dealing with a nanoscale system.

A more practical approach for larger systems is to neglect the particulate nature of matter and treat the system as if it consists of material that is continuously distributed in space, indicated by the middle panel of Fig. 2.4. We will evaluate the validity of that assumption shortly. This *microscopic* approach uses the conservation of mass, charge, momentum, and energy to the microsystem. Empirical relationships are used to relate fluxes of heat, mass, momentum, and electrical

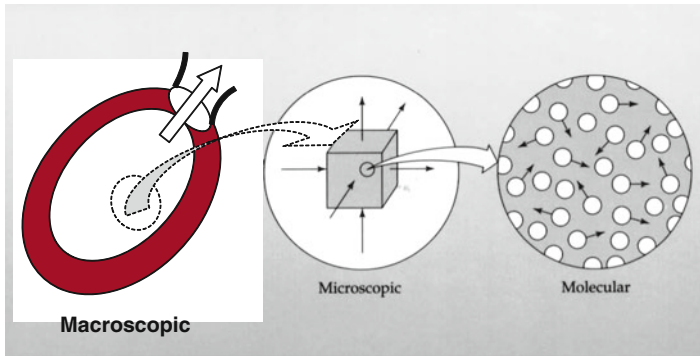


Fig. 2.4 Transport scales

charge (i.e., extrinsic or “through variables”) through the microsystem to gradients of driving “forces” such as temperature, concentration, pressure, or electrical potential (intrinsic or “across variables”). The resulting relations allow us to determine how transport variables vary with position (x, y, z) and time (t).

At the *macroscopic* scale, we are interested in how the average momentum, heat, mass, and electrical charge vary with time inside the system as a whole. Consider the system in the left panel of Fig. 2.4 which consists of the blood within the left ventricle. If the blood is well mixed, then variations in the transport variables change only with time and do not change with position within the system. In many situations, even if the system is not well mixed, we are only interested in how the average temperature, mass, or concentration varies in the system, so a macroscopic approach is appropriate.

Transport processes in living systems are manifested across length scales extending from physiological to molecular. Until recently, most analysis has been focused on processes that can be measured and analyzed at the macroscopic and microscopic levels. Advances in adjuvant sciences such as molecular biology have demonstrated that heat transfer can be used to manipulate the genetic expression of specific molecules for purposes of prophylaxis and therapy for targeted medical disease states. An illustrative example is the application of a spatially and temporally varying macroscopic scale thermal stress to control the pattern of genetic expression of specific proteins within cells of a tissue.

Common transport processes and their effects have been identified across a broad range of length scales. The greatest length is on the order of the size of the human body (1 m) and is typically encountered in environmental thermal interactions at the surface of the skin. At the opposite extreme is the profound effect of temperature on the genetic expression of individual protein molecules. In many instances, there is a direct coupling of the transport processes across disparate length scales. For example, transport originating at the physiologic scale can have its most important manifestation within individual cells.

There also exists a wide range of time scales for physiological transport, from near instantaneous to days, weeks, and longer. Here again coupling across time

scales is significant. The feedback control systems that regulate all aspects of life are among the most complex encountered in nature. Typically there exist many options for parallel pathways and for counterbalancing effects. There can be an interaction among transport processes having very different scales of length and time that is not apparent by superficial inspection. These differences in scales can provide a major challenge to modeling the integrated behavior of a physiological system. When encountering new arenas of application, it may be important to ensure that multiscale effects are accounted for.

Improved understanding of the constitutive behavior of living systems across the full range of scales has enabled meaningful application of biotransport modeling techniques which were not previously possible. It has been a continual challenge to develop mechanistically accurate models of biotransport processes since these are highly coupled and generally of a more complex nature than are processes in inanimate systems. The recent acceleration in learning about life at the cellular and molecular scales will lead to the development of more accurate and comprehensive biotransport models.

Complex geometric and nonlinear properties of living systems must be accounted for in building realistic models of living systems. This requirement remains one of the major challenges in the field of biotransport. Recent dramatic improvements in medical imaging techniques enable acquisition of more complete and accurate geometric and property data that can be used for developing patient specific models. This area of analysis holds great potential for future exploitation with applications such as computer-controlled surgical procedures using energy-intensive sources.

A primary conclusion of these observations is that currently there is a great potential for defining and solving new and important problems in biomedical transport (Schmid-Schönbein and Diller 2005). It is anticipated that there will be forthcoming significant advances in both theory and applications of biotransport in the near future.

In this text, we will be concerned primarily with treatments at the macroscopic and microscopic scales. In addition, the bulk of the text deals with the transport of uncharged species.

2.3.1 *Continuum Concepts*

How do we define the density at a specific point (x_0, y_0, z_0) in a system? The classic mathematical definition of density in a truly continuous system (i.e., a continuum) would be to measure the mass per unit volume as the volume approaches zero. However, because of the molecular nature of the material, the density can oscillate wildly as molecules jump into and out of a molecular sized control volume, ΔV (Fig. 2.5). If our point (x_0, y_0, z_0) is centered on one of the molecules, the final density would approach that of a nucleon. But an instant later the molecule might move away and the density would be zero. We are not interested in whether or not

Fig. 2.5 Volume of molecular proportions

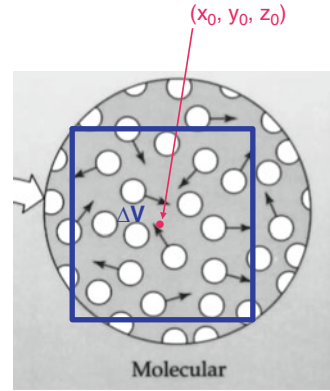
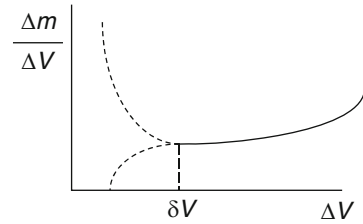


Fig. 2.6 Local density versus volume



molecules are present at the point, but rather in the average local density in the neighborhood of the point.

At what volume can we safely ignore the molecular nature of matter, but still compute a representative local density? As we reduce the local volume surrounding the point (x_0, y_0, z_0) , the mass per unit volume will change. At large volumes this reflects true differences in density caused by spatial variations. However, as the volume gets smaller, the computed density will eventually become independent of the size of the control volume, representing the true local density in the vicinity of the point (x_0, y_0, z_0) . As the volume drops below a critical value, δV , the density will oscillate in time between the two dotted lines in Fig. 2.6 as molecules move in and out of the volume. A practical definition for the *local density* would be:

$$\rho(x_0, y_0, z_0) = \lim_{\Delta V \rightarrow \delta V} \left\{ \frac{\Delta m}{\Delta V} \right\}. \quad (2.1)$$

How big is δV ? Let us postulate that the critical volume δV is reached when the point (x_0, y_0, z_0) , is surrounded by 1,000 molecules. Consider first the volume occupied by 1,000 molecules of an ideal gas. We can use Avogadro's number (number of molecules per mole) and the ideal gas law. Assuming a pressure of

1 atmosphere and a temperature of 298 K, we find this volume to be equivalent to a cube with each side having a length of $0.0344 \mu\text{m}$. By comparison, the smallest structural unit in the lung, an alveolus, has a diameter of about $300 \mu\text{m}$. For all practical purposes, air can be considered a continuum.

The value of δV will be even smaller in a liquid. To calculate the volume occupied by 1,000 molecules of water, we use Avogadro's number and the molar density of water at a pressure of 1 atmosphere and a temperature of 298 K. We find this volume to be equivalent to a cube with each side having a length of $0.0031 \mu\text{m}$ (3.1 nm). By comparison, a red blood cell has a volume that is more than a billion times larger than the critical volume. Again, for all practical purposes, problems involving biological materials of interest can be treated using the *continuum approach*.

2.4 Conservation Principles

In its simplest form, biotransport can be considered as the study of the movement of extensive properties across the boundaries of a biological or biomedical system. The first step in formulating a biotransport problem is to identify the system and its boundaries. The next step is to apply the appropriate conservation principles governing the movement of an extensive property, such as mass or energy. A general *conservation statement* for any extensive quantity can be expressed in words as:

$$\left\{ \begin{array}{c} \text{Rate of} \\ \text{accumulation} \\ \text{of the quantity} \\ \text{within a system} \end{array} \right\} = \left\{ \begin{array}{c} \text{Net rate the} \\ \text{quantity is produced} \\ \text{within the system} \end{array} \right\} + \left\{ \begin{array}{c} \text{Net rate the} \\ \text{quantity enters} \\ \text{through the} \\ \text{system boundary} \end{array} \right\}. \quad (2.2)$$

Let us refer to an extensive property of interest as “ X ”. The rate of accumulation of X within the system refers to the change in X per unit time. The accumulation of X in the system between times t and $t + \Delta t$ is $X(t + \Delta t) - X(t)$, and the rate of accumulation can be found by dividing this difference by the time increment Δt as it becomes very small:

$$\left\{ \begin{array}{c} \text{Rate of} \\ \text{accumulation of } X \\ \text{within a system} \end{array} \right\} = \lim_{\Delta t \rightarrow 0} \left\{ \frac{X(t + \Delta t) - X(t)}{\Delta t} \right\} = \frac{\partial X}{\partial t}. \quad (2.3)$$

If the rate of accumulation of X is positive, then X will increase with time, and if it is negative, X will decrease within the system as time increases.

The net rate of production of the quantity X in (2.2) refers to the rate at which X is produced or generated within the system minus the rate at which X is being consumed or depleted within the system. The net rate of production of quantities that are truly conserved such as mass, net electrical charge, and total energy is zero. Those quantities can only change if there is a net movement through the boundary. For this reason, some scientists prefer to call (2.2) an “accounting equation”, rather than a conservation equation. Quantities that are not conserved, such as the mass of cations or anions in a system, can change because of chemical dissociation or reaction without any cations or anions entering the system. Similarly, molecular species can be produced or depleted in the system by chemical reaction, irrespective of whether the species traverse the system boundary. Momentum in a system can be changed without momentum entering or leaving through the system boundaries. According to Newton’s second law, momentum will be altered if a net force is applied to the system. Heat can be produced in a system by viscous dissipation or chemical reaction; so the production term in the conservation relationship must be included if those sources of heat are present.

2.5 Transport Mechanisms

The final step necessary in the formulation of a biotransport problem is to identify appropriate expressions for the last term in (2.2) that accounts for the movement of extensive properties across the boundary. To answer this question, it is useful to first take a look at equilibrium situations. A system in *equilibrium* with its surroundings has no net exchange of any extensive property, such as mass or energy, with its surroundings. Thus, the net mass flow of each individual species between system and surroundings is zero. Consequently, there will be no current flow or total mass flow into or out of the system. Finally, there cannot be any net heat gain or loss from a system in equilibrium.

In addition, if we were to measure the temperature at all positions within a system that is in equilibrium with its surroundings, we would find no spatial variations. Similarly, we would find no spatial variations in pressure or in the concentrations of any of the molecular species within a system that is in equilibrium with its surroundings. The temperature and pressure within the system would be the same as the temperature and pressure of the surroundings. However, the concentration of each species within the system may be different than the concentration of the same species in the surroundings. This is because the solubility of a species in the system can be different than the solubility of the species in the surroundings. For example, if the system is a pane of glass immersed in the ocean, the solubility coefficients for various salts in glass are generally much lower than they are in water. Consequently, under equilibrium conditions, even though there is no net movement of any salt between system and surroundings, the salt concentrations in the system will generally be different than the concentrations of the same salts in the surroundings.

Now, consider two systems in contact that are not in equilibrium. If the temperatures of the two systems are different, then heat will flow from the system having the greater temperature to the system having the lower temperature. Consequently, the temperature difference between two systems that are not in equilibrium is an appropriate driving force for inducing heat transfer between the systems. However, a simple concentration difference cannot be considered as an appropriate driving force for mass transfer between systems because differences in species concentration can occur under equilibrium conditions, where no mass transport can occur. Instead, the appropriate driving force would be the concentration in the first system minus the concentration in the second system that would be in equilibrium with the concentration in the first system.

What causes heat, momentum, and mass to flow under nonequilibrium conditions? There are two basic transport mechanisms: random molecular motion and bulk fluid motion. Heat, momentum, mass, and electrical charge can be transported by both of these mechanisms. Other important transport mechanisms also exist, including radiation, evaporation, condensation, and freezing.

2.5.1 Molecular Transport Mechanisms

Let us begin with a description of transport by molecular motion. If we open a bottle containing an odiferous gas at the center of a large room containing stagnant air, we will smell the gas several feet away within a short time. The transport of the gas is by random molecular motion, known as diffusion. The more molecules of gas present at the release site, the greater will be the movement of gas away from the release site. Consequently, the higher the concentration gradient in a particular direction, the greater will be the movement of gas in the opposite direction.

This and other transport processes can be described in terms of a constitutive equation. A *constitutive relationship* for molecular transport mechanisms is an empirical equation relating the motion of an extensive transport property to the negative gradient of an intensive transport property. A unique constitutive equation is associated with each transport process, and many of these equations have been known for more than a century based on the observation of naturally occurring transport phenomena. The constitutive equations are usually written in terms of the transport flux in a particular coordinate direction n and the precipitating potential gradient in that direction. This can be expressed as:

$$\text{Flux}_n = (\text{constitutive property}) \cdot \left[-\frac{\partial(\text{potential})}{\partial n} \right]. \quad (2.4)$$

Let us formally define flux and gradient. The *flux* of a quantity X (e.g., species, mass, momentum in the n -direction, heat, charge) at a point (x_0, y_0, z_0) is a vector

representing the rate at which X passes through a unit area A that is perpendicular to the n -direction per unit time (Fig. 2.7):

$$(\text{Flux of } X)_{x_0, y_0, z_0} = \frac{1}{A} \left(\frac{\partial X}{\partial t} \right)_{x_0, y_0, z_0} . \quad (2.5)$$

Let us define a potential Ψ , which is an intensive property responsible for inducing the flux of X . In the case of heat transfer, Ψ would be temperature and X would be heat. The *gradient* of the potential Ψ in the n -direction at the point (x_0, y_0, z_0) is simply the rate at which the potential varies in the n -direction at that point:

$$(\text{Gradient of } \Psi)_{x_0, y_0, z_0} = \left(\frac{\partial \Psi}{\partial n} \right)_{x_0, y_0, z_0} . \quad (2.6)$$

In general, the potential is a scalar property, and the flux is a vector expressed as the flow per unit area normal to the direction of the applied potential gradient.

The *constitutive property* is a measure of the ability of the system material to facilitate the transport process. It is dependent on the chemical composition of the system material and the state of the system. For example, changes in temperature and pressure can often cause significant alterations in the flux of extensive properties, and the magnitude of the effect will depend on the composition of the system.

Because of the random nature of molecular collisions, regions of space with an initially high population of molecules possessing a particular transport characteristic will lose some of those molecules to surrounding regions with time. Energy and momentum can also be exchanged to surrounding regions via molecular collisions. A completely random process cannot concentrate mass, charge, momentum, or energy. This would violate the second law of thermodynamics. In a random process, each of these quantities must move from regions of high potential to low potential. A positive potential gradient is one in which the potential increases with n . Therefore, the flux of transport quantities such as mass, momentum, charge, and heat must be in the opposite direction as the potential gradient. Consequently, the flux in the constitutive equation is proportional to the negative of the potential gradient. To generate a transport flow with a positive vector, it is necessary to apply

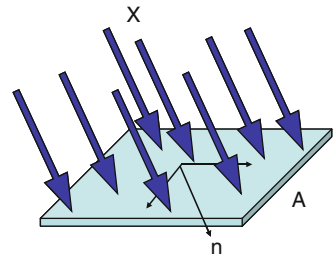
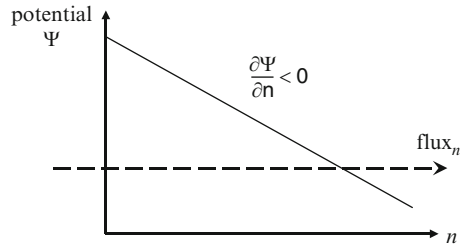


Fig. 2.7 Flux in n -direction through a surface with area A that is perpendicular to n

Fig. 2.8 One-dimensional flux of X generated in a positive direction by application of a negative gradient in driving potential along the axis of flow



a negative potential gradient, i.e., with a magnitude decreasing along the coordinate axis (Fig. 2.8).

2.5.1.1 Basic Constitutive Equations for Molecular Transport

There are characteristic constitutive equations that are applied uniquely to describe all observed transport processes. However, processes based on random molecular motion all have analogous constitutive equations even though they have been derived for processes in different domains. The diffusion of chemical species in dilute solutions is represented by a constitutive equation known as *Fick's law of diffusion*, which states that the transfer of species A in a binary mixture of A and B is expressed for a one-dimensional Cartesian coordinate as:

$$J_{Ax} = -D_{AB} \frac{dc_A}{dx} \quad (\text{diffusion}), \quad (2.7)$$

where J_{Ax} (mol/(s m²)) is the molar flux of species A in the x -direction, c_A (mol/m³) is the molar concentration of species A in solution, and D_{AB} (m²/s) is the binary diffusion coefficient of species A in the mixture. Fick's law is also used in mixtures that are not binary mixtures if species A is dilute. For multidimensional applications, (2.7) can be written in vector form as:

$$\vec{J}_A = -D_{AB} \vec{\nabla} c_A = -D_{AB} \left(\vec{i} \frac{\partial c_A}{\partial x} + \vec{j} \frac{\partial c_A}{\partial y} + \vec{k} \frac{\partial c_A}{\partial z} \right). \quad (2.8)$$

For the transport of heat, the equivalent constitutive equation is known as *Fourier's law of conduction* or thermal diffusion. One-dimensional heat flux in Cartesian coordinates is given by:

$$q_x = \frac{\dot{Q}_x}{A} = -k \frac{dT}{dx} \quad (\text{conduction}), \quad (2.9)$$

where x is the direction of heat flow, q_x is the heat flux in that direction (W/m²), \dot{Q}_x is heat flow (W), k (W/(m K)) is the thermal conductivity, T (K) is the local

temperature within the system, and A (m^2) is the area normal to the temperature gradient. If heat also flows in the y and z directions, then a more general expression for the heat flux is written as a vector quantity, \vec{q} :

$$\vec{q} = -k\vec{\nabla}T = -k\left(\vec{i}\frac{\partial T}{\partial x} + \vec{j}\frac{\partial T}{\partial y} + \vec{k}\frac{\partial T}{\partial z}\right). \quad (2.10)$$

For the transport of electrical charge, Q (Coulombs), *Ohm's law* can be written on a molecular scale as:

$$i_x = \frac{I_x}{A} = \frac{1}{A} \frac{\partial Q}{\partial t} = -\frac{1}{\mathfrak{R}_e'} \frac{dE}{dx} = -k_e \frac{dE}{dx}, \quad (2.11)$$

where i_x is the flux of electrical charge or the current density, I_x is the current, E is the electrical potential, \mathfrak{R}_e' is the electrical resistivity, k_e is its inverse, or electrical conductivity, and A is the area normal to the electrical potential gradient. In more general terms, the current density can be written as a vector:

$$\vec{i} = -k_e \vec{\nabla}E. \quad (2.12)$$

If you move your hand in the x -direction through a fluid, like water, fluid layers above and below your hand will also move in the x -direction. The fluid closest to your hand will move the fastest, while fluid far from your hand will be nearly stationary. Because of the viscous or frictional nature of the fluid, x -momentum induced in the fluid layer next to your hand will be transmitted in the y -direction, perpendicular to the direction of movement. *Newtonian fluids* are those in which the flux of x -momentum in the y -direction is proportional to the negative of the velocity gradient. *Newton's law of viscosity* can be written:

$$\tau_{yx} = -\mu\dot{\gamma} = -\mu \frac{dv_x}{dy}, \quad (2.13)$$

where $\dot{\gamma}$ is the shear rate in the fluid, which is the velocity gradient orthogonal to the flow vector, in units of (1/s). The constant of proportionality μ is called the viscosity in units of (N s/m^2) or (Pa s). The momentum flux can also be interpreted as the shear stress τ_{yx} that acts on a plane normal to the y axis in the direction of the x axis in units of (N/m^2). These interpretations will be discussed in Chap. 4.

Other transport mechanisms are known to exist. A large temperature gradient can induce a mass flux (*Soret effect*) and a large concentration gradient can induce an energy flux (*Dufour effect*). However, in biomedical applications, these effects are expected to be negligible. The basic constitutive relations for one-dimensional molecular transport are summarized in Table 2.1. There are clear analogies between these four relations, showing why these transport mechanisms are often studied together.

Table 2.1 Constitutive relationships for 1D molecular transport [$x = n$ in (2.4)]

	Species	Momentum	Heat	Electrical charge
Extensive variable (flux)	Molar flux	x -Momentum flux in y -direction	Heat flux	Current density
	J_{Ax}	τ_{yx}	q_x	i_x
Intensive variable (potential)	Molar concentration	Velocity in x -direction	Temperature	Electrical potential
	c_A	v_x	T	E
Transport coefficient or property	Diffusivity of A in B	Fluid viscosity (Newtonian)	Thermal conductivity	Electrical conductivity
	D_{AB}	μ	k	k_e
Constitutive relation	$J_{Ax} = -D_{AB} \frac{dc_A}{dx}$	$\tau_{yx} = -\mu \frac{dv_x}{dy}$	$q_x = -k \frac{dT}{dx}$	$i_x = -k_e \frac{dE}{dx}$

2.5.1.2 Molecular Transport Properties

The ability of a material to participate in a particular type of transport is related to its molecular structure. Consequently, solids, liquids, and gases will vary in their ability to enable different types of transport processes. This ability can be quantified and measured in terms of a unique property value associated with each mechanism of transport. These features of a material are called constitutive properties, and they are used in constitutive equations, as described in the foregoing section, to calculate the magnitude of a transport flow in a particular type of material subjected to a driving potential. The value of a property gives a measure of the rate at which a transport flow will occur in response to a given driving potential.

Values for many transport properties are available in tables, some of which can be found in Appendix C of this text. These values are obtained by monitoring transport processes in specific materials under very tightly controlled experimental conditions. Fluid viscosity of Newtonian fluids, for instance, is computed from direct measurements of wall force and shear rate in a viscometer having a known wall area. When these measured values are inserted in the appropriate constitutive equation (2.13), the only unknown is the fluid viscosity. Similar experiments can be designed to provide direct measures of other constitutive properties, such as thermal conductivity and diffusion coefficients. This approach to analysis is termed the “inverse solution method”, since it contrasts with the common application where a constitutive equation is used to calculate a transport flow from known values of the applied driving potential and the transport property.

Transport properties generally depend on the state conditions of the material under investigation, particularly temperature and pressure. Therefore, it is important that state variables be controlled in experiments designed to measure transport properties. Likewise, when attempting to identify transport properties for a particular application, it is important to ensure that the transport properties selected are valid under the applicable state conditions.

In some cases, large variations in state variables may exist in particular transport processes. This situation may arise frequently for heat transfer applications where

large temperature gradients are applied to a system. An analogous situation may arise for fluid flow resulting from a steep gradient in applied pressure. In such cases, transport properties might vary significantly with position. If significant property gradients are present, it will be necessary to either use an average approximation for the magnitude of the property throughout the system or to account for local property variations when applying the constitutive relation.

Sometimes, it is useful to combine constitutive properties with other properties to form a new property that has particular physical significance. Examples include the *kinematic viscosity*, ν , and the *thermal diffusivity*, α , both of which have units of (m^2/s):

$$\nu = \frac{\mu}{\rho}. \quad (2.14)$$

$$\alpha = \frac{k}{\rho c_p}. \quad (2.15)$$

The quantity c_p is the *heat capacity per unit mass at constant pressure* (or simply *specific heat*) of the material. It is not accidental that the properties ν and α from fluid and heat transport match the units for the diffusion coefficient, D_{AB} , for mass transport. We will discuss the analogies among the different transport domains in the next section.

2.5.1.3 1D Molecular Transport Analogies

An extensive variable can be converted to an intensive variable by dividing by the volume of the system. For example, the number of moles of species A in a system N_A , an extensive variable, can be converted to the average molar concentration of species A, c_A , an intensive variable, by dividing by the system volume. The flux of an extensive property X can be written as the product of a transport coefficient γ_X and the negative gradient of the same extensive property per unit volume, \tilde{X} , where the tilde above the symbol can be interpreted as the quantity “per unit volume.” For one-dimensional transport in the y -direction:

$$\text{Molecular flux of } X \text{ in } y\text{-direction} = -\gamma_X \frac{\partial \tilde{X}}{\partial y}. \quad (2.16)$$

A consequence of writing the flux equation in this form is that the dimensions of the transport coefficient γ_X will always be the same. The flux of X will have dimensions of X per unit time per unit length squared and the dimensions of $\partial \tilde{X}/\partial y$ will be the dimensions of X per unit length to the fourth power. Consequently, γ_X will have dimensions of $\text{length}^2/\text{time}$.

Returning to our previous example, if the extensive property X is the number of moles of species A, then:

$$\begin{aligned} X &= N_A, \text{ number of moles} \\ \text{Molecular flux of species A in } y\text{-direction} &= J_{Ay} \text{ (molar flux by diffusion)} \\ \tilde{X} &= \tilde{N}_A = c_A \text{ (moles per unit volume or concentration)} \end{aligned}$$

Therefore, according to (2.16):

$$J_{Ay} = -\gamma_{N_A} \frac{\partial c_A}{\partial y}. \quad (2.17)$$

Comparing this with Fick's law of diffusion (2.7), we found that the transport coefficient γ_{N_A} is equal to the diffusion coefficient D_{AB} , which has the appropriate dimensions of $\text{length}^2/\text{time}$.

If the extensive variable is the internal energy, U , then:

$$\begin{aligned} X &= U = mc_p(T - T_R), \text{ where } T_R \text{ is a reference temperature.} \\ \text{Molecular flux of energy in } y\text{-direction} &= q_{Ay} \text{ (conduction heat flux)} \\ \tilde{X} &= \tilde{U} = \rho c_p(T - T_R), \text{ internal energy per unit volume} \end{aligned}$$

Therefore, according to (2.16):

$$q_y = -\gamma_U \frac{\partial \tilde{U}}{\partial y} = -\gamma_U \frac{\partial}{\partial y} (\rho c_p T). \quad (2.18)$$

Comparing this with Fourier's law of conduction (2.9), we find $\gamma_U = k/\rho c_p = \alpha$, the thermal diffusivity, from (2.15). Indeed, this has the same dimensions as the diffusion coefficient.

Finally, let us take x -momentum as our extensive variable:

$$\begin{aligned} X &= mv_x \\ \text{Molecular flux of } x\text{-momentum in the } y\text{-direction} &= \tau_{yx} \\ \tilde{X} &= \rho v_x. \end{aligned}$$

The flux equation becomes:

$$\tau_{yx} = -\gamma_{mv_x} \frac{\partial(\rho v_x)}{\partial y}. \quad (2.19)$$

Comparing this with Newton's law of viscosity, (2.13), the transport variable γ_{mv_x} must be μ/ρ , which is the kinematic viscosity ν defined previously in (2.14). Again, the momentum transport variable will have dimensions of $\text{length}^2/\text{time}$.

Equations (2.17)–(2.19) all have similar forms and have transport coefficients with the same dimensions: D_{AB} , α , and v . The similarities in the relations between the fluxes and gradients for 1D transport are known as the *transport analogies*.

2.5.2 Convective Transport Mechanisms

The second major transport mechanism is the transport of materials, energy, momentum, and charge by bulk fluid motion. This is known as convective transport. Let us take as an example the flow of a fluid into a control volume as shown in Fig. 2.9. Recall that the flux of a quantity X is the rate of change of X per unit area per unit time. Let us apply that definition to an element of mass Δm that enters a system in the x -direction in a time interval Δt . The bolus passes through a cross-sectional area A_c in time Δt by bulk fluid motion. The mass that enters is equal to the fluid density times the fluid volume that enters the control volume. The volume of fluid entering the system in time Δt is equal to the cross-sectional area times the length of the bolus ΔL . But the length of the bolus relative to the time it enters is simply equal to the fluid velocity in the x -direction. Therefore, the convective mass flux in the x -direction is found to be ρv_x :

$$\text{Convective mass flux} = \frac{1}{A_c} \frac{\Delta m}{\Delta t} = \frac{1}{A_c} \frac{\rho A_c \Delta L}{\Delta t} = \rho \frac{\Delta L}{\Delta t} = \rho v_x. \quad (2.20)$$

Note that this is also equal to the x -momentum of the entering fluid per unit volume. In a similar manner, if species A also enters the control volume, the convective molar flux of A will be equal to $c_A v_x$:

$$\text{Convective molar flux of } A = \frac{1}{A_c} \frac{c_A A_c \Delta L}{\Delta t} = c_A \frac{\Delta L}{\Delta t} = c_A v_x. \quad (2.21)$$

Using the same procedure, the convective momentum flux is found to be ρv_x^2 :

$$\text{Convective } x\text{-momentum flux} = \frac{1}{A_c} \frac{\Delta(mv_x)}{\Delta t} = \rho v_x^2. \quad (2.22)$$

The convective heat flux arises primarily from the transport of internal energy U into the system by bulk fluid movement. This is equal to product of the mass flux,

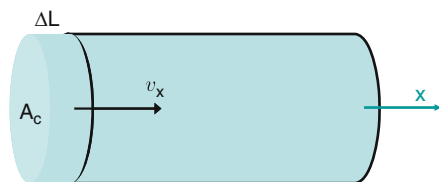


Fig. 2.9 Convection of volume $A_c \Delta L$ into control volume

the specific heat capacity at constant pressure, and the temperature relative to some standard reference temperature T_R :

$$\text{Convective heat flux} = \frac{1}{A_c} \frac{\Delta U}{\Delta t} = \frac{1}{A_c} \frac{\Delta [mc_p(T - T_R)]}{\Delta t} = \rho v_x c_p (T - T_R). \quad (2.23)$$

In the case of heat transfer, we also need to consider a third mechanism, radiation heat flux, which will be introduced in Chap. 8. The total flux in 1D flow situations can be found by adding the flux contributions from all mechanisms. Neglecting all but molecular and convective fluxes, the total fluxes are:

$$\text{Total mass flux} = \rho v_x. \quad (2.24)$$

$$\text{Total flux of } x\text{-momentum} = \rho v_x^2 + \tau_{yx} = \rho v_x^2 - \mu \frac{dv_x}{dy}. \quad (2.25)$$

$$\text{Total molar flux of species } A = N_{Ax} = c_A v_x + J_{Ax} = c_A v_x - D_{AB} \frac{dc_A}{dx}. \quad (2.26)$$

$$\text{Total heat flux} = \rho v_x c_p (T - T_R) + q_x = \rho v_x c_p (T - T_R) - k \frac{dT}{dx}. \quad (2.27)$$

The student should be aware that some texts refer to transport by bulk fluid motion as *advection* and the combined transport by molecular motion and bulk fluid motion as *convection*. Most engineering texts, including this one, associate convection with transport by bulk fluid motion.

2.6 Macroscopic Transport Coefficients

In many situations, we are interested only in transport at the macroscopic scale where convection and molecular motion may both play a role. Rather than applying the expressions for molecular and convective fluxes derived in previous sections, a more empirical approach involving the use of dimensional analysis has proven to be quite fruitful. Details of the general approach will be presented in Chap. 3 and applications will be presented in Chaps. 5, 9, and 13. For macroscopic transport in a single medium, we can express the flow of an extrinsic transport quantity as the product of a transport coefficient and a driving force. To use a familiar example, the flow of charge in an electrical wire is expressed as:

$$I = \frac{\Delta E}{\mathfrak{R}_e}, \quad (2.28)$$

where I is the electric current in the wire, ΔE is the electrical potential difference across the wire, and \mathfrak{R}_e is the electrical resistance. In some instances, the electrical

resistance is nearly constant and in others it may depend on the potential difference. For a wire with length L and cross-sectional area A_c , the average flux of electrical charge or *current density* $\langle i \rangle$ can be found by dividing (2.28) by A_c :

$$\text{Average charge flux} = \langle i \rangle = \frac{I}{A_c} = \frac{\Delta E}{A_c \mathcal{R}_e} = \left(\frac{L}{A_c \mathcal{R}_e} \right) \frac{\Delta E}{L}. \quad (2.29)$$

A quantity in braces $\langle \rangle$ is defined in this text as the *average value* of that quantity over the cross-section of the system. Since ΔE is the inlet potential minus the outlet potential, then the average gradient of electrical potential in the wire over its length L is $-\Delta E/L$. Therefore, (2.29) can be interpreted as a macroscopic version of (2.11), a constitutive relationship between the average current density and the average negative gradient of electrical potential. In this case, the electrical resistance is directly proportional to the electrical resistivity of the material, $\mathcal{R}_e = \mathcal{R}_e' L/A_c$, or $\mathcal{R}_e = L/k_e A_c$, where k_e is the electrical conductivity of the material.

An empirical expression analogous to (2.28) can be written for the *volumetric flow rate* Q_V of fluid through a horizontal conduit:

$$Q_V = \frac{\Delta P}{\mathcal{R}_f}. \quad (2.30)$$

ΔP is the hydrostatic pressure difference between inlet and outlet of the conduit and \mathcal{R}_f is the resistance to flow. The resistance will depend on conduit geometry, fluid properties, and flow rate. If the cross-sectional area of the conduit is constant and flow is laminar, then resistance is constant. However, if flow is turbulent, the resistance will depend on the pressure difference and empirical methods relating the flow resistance to a friction factor must be used. The technique is described in Sect. 5.6. If the conduit is not horizontal, then (2.30) must be modified to include gravitational effects, as described in Sect. 5.5.

Total *mass flow* w through a conduit is equal to the volumetric flow multiplied by the fluid density:

$$w = \rho Q_V = \frac{\rho \Delta P}{\mathcal{R}_f}. \quad (2.31)$$

The area perpendicular to the direction of flow in a conduit is the cross-sectional area of the conduit, A_c . If A_c is constant for the entire length L of the conduit, the average mass flux can be found by dividing the mass flow by A_c :

$$\text{Average mass flux} = \frac{w}{A_c} = \rho \frac{Q_V}{A_c} = \rho \langle v \rangle = \frac{\rho \Delta P}{\mathcal{R}_f A_c} = \frac{\rho L}{\mathcal{R}_f A_c} \left(\frac{\Delta P}{L} \right). \quad (2.32)$$

The quantity $\langle v \rangle$ is defined as the *average velocity* in the conduit. Since ΔP is the upstream pressure minus the downstream pressure, then $-\Delta P/L$ is the average

pressure gradient in the conduit. Therefore, (2.32) can be interpreted as a macroscopic version of a constitutive relationship between the average mass flux and the average negative pressure gradient, with the transport coefficient equal to $\rho L/(\mathfrak{R}_t A_c)$.

Since heat flows from regions of high temperature to low temperature, an empirical expression for the flow of heat through a material can be written as:

$$\dot{Q} = \frac{\Delta T}{\mathfrak{R}_T}. \quad (2.33)$$

where \dot{Q} is the *flow of thermal energy or heat flow*, ΔT is the temperature difference across the media, and \mathfrak{R}_T is the thermal resistance. The thermal resistance in a solid will depend on geometry and material properties such as thermal conductivity and density. Thermal resistance in fluids will also depend on how the velocity is distributed in the fluid, which in turn depends on other fluid properties, such as viscosity.

If the area perpendicular to the direction of heat flow is constant and equal to A , and the material has length L , then the average heat flux $\langle q \rangle$ will be:

$$\text{Average heat flux} = \frac{\dot{Q}}{A} = \langle q \rangle = \frac{\Delta T}{\mathfrak{R}_{TA}} = \frac{L}{\mathfrak{R}_T A} \left(\frac{\Delta T}{L} \right). \quad (2.34)$$

The average temperature gradient in a solid material under these conditions is $-\Delta T/L$. Consequently, (2.34) can be thought of as a macroscopic version of the constitutive relation for 1D conduction, (2.9). In that case, the thermal resistance can be shown to be inversely proportional to the thermal conductivity of the material ($\mathfrak{R}_T = L/kA$). However, if the material is a flowing fluid, the thermal resistance will also depend on other fluid properties, on the velocity distribution, and on whether the flow is laminar or turbulent. Thus, the macroscopic thermal resistance must account for both convective and molecular heat transfer.

The macroscopic expression for molar flow W_A of species A through a solid material B is:

$$W_A = \frac{\Delta c_A}{\mathfrak{R}_{AB}}, \quad (2.35)$$

where \mathfrak{R}_{AB} is the resistance to the transport of species A in material B and Δc_A is the difference in concentration of species A between the two ends of the material. For a solid material or stationary fluid with length L and with area A perpendicular to the direction of flow, the average molar flux $\langle N_A \rangle$ is:

$$\langle N_A \rangle = \frac{W_A}{A} = \frac{L}{\mathfrak{R}_{ABA}} \left(\frac{\Delta c_A}{L} \right). \quad (2.36)$$

This is a macroscopic version of (2.7), with $\mathfrak{R}_{AB} = L/(D_{AB}A)$ for a solid. However, as in the case of heat transfer, if the material is a flowing fluid, then convective transport mechanisms will contribute to the mass transfer resistance.

Table 2.2 Relationships for 1D macroscopic transport

	Species	Mass	Heat	Electrical charge
Extensive variable (flow)	Molar flow W_A	Mass flow w	Heat flow \dot{Q}	Current flow I
Intensive variable (difference)	Molar concentration Δc_A	Pressure ΔP	Temperature ΔT	Electrical potential ΔE
Empirical relation	$W_A = \frac{\Delta c_A}{\mathfrak{R}_{AB}}$	$w = \frac{\rho \Delta P}{\mathfrak{R}_f}$	$\dot{Q} = \frac{\Delta T}{\mathfrak{R}_T}$	$I = \frac{\Delta E}{\mathfrak{R}_e}$
Constitutive relation	$\langle N_A \rangle = \frac{L}{\mathfrak{R}_{ABA}} \left(\frac{\Delta c_A}{L} \right)$	$\rho \langle v \rangle = \frac{\rho L}{\mathfrak{R}_{fA_c}} \left(\frac{\Delta P}{L} \right)$	$\langle q \rangle = \frac{L}{\mathfrak{R}_{TA}} \left(\frac{\Delta T}{L} \right)$	$\langle i \rangle = \frac{L}{\mathfrak{R}_{eA_c}} \left(\frac{\Delta E}{L} \right)$
Transport coefficient	$L/(\mathfrak{R}_{ABA})$	$\rho L/(\mathfrak{R}_{fA_c})$	$L/(\mathfrak{R}_{TA})$	$L/(\mathfrak{R}_{eA_c})$

The macroscopic transport relationships are summarized in Table 2.2.

The analogous nature of these expressions provides motivation for studying these transport phenomena together.

2.7 Interphase Transport

By interphase transport, we refer to transport across the interface separating two media. For example, we might be interested in the transport of energy, momentum, or species between a swimmer and the water or between blood and the wall of a blood vessel.

Let us consider first the transport of momentum. Since fluid exhibits the phenomenon of “no slip”, the motion of a swimmer’s hand will impart momentum to the fluid in contact with the hand, and because water is viscous, momentum will be transferred from the water in contact with the hand to the water far away from the hand. The flow of momentum has the dimensions of momentum flux multiplied by area. Since momentum flux ρv^2 has the same dimensions as a force per unit area, the force F_s exerted by the hand on the fluid would be expected to be proportional to the product of area and the change in momentum flux:

$$F_s = \frac{f}{2} A [\rho v_s^2 - \rho v_\infty^2], \quad (2.37)$$

where v_s is the velocity of the solid (hand), v_∞ is the fluid velocity, f is defined as a *friction factor*, and A is a characteristic area, defined differently for internal and external flow situations. The factor of 2 arises from the fact that f was originally defined in terms of the kinetic energy per unit volume ($\frac{1}{2}\rho v^2$). In many instances, we are interested in the force exerted by the fluid on a stationary object ($v_s = 0$), such as the force of flowing blood on a vessel wall or the force on a fisherman standing in a flowing river. This force by the fluid on the solid is commonly referred to as the *drag force* ($F_D = -F_s$). In this case, the velocity will vary from zero at the

wall to v_∞ in a thin fluid layer near the solid, referred to as a *boundary layer*. The friction factor will depend on the thickness of the boundary layer, which in turn depends on fluid properties and the average fluid velocity.

For external flow past a stationary body, the drag force is:

$$F_D = fA_f \left(\frac{1}{2} \rho v_\infty^2 \right) \quad (\text{external flow}). \quad (2.38)$$

The area A_f used to define the friction factor for external flow is the frontal area of the object or the area that the object projects onto a plane that is perpendicular to the flow. For internal flow in a conduit, the wetted surface area of the conduit S_w and the average fluid velocity $\langle v \rangle$ in the conduit are used to define the friction factor f . For steady flow through the conduit, the drag force on the conduit wall is equal to the pressure difference across the ends of the conduit ΔP multiplied by the cross-sectional area of the conduit A_c :

$$F_D = \Delta P A_c = f S_w \left(\frac{1}{2} \rho \langle v \rangle^2 \right) \quad (\text{internal flow}). \quad (2.39)$$

This can be used to find the pressure difference across a tube for a given geometry and flow rate. The friction factors for both internal and external flows depend on the geometry of the object and properties of the fluid.

A *thermal boundary layer* will also exist in the fluid region near the interface. This is defined as the region where the temperature varies from the interfacial temperature to a value that is very near the fluid temperature far from the interface. For external flow past a solid object, heat transfer across the interface is governed by *Newton's Law of cooling*. This states that the heat flux across the interface from solid to fluid is proportional to the difference in temperature between the solid surface T_s at the interface and the fluid temperature far from the interface T_∞ :

$$q = \frac{\dot{Q}_s}{S} = h[T_s - T_\infty] \quad (\text{external flow}). \quad (2.40)$$

A positive value of the heat flux q or heat flow \dot{Q}_s indicates heat loss from the surface with area S (cooling). The proportionality factor h is known as the *convective heat transfer coefficient*. For internal flow, the heat transfer coefficient is defined slightly differently:

$$q = h[T_w - T_m] \quad (\text{internal flow}). \quad (2.41)$$

T_m is the mixing cup temperature or the bulk fluid temperature in the fluid flowing through the conduit and T_w is the wall temperature (i.e., interface temperature). T_m is also known as the *flow averaged temperature*, which is the temperature that would be measured if the conduit were cut at the axial location of interest, the fluid collected in a cup, and the temperature of the well-mixed fluid in the cup

measured. The heat flux is positive when heat flows from the wall to the fluid. The interfacial heat transfer coefficient h is a transport coefficient that depends on the thermal boundary layer and is normally determined experimentally.

The flow of species A across a fluid–solid interface is slightly more complex. Within the fluid phase, we can rewrite (2.36) in a manner analogous to Newton’s law of cooling for external and internal flow situations:

$$N_A = k_{Af}([c_{Af}]_S - [c_{Af}]_\infty) \quad (\text{external flow}). \quad (2.42)$$

$$N_A = k_{Af}([c_{Af}]_w - [c_{Af}]_m) \quad (\text{internal flow}). \quad (2.43)$$

The subscripts are analogous to those used for heat transfer, with $[c_{Af}]_m$ representing the flow averaged mixing cup or bulk concentration of species A in fluid f. These expressions serve as definitions for k_{Af} , the *convective mass transfer coefficient for species A in fluid f*. The mass transfer coefficient depends on geometry, fluid properties, and the distribution of velocity in the boundary layer. The factor k_{Af} is the inverse of $\mathcal{R}_{AB}A$ in (2.36). Concentrations in (2.42) and (2.43) reflect concentrations of species A *in the fluid phase*, as indicated by the subscripts “Af”. Similar expressions could also be written for the transport of species A through the solid. Since species A may have a different solubility in the fluid than in the solid, a concentration difference will normally exist between the fluid and solid at the interface, even when the flux of species A is zero. Let us define a *partition coefficient* Φ_{A12} as the equilibrium ratio of concentration of species A in material 1 (c_{A1})_{eq} relative to material 2 (c_{A2})_{eq}:

$$\Phi_{A12} = \left[\frac{c_{A1}}{c_{A2}} \right]_{\text{eq}}. \quad (2.44)$$

In this case, material 1 is the fluid f and material 2 is the solid s. Φ_{Afs} should be interpreted as the partition of species A in the fluid relative to the solid under equilibrium conditions. The order of the last two subscripts is important. Alternatively, we could define a partition coefficient Φ_{Afs} for species A between the solid relative to the liquid under equilibrium conditions:

$$\Phi_{Afs} = \left[\frac{c_{As}}{c_{Af}} \right]_{\text{eq}} = \frac{1}{\Phi_{Afs}}. \quad (2.45)$$

The two partition coefficients are inversely related to each other. If we assume that local equilibrium occurs at the interface, then:

$$[c_{Af}]_{\text{interface}} = \Phi_{Afs}[c_{As}]_{\text{interface}}. \quad (2.46)$$

Although the fluid far from the interface is not in equilibrium with the solid, a key assumption made in interfacial transport is that species A in the fluid and solid are in local equilibrium *at the interface*. For the internal flow situation, the interface

represents the conduit wall. Substituting (2.45) and (2.46) into (2.43) provides an expression for the mass flux in terms of the concentration of A in the solid at the interface and the bulk concentration of A in the fluid:

$$N_A = k_{Af} (\Phi_{Afs} [c_{As}]_w - [c_{Af}]_m) \quad (\text{internal flow}). \quad (2.47)$$

Therefore, the appropriate driving force for the movement of species A across the interface is not $[c_{As}]_w - [c_{Af}]_m$, but rather $\Phi_{Afs} [c_{As}]_w - [c_{Af}]_m$. The convective mass transfer coefficient k_{Af} accounts for both convective and diffusive fluxes.

For external flow situations, the bulk concentration in the liquid is replaced by the concentration far from the wall, $[c_{Af}]_\infty$, and the concentration in the solid at the interface is $[c_{Af}]_s$. The flux of species A from wall to fluid, N_A , can be computed from the empirical relation:

$$N_A = k_{Af} [\Phi_{Afs} [c_{As}]_s - [c_{Af}]_\infty] \quad (\text{external flow}). \quad (2.48)$$

Unfortunately, we rarely know the interfacial concentration in either the fluid or the solid at a solid–fluid interface. For an internal flow application, where the solid represents the conduit wall, it is more common to know the concentration at the outside surface of the conduit wall, $[c_{As}]_o$, rather than the concentration at the inside surface. Applying an analog of (2.43) to the flux of species A through the conduit wall:

$$N_A = k_{As} ([c_{As}]_o - [c_{As}]_w). \quad (2.49)$$

The factor k_{As} is a mass transfer coefficient governing the transport of species A in the conduit wall. It is directly proportional to the diffusion coefficient D_{As} for species A in the wall material. Assuming steady-state transport, we can eliminate $[c_{As}]_w$ from (2.47) to (2.49), to provide the flux in terms of the outside wall concentration and the bulk fluid concentration:

$$N_A = P_A (\Phi_{Afs} [c_{As}]_o - [c_{Af}]_m). \quad (2.50)$$

P_A is defined as the *permeability of species A* and is related in this case to the mass transfer coefficients in the fluid and solid as follows:

$$\frac{1}{P_A} = \frac{1}{k_{Af}} + \frac{\Phi_{Afs}}{k_{As}}. \quad (2.51)$$

In biotransport applications, we are often interested in finding the flux of solutes from one fluid region to another across a barrier, such as a cell membrane or a capillary wall. This actually involves transport across three barriers in series: two fluid–solid interfaces and a barrier material. Although the concentrations at either fluid–barrier interface are not generally known, an analysis that includes all three

Table 2.3 Interphase transport relationships

	Species	Momentum	Heat
Through variable (flux)	Molar flux N_A	Momentum flux F_{Dx}/A	Heat flux q
Across variable (external)	Molar concentration $[c_{Af}]_S - [c_{Af}]_\infty$ or $\Phi_{Afs}[c_{As}]_S - [c_{Af}]_\infty$	KE per unit volume $\frac{1}{2}\rho v_\infty^2$	Temperature $T_S - T_\infty$
Across variable (internal)	Molar concentration $[c_{Af}]_w - [c_{Af}]_m$ or $\Phi_{Afs}[c_{As}]_w - [c_{Af}]_m$ (interface) or $C_{A2} - \Phi_{A21}C_{A1}$ (across barrier)	KE per unit volume $\frac{1}{2}\rho\langle v \rangle^2$	Temperature $T_w - T_m$
Transport coefficient	Mass transfer coefficient k_{Af} or P_A	Friction factor f	Heat transfer coefficient h

barriers (see Chap. 12) allows us to express the flux from side 2 to side 1 in terms of bulk concentrations on the two sides of the barrier, $[c_{A1}]_m$ and $[c_{A2}]_m$:

$$N_A = P_A([c_{A2}]_m - \Phi_{A21}[c_{A1}]_m) = P_A(C_{A2} - \Phi_{A21}C_{A1}). \quad (2.52)$$

We use an uppercase “C” to refer to mixing cup or bulk concentrations in the two fluids. The *permeability* P_A of the membrane to species A is an overall mass transfer coefficient that includes effects of the boundary layers on each side of the barrier and conductance through the barrier itself.

A summary of empirical relationships used to describe interfacial transport of momentum, species, and heat is shown in Table 2.3.

2.8 Transport in Biological Systems: Some Unique Aspects

Transport phenomena are studied by students in many disciplines of engineering and science, and they are analyzed and used in design by professionals in a very wide range of occupations. Although the spectrum of applications in transport is large, there is a common thread of principles and methods that runs through all of these different domains. However, it is our observation over decades of research and teaching that biotransport tends to fall at an extreme end of this spectrum owing to unique features of the systems that are frequently encountered.

In multiple ways, biological and biomedical systems tend to give rise to more complex transport processes than do inanimate systems. It is helpful to be aware of some of the more commonly encountered features unique to living systems to plan

the best problem-solving strategies. The following list is not exhaustive, but it presents a flavor of some of the characteristics and behaviors that can make dealing with biological systems challenging.

- Biotransport often occurs in systems having irregular-shaped geometries. Organs, limbs, muscles, tissues, vasculature and respiratory networks, bones, and many other biological structures have shapes that are asymmetric, curvilinear, and three-dimensional. These geometries are typically not compatible with standard coordinate systems, requiring simplifying assumptions, approximations to closed form mathematical solutions, or numerical solution methods such as finite difference and finite element that can accommodate specific geometries via meshing techniques.
- Many biotransport processes are nonlinear in which the behavior is not a simple function of the inputs that cause a process to occur. As a consequence, the constitutive relations that describe these behaviors can introduce mathematical functions that are difficult to incorporate into analytical functions. An example is that blood flow can be altered drastically as a function of many different tissue properties such as temperature, pressure, and mechanical stress, as well as systemic functions such as heart rate and muscle work level. As a consequence, the behavior of a system can be altered due to internally driven changes causing nonlinear function. Again, numerical and approximation methods can be applied to obtain a solution.
- Nearly all biological materials are composite, consisting of areas that have differing properties. Since the spatial domain is not homogeneous, it is difficult to apply a simple analytical solution for the entire process. At material interfaces it is necessary to ensure that the boundary conditions embody both continuity of potential (such as concentration and temperature) and flow (such as molecules and heat).
- Many biological materials have anisotropic properties, meaning that their behavior is directionally dependent. This is another feature that makes the use of closed form analytical solutions problematic.
- Some biological systems may change their properties and/or phase state during a process in response to imposed stresses. Examples are the denaturation of molecules at elevated temperatures and the freezing of tissues at subzero temperatures. The result is that there can be dramatic changes in properties over both time and position during a process.

Since all of these unique features of biological systems make the most simple closed form analytical solutions problematic, numerical simulations find very widespread use in biomedicine. Fortunately, there now exists commercial software that is powerful and user friendly so that the difficult process of self-generating code is no longer an impediment in many cases. The theory behind the use of these advanced techniques is largely beyond the scope of this introductory text. Many excellent sources are available that present directions and details for these methods.

All of these phenomena require that special experimental methods be applied to characterize the phenomena and to measure the relevant transport properties. The availability of accurate constitutive property values is important in successfully modeling and solving biotransport problems. Despite these complexities, the fundamental principles and methods of analysis presented in this text will provide a good starting point for approaching all biotransport problems and will often provide good first-order approximations to their solutions.

2.9 Summary of Key Concepts

In Chap. 1, we presented the Generate Ideas Model, which provides a systematic way of thinking about a biotransport problem before attempting to solve the problem. In this chapter, we consider the essential components of the problem that should be resolved before a formal analysis is attempted.

Fundamental Concepts. We introduce the fundamental concepts that define the field of biotransport, and will refer back to these over and over again throughout the text. In Sect. 2.2 we discuss how to define the system of interest and all of the interactions that the system has with the environment at the system boundaries. We define the extensive transport properties that cross the boundaries and the intensive properties that tend to cause the motion. In Sect. 2.3, we discuss how to identify the appropriate scale of interest. The two scales of interest in most biotransport applications are the macroscopic scale, in which average properties are of interest, and the microscopic scale, in which spatial variations in properties are of interest.

Conservation Relationships. Once a system and the appropriate transport properties have been identified, and a scale selected, the appropriate conservation relationship for each extensive property must be selected. General conservation principles applied to mass, momentum, energy, species, and electrical charge can be stated simply as in (2.2):

$$\left\{ \begin{array}{c} \text{Rate of} \\ \text{accumulation} \\ \text{of the quantity} \\ \text{within a system} \end{array} \right\} = \left\{ \begin{array}{c} \text{Net rate the} \\ \text{quantity is produced} \\ \text{within the system} \end{array} \right\} + \left\{ \begin{array}{c} \text{Net rate the} \\ \text{quantity enters} \\ \text{through the} \\ \text{system boundary} \end{array} \right\}.$$

Constitutive Relationships. The final components that must be assembled before a biotransport problem can be analyzed are the constitutive relationships that govern the transport of extensive properties across the system boundaries. For microscopic systems, the molecular flux of an extensive property is proportional to the negative gradient of an appropriate intensive property, given by (2.4):

$$\text{Flux}_n = (\text{constitutive property}) \cdot \left[-\frac{\partial(\text{potential})}{\partial n} \right].$$

The flux of an extensive property is defined as the rate the property crosses a boundary per unit time per unit area of the boundary. Specific examples that will be used often in this text are Newton's law of viscosity (2.13), Fourier's law of thermal conduction (2.9), Fick's law of diffusion (2.7), and Ohm's law of electrical conduction (2.11). The analogies between these molecular transport mechanisms are summarized in Table 2.1 and in Sect. 2.5.1.3, providing motivation for studying these concepts together. If the process involves fluid motion, then we must consider convection of the properties of interest in addition to molecular motion (Sect. 2.5.2).

Macroscopic Relationships. In macroscopic applications, the constitutive relationship often relates flow of an extensive property to a difference in the potential across the system:

$$\text{Flow} = \frac{\Delta(\text{potential})}{\mathfrak{R}},$$

where \mathfrak{R} is the resistance to flow. These relationships are summarized in Table 2.2.

Transport Coefficients (Internal Flow). When fluid flows past an object, the empirical relationships that govern transport from the fluid in contact with the boundary and fluid far from the boundary can be summarized as:

$$\text{Flux} = (\text{transport coefficient}) \cdot (\Psi_s - \Psi_\infty) \text{ (external flow)}.$$

For heat transfer applications, this is known as Newton's law of cooling, with the flux equal to the heat flux q away from the surface, the transport coefficient equal to the heat transfer coefficient h , Ψ_s equal to the surface temperature, and Ψ_∞ equal to the temperature in the fluid far away from the system surface. For mass transfer applications, the flux represents the flux of species A, N_A , away from the surface, the transport coefficient is called the mass transfer coefficient k_A , and the potential difference is the difference in concentration between the fluid in contact with the system surface and fluid far from the surface. In fluid momentum applications, the flux represents the momentum flux or shear stress at the wall, the transport coefficient is the friction factor, and the potential difference is the kinetic energy per unit mass of the fluid flowing past the object.

Transport Coefficients (External Flow). If the fluid flows inside a conduit, the flux at the surface is given by the following expression:

$$\text{Flux} = (\text{transport coefficient}) \cdot (\Psi_w - \Psi_m) \text{ (internal flow)}.$$

The potential difference in this case represents the difference between the potential at the wall and the mean (flow averaged or mixing cup) potential in the fluid flowing through the conduit. The analogous expressions are given in Table 2.3.

Interphase Transport. The analogy between heat and mass transport breaks down when dealing with macroscopic transport from one phase to another or across a barrier connecting two materials. In general we can write:

$$\text{Flux}_{1 \rightarrow 2} = (\text{transport coefficient}) \cdot (\Psi_{1m} - \Phi \Psi_{2m}) \text{ (across barrier)}.$$

The subscripts “m” refer to mean properties in the materials. The factor Φ equals unity for the case of heat transfer and equals the equilibrium partition coefficient between materials 1 and 2 (2.44) for the case of mass transfer.

2.10 Questions

- 2.10.1. Why do we study momentum, heat, and mass transfer together?
- 2.10.2. Distinguish between a closed system and an open system.
- 2.10.3. What separates a system from the environment?
- 2.10.4. Distinguish between intensive (intrinsic) and extensive (extrinsic) properties and give examples of each.
- 2.10.5. Distinguish between macroscopic and microscopic approaches to transport problems. Which independent variables will not appear in macroscopic problems?
- 2.10.6. Should a microscopic or a macroscopic species mass balance be used to determine blood concentration as a function of position from the inlet of an alveolar capillary sheet? Justify your answer.
- 2.10.7. Under what circumstances can matter be treated as a continuum?
- 2.10.8. Give an example where the assumption that matter can be treated as a continuum is probably invalid.
- 2.10.9. Write the general expression for the conservation of a quantity “X” in a system.
- 2.10.10. Which conservation statement describes the conservation of oxygen inside a red blood cell?
- 2.10.11. Can a system in equilibrium with its surroundings exchange mass, energy, or momentum with the surroundings?
- 2.10.12. Two systems are in equilibrium. Can the temperatures of the two systems be different? Can the concentrations of species “A” in each system be different?
- 2.10.13. Can a system that is in equilibrium with its surroundings have a temperature gradient at the system boundary?
- 2.10.14. Explain the negative sign in the molecular flux vs. gradient expressions for momentum, heat, and species transport.
- 2.10.15. How do molecular and convective transport mechanisms differ?
- 2.10.16. Distinguish between flux, diffusive flux, and convective flux for mass transfer of species “A.”
- 2.10.17. What are Newton’s Law of viscosity, Fick’s Law of diffusion, and Fourier’s Law of conduction? What quantities in these equations are analogous? Define any symbols used.
- 2.10.18. What transport mechanisms are involved in lung CO₂ exchange?
- 2.10.19. Which *gradients* influence the total passive flux of Cl[−] ions through a channel in a cell membrane? (Assume that there is a net flow of water through the same channel.)

- 2.10.20. In an electrical system, current is the “flow variable” while a voltage difference provides the driving force. A fluid mechanics system may be modeled similarly if we treat volumetric flow as the flow variable and which variable as the driving force?
- 2.10.21. Distinguish between resistance and conductance.
- 2.10.22. How are heat transfer and mass transfer coefficients defined for internal and external flow situations?
- 2.10.23. What area is used when converting fluxes to flows?
- 2.10.24. How is a heat transfer coefficient related to thermal resistance?
- 2.10.25. What factors influence heat and mass transfer coefficients for internal and external flow situations?
- 2.10.26. Two materials in contact are assumed to be in “local equilibrium” at the interface. What does this mean in terms of the temperature of each material at the interface? What does this mean in terms of the concentrations of nonreacting chemical species in each material at the interface?
- 2.10.27. The concentration of O_2 in a cell membrane is higher than the concentration of O_2 in the intracellular fluid. O_2 will: (a) be transported into the cell, (b) be transported out of the cell, (c) not be transported into or out of the cell, or (d) not enough information is given. Justify your answer.
- 2.10.28. The concentration of CO_2 in the cell membrane near the intracellular side is higher than the concentration of CO_2 in the membrane near the extracellular side. CO_2 will: (a) be transported into the cell, (b) be transported out of the cell, (c) not be transported into or out of the cell, or (d) not enough information is given. Justify your answer.
- 2.10.29. Species A can diffuse from material B to material C even though the concentration of A in C is higher than the concentration of A in B if: (a) the solubility of A in C is higher than the solubility of A in B; (b) the solubility of A in B is lower than the solubility of A in C, (c) the solubility of A in B is equal to the solubility of A in C, or (d) species A cannot move from B to C under these circumstances
- 2.10.30. What is a partition coefficient? Why is it important? Explain the subscript convention used for Φ_{ABC} .
- 2.10.31. Why doesn't the partition coefficient appear in equations (2.42) and (2.43)? Why does it appear in (2.47) and (2.48)?
- 2.10.32. What factors affect membrane permeability?

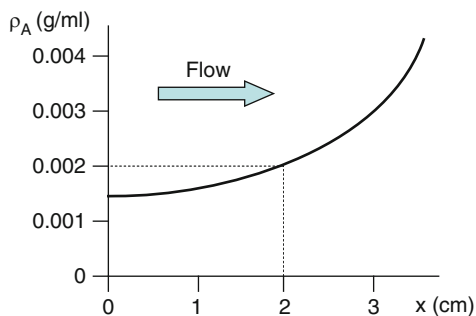
2.11 Problems

2.11.1 Transport Examples

Identify one specific example each of heat, mass, and momentum transport in a mammalian system. Briefly describe each example and identify the driving force and the resistance. In each example, identify a parameter that can change in value,

how that parameter is likely to change, and the effects of that change on heat, mass, or momentum transfer in your example.

2.11.2 Convective and Diffusive Fluxes



A solution containing species A in water moves to the right with a mass average velocity of 0.06 cm/min. Species A obeys Fick's law with a diffusion coefficient of 10^{-5} cm²/s. The mass concentration of species A vs. position is shown in the figure. Find the diffusion flux and convective flux of species A at the position $x = 2$ cm. Is the total flux of A greater or less than the convective flux of A? Justify your answer.

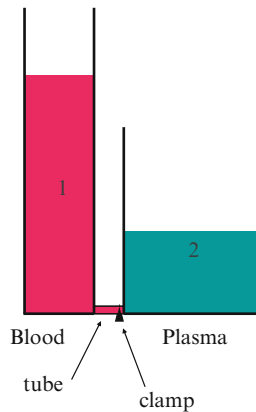
2.11.3 Relation Between Macroscopic and Microscopic Transport Coefficients, Heat Transfer

Show that the resistance to heat transfer is inversely proportional to the thermal conductivity, $\mathcal{R}_T = L/kA$, for steady-state, 1D conduction through a slab of material with thickness L and cross-sectional area A .

2.11.4 Relation Between Macroscopic and Microscopic Transport Coefficients, Mass Transfer

Show that the resistance to mass transfer is inversely proportional to the diffusion coefficient, $\mathcal{R}_{AB} = L/D_{AB}A$, for steady-state, 1D diffusion of species A through a slab of material B with thickness L and cross-sectional area A .

2.11.5 Conservation Principles



Blood in reservoir 1 is separated from plasma in reservoir 2 by a rubber tube, which is initially clamped. The height of blood in reservoir 1 is greater than the height of plasma in reservoir 2, and the initial blood temperature is different than the initial plasma temperature. The hematocrit value (i.e., ratio of cell volume to total volume) of the blood in reservoir 1 is 0.45. After the clamp is released, blood from reservoir 1 flows into reservoir 2. We wish to predict how the following factors vary with time: height in each reservoir, pressure difference across the tube, blood flowrate from reservoir 1 to reservoir 2, hematocrit value in each reservoir, and temperature in each reservoir. How would you go about setting up this problem? What principles will you apply? What assumptions will you make? What additional information do you need?

2.11.6 Conservation and Chemical Reaction

Species A and species B are added to a well-mixed volume of water V , where they combine chemically $A + 2B \rightarrow C$. Write molar conservation equations for each species if the rate of production of species C (mol/s) is proportional to the product of the molar concentration of A and the molar concentration of B squared. The proportionality factor is k . What additional information do we need to know before we can predict the concentrations of A, B, and C as functions of time? (Do not solve).

2.11.7 Measurement of Lung Gas Volumes

A pneumotachograph is a device used to measure airflow at the mouth. Air flow rate is computed from the pressure drop measured across a fixed resistance such as a fine screen or honeycomb structure during breathing. Integration of the flow provides the

volume of air that passes through the mouth. The amount of air left in the lung after a maximal expiration is known as the residual volume (RV). The amount of air in the lung at the end of a maximal inspiration is known as the total lung capacity (TLC). The amount of air left in the lung at the end of a normal expiration is known as the functional residual capacity (FRC). FRC, TLC, and RV cannot be detected with a pneumotachograph since all of the air in the lung does not flow through the device. However, several important lung volumes can be measured with this device. Design a procedure that uses a pneumotachograph to measure the following lung volumes:

- (a) Expiratory reserve volume (ERV) = $FRC - RV$
- (b) Inspiratory capacity (IC) = $TLC - FRC$
- (c) Tidal volume (TV) = volume at the end of a normal inspiration minus FRC
- (d) Inspiratory reserve volume (IRV) = $IC - TV$
- (e) Vital capacity (VC) = $TLC - RV$

2.11.8 Measurement of FRC or RV

FRC or RV cannot be measured using a pneumotachograph, since, by definition, RV cannot pass through the device. These volumes can be detected by breathing in a gas mixture containing a small amount of a tracer gas that does not penetrate the alveolar wall. Apply conservation of tracer before and after inspiring a gas mixture with known volume and tracer concentration to estimate the total volume of gas in the lung. Describe a procedure that involves the pneumotachograph and inspiration of the gas mixture to compute FRC or RV. Neglect the volume of the conducting airways in relation to alveolar volume.

2.11.9 Continuum Concepts

The volume of air that contains 1,000 molecules at standard temperature and pressure is approximately $4 \times 10^{-7} \text{ cm}^3$. This is small enough that we can consider it to be a “point” in space. Outer space consists primarily of hydrogen atoms with a density of $1.66 \times 10^{-24} \text{ g/cm}^3$. What volume of outer space contains 1,000 molecules? Compare that with the volume of air above.

2.12 Challenges

2.12.1 Preliminary Research, Design of a Heart–Lung Machine

Background: New surgical devices and procedures have helped to improve cardiac care of many patients. Open heart surgery requires opening the chest cavity which collapses the lungs, and the heart is usually stopped so that a surgeon can perform

techniques such as a bypass or valve replacement. The functions of the heart and lung must be maintained, not to mention preservation of the heart tissue once it has stopped beating. A young biotechnology company produces various medical devices such as IV units and blood filtration systems. They believe that they could use some of their technology to design an advanced heart lung machine. The company hires you, a biomedical engineer, to conduct a feasibility study. *Challenge:* You are to determine which major components the system should contain, and you must consider the potential design challenges these systems may encounter while interfacing with the human body. *Generate Ideas:* What are the important system variables that you should consider in your design? What system components would you recommend? If these components were placed in series, in what order would you place them? Why?

2.12.2 Alternate Applications for a Device

The company that hired you as a consultant on a heart–lung machine project is concerned that an open heart surgery application for the proposed device is too specialized. *Challenge:* Are there other applications that you might suggest that will expand the market for this device? *Generate ideas:* Use the transport principles presented in this chapter to provide a list of applications that might convince the company executives to build the device.

2.12.3 Design of a Heart–Lung Machine

The company decides to move ahead with the project and assigns you to lead the team that designs and builds the machine. *Challenge:* Suggest preliminary designs for each subsystem. *Generate Ideas:* Estimate specific input values for each subsystem. What are the desired output variables of each subsystem? Suggest a specific design for each subsystem that can provide the desired outputs. What conservation relationships are relevant for each subsystem? What constitutive relationships are relevant for each subsystem? What additional information will you need before you can actually design a heart–lung machine that provides the desired outlet variables?

2.12.4 Heat Loss by Conduction

The temperature difference across the skin layer of a resting individual is measured to be 1°C. *Challenge:* Assuming all steady-state heat loss from the body is by conduction through the skin, estimate basal metabolic rate (BMR) of the body. *Generate Ideas:* What general principle governs the conduction of heat through the skin? Should we use a macroscopic or microscopic approach to determine heat flow

through the skin? What system should be analyzed to determine BMR? What conservation principle applies? What additional information is required if we are to solve this problem? Search the literature to find this information and estimate BMR. Compare this with values found in the literature and provide explanations if the values are different.

2.12.5 Respiratory Heat Loss

Tidal volume for an average human is of 500 ml of air and normal breathing rate is about 12 breaths/min. *Challenge:* What is the rate that heat is lost via respiration if inspired air at 20°C is heated to body temperature by the time it is expired? *Generate Ideas:* What system should be analyzed? What assumptions will you make? Is a macroscopic or microscopic analysis appropriate? What additional information is needed? Perform a literature search to find any missing information and estimate the respiratory heat loss. What fraction of normal heat generated by the body does this represent?

References

Schmid-Schönbein GW, Diller K (2005) Transport processes in biomedical systems: a roadmap for future research directions. *Ann Biomed Eng* 33:1136–1141

<http://www.springer.com/978-1-4419-8118-9>

Biotransport: Principles and Applications

Roselli, R.J.; Diller, K.R.

2011, XX, 1286 p. 578 illus., 305 illus. in color.,

Hardcover

ISBN: 978-1-4419-8118-9