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P. A. Ramachandran
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Introduction

Learning objectives

You will learn from this chapter

- the basic concepts and the framework for analysis of transport problems;
- the notion of conservation laws and the transport laws, including their use in setting up models for some simple problems in transport;
- the various hierarchical levels (micro, meso, and macro) at which the models for transport processes can be developed;
- the interrelation between models of different levels;
- the need for and the definition of parameters such as friction factors and heat and mass transfer coefficients for macro- and meso-scale models;
- the range of application areas where the transport phenomena and the models have been and can be used.

Mathematical prerequisites

- The notion of scalars and vectors.
- Common coordinate systems (rectangular, cylindrical, and spherical) and the notion of components of vectors in various coordinates.
- The gradient of a scalar field and its physical significance.
- The dot product of two vectors.
- The definition and meaning of the directional derivative.
- The expression for gradient in common coordinate systems.

The goal of this chapter is to introduce the scope of the subject matter of transport phenomena, which essentially deals with flow of fluids, flow of heat, and flow of mass. This subject provides us with the basic tools to build models for systems or processes. These tools find application in a wide range of areas drawn from different disciplines. The analysis of transport processes which you will learn from this book

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can be effectively used in these areas. At the end of this chapter we will provide a run-down of some of these important areas of applications.

The chapter starts off with an introduction of the basic methodology of analysis and modeling of transport processes. Some important definitions and terminology that will reappear throughout the text are presented. Since transport phenomena are closely related to model development, we then provide a general discussion on the (philosophy of) modeling of processes and systems. The need for modeling at different levels and scales is emphasized and ”information flow” from one scale to another is discussed. Simple examples are then given to show how models of different levels can be developed and what information is needed to complete the model formulation. These examples are important in order to get a feel for the problems which we will study in detail in later chapters and hence it is sufficient to understand only the basic ideas from this chapter. The idea is to start speaking the language. The problems at the end of the chapter will help you to practice the words. If you have already taken similar undergraduate courses, you can use these problems as a refresher.

Transport models are developed on the basis of a continuum hypothesis, assuming that matter is distributed continuously in space. Hence the molecular structure of matter is not reflected in the analysis and is captured by using transport properties. Some common transport properties are the viscosity and thermal conductivity of the fluid/material and diffusion coefficients. These properties are, however, related to the molecular structures of the species under consideration. Hence an understanding of the molecular-level models and how they can interact with transport-phenomena models is important, and a brief introduction is provided in this chapter. The detailed study of molecular models is outside the scope of this book.

The chapter concludes with a brief indication of the historical developments in transport phenomena and some thoughts on the future.

1.1 What, why, and how?

1.1.1 What?

The subject matter of transport phenomena is the unified study of the heat, mass, and momentum transport and applications to systems of importance in engineering analysis. Traditionally this subject has been a core course in chemical engineering education but it is now an integral part of most branches of engineering.

Most chemical transformation and biological processes involve one or all of the above-mentioned transport processes: the momentum transport (fluid flow), transport of heat, and mass diffusion and convection. These processes are often accompanied by chemical reactions as well. Hence a unified study of the principles governing these transport processes provides an underpinning for the development of process models and system analysis. Such a study is the focus of this book. Some application areas are indicated in Section 1.9 to indicate the range of problems amenable to this type of analysis.

Transport phenomena are encountered in our everyday life. In the morning we boil a pot of water to make the coffee, which is a two-phase heat-transfer process with a phase change.

What is the rate of boiling as a function of the rate of heat input?

We then add a lump of sugar to the coffee. If we do not stir the cup, the sugar dissolves by a process of diffusion. If we stir it, the dissolution takes place by the combined action of diffusion and convection.

How much time is needed to dissolve the sugar?

The car we drive to work is fitted with a catalytic converter, which is a set of flow channels coated with an active layer of catalyst such as Pt. This is an example of a flow system accompanied by mass transfer and chemical reaction to reduce the pollutants such as CO, NO_x, etc. The extent of pollutant removal depends on the flow rate of the gas, the temperature, the rate of mass transfer to the catalytic surface, and the rate of reaction at the surface itself.

How does the extent of pollutant removal change with the gas flow rate in the channel? How does it vary in the start-up period when the engine is cold?

The heart of the computer you use is made of a silicon chip, but the electronic activity arises due to the fact that the chip has undergone a diffusion process to incorporate phosphorus, boron, or other dopants.

If phosphorus diffusion is done for 2 hours, to what depth does phosphorus penetrate into the silicon substrate?

Relation to system analysis

Transport phenomena can be viewed as a subset of the general field of mathematical modeling and system analysis. Mathematical modeling involves the quantification of a process and developing an understanding of it. System analysis involves relating the effects of the input variables to the system outputs. Transport phenomena are closely related to these subjects; of course one deals primarily with chemical and biological systems. A system is an interconnected entity intended to achieve a desired objective. The human body can be thought of as a very complex and well-designed biological system. A simple example of a chemical system is a packed-bed reactor, which is simply a tube packed with solid catalyst particles. A knowledge of transport-phenomena principles is an essential prerequisite to build such system models. This connection of transport with modeling and system analysis is not often clearly stated and emphasized in some textbooks. You should always keep the perspective of system analysis when you study the various transport processes in this book. Thus one of the goals of this study would be to understand the basic principles so that you can build a mathematical model for a given system. You can then use this model for various purposes as discussed later in Section 1.6.

1.1.2 Why?

Three distinct subjects, *viz.* fluid dynamics, heat transport, and mass diffusion, are studied together in transport phenomena. Why should they be studied together rather than in three separate courses? The answer is the basic premise that all three modes of transport can be analyzed using the same (or similar) methodology. In fact, a close analogy exists between the model equations which describe the transport of heat and mass, and these models are often used interchangeably with only changes in the definitions of the parameters. The analogy between momentum transport and heat/mass transfer is not so close, which will become evident as we go along. In spite of this and some other differences, the method of problem formulation and solution techniques for all three modes of transport are closely related and therefore provide motivation for a unified study.

A second reason for a unified study is that systems of practical importance rarely have only one mode of transport. Thus a basic problem in momentum transfer is the flow of a fluid in a pipe under isothermal conditions. But in process industries the flow is often accompanied by heat transfer or mass transfer, and the system may also undergo a chemical transformation. Hence all three modes of transport often need to be analyzed together. A unified study is therefore very important and provides the framework to analyze such coupled effects in a systematic manner.

Examples of coupled problems

As an example consider the hot-water radiator which is used in many old homes in St. Louis. This can be a blessing on a chilly wintry night but certainly puts a burden on the utility payments in the winter and indirectly contributes to global warming. But here we are more interested in the mechanism of heat transfer from hot water to air. The phenomenon is referred to as natural convection heat transfer. Here the heat is transferred from the water to the surface of the radiator. The heat is then transferred from the surface to air by conduction, and the air gets heated. The hot air rises due to buoyancy, creating a natural circulation flow in the system. The flow in turns causes additional heat to be transferred from the radiator to air by convection, and hence the process has a feedback effect due to the coupling between the momentum transfer and heat transfer. The rate of heat transport cannot be calculated in isolation, and one needs information on the velocity profile, which in turn depends on the rate of heat transfer. An illustrative plot of the upward fluid velocity and temperature distribution near a hot vertical plate is shown in Fig. 1.1 and serves as a prototype problem in natural convection heat transfer, which is a coupled problem in flow and heat transfer.

As a second example, consider a continuous-flow tubular reactor. This is simply a tube into which the reactants are fed at one end and from which the products are withdrawn at the other end. Now, in a fluid, the different fluid elements have different (axial) velocities, with the fluid at the center of the tube moving a lot faster than the fluid near the walls. The extent of reaction depends on the residence time of the fluid elements, as discussed later, and hence is different at different radial positions in the tube. The difference in the extent of reaction at various locations sets up a concentration difference, which causes diffusion to occur. Hence it is obvious that the performance of a tubular reactor is strongly affected by the fluid flow pattern in the tube and by mass diffusion. Chemical kinetics (the rate at which a species reacts) alone is not sufficient to predict the reactor's performance. Reactions are also either exothermic or endothermic; therefore, the extent of heat generation, the rate of heat transport, and the temperature distribution in the reactor are also of importance. It may be noted that the rate of reaction is usually an exponential function of temperature, and hence this coupling can be quite strong. Thus we encounter here a coupled problem involving flow and heat and mass transfer accompanied by a chemical reaction, which can

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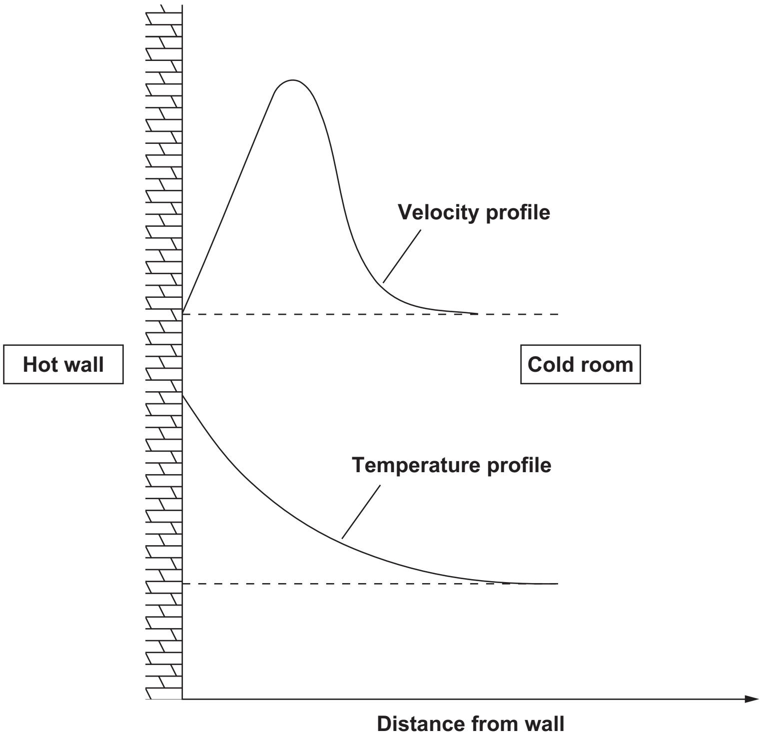

Figure 1.1 A simple example of a coupled momentum and heat-transfer problem, namely natural convection near a radiator. Velocity and temperature profiles near a hot vertical plate are shown schematically, and later we shall calculate these.

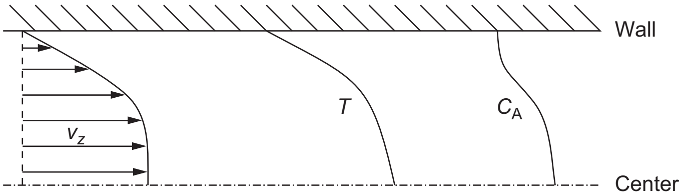

Figure 1.2 Schematic velocity, temperature, and concentration profiles in a tubular reactor. An example would be a polymerization reactor where the molecular weight (more formally, relative molecular mass) changes as the reaction proceeds, causing a dramatic change in fluid viscosity. This significantly alters the velocity profile in the reactor, which in turn affects the temperature and concentration profiles.

be quite challenging to compute. It can be said without exaggeration that the central theme in reactor design and scaleup is the question of how to evaluate the coupling between transport and chemical reaction.

Illustrative velocity, temperature, and concentration profiles in a tubular reactor with an exothermic reaction are shown in Fig. 1.2.

How do we calculate these? What are the governing equations?

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1.1.3 How?

This is the main focus of the book. It will be shown that the analysis can be done on many levels and at many scales as well. But the basic methodology is to define a control volume and then apply the basic conservation laws of physics to this control volume. The conservation laws are the energy balance (heat transport), the mass balance for total mass and for each species constituting the mixture (mass transport), and Newton's second law (momentum transport).

A system or control volume can be defined as any part of the equipment, the entirety of the equipment, or even a large-scale system as a whole. The basic conservation laws apply to the system. Thus the total mass and energy content of the system are conserved. The change in a species' mass depends on the extent of chemical reaction that the species has undergone. The rate of change of momentum in the system has to be balanced by the forces acting on the system in accordance with Newton's second laws. These are universal principles of physics. The application of conservation laws is, therefore, the starting point of each analysis of transport processes. Translation of these principles into mathematical equations leads to a basic model for the system.

The system model based on the application of conservation laws alone (which we call the basic model) is, however, not complete. Additional equations governing the rate of transport are needed, which are referred to as constitutive equations or, more generally, as transport models. These equations are specific to the chemical composition of the system and are not universal, unlike the conservation laws. Basic models supplemented with transport laws then provide the system model. The methodology can therefore be shown in the simple-minded diagram illustrated in Fig. 1.3. We first elaborate on the use of conservation laws to start building the model.

1.1.4 Conservation statement

The conservation principle is rather simple. For example, the total mass is conserved in the system. Mass can enter and leave through the system boundaries, which are also called control surfaces. Mass can also accumulate in the system if the control volume size is changing in time. The conservation law is simply a balance of these quantities as discussed below.

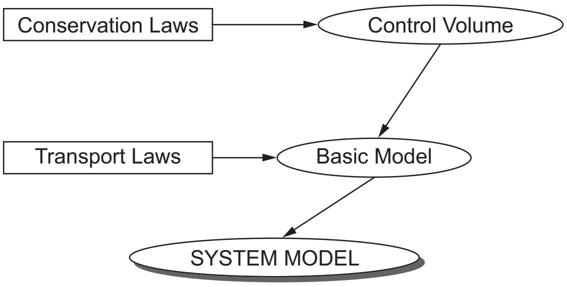

Figure 1.3 A schematic flowchart of the basic methodology for development of system models.

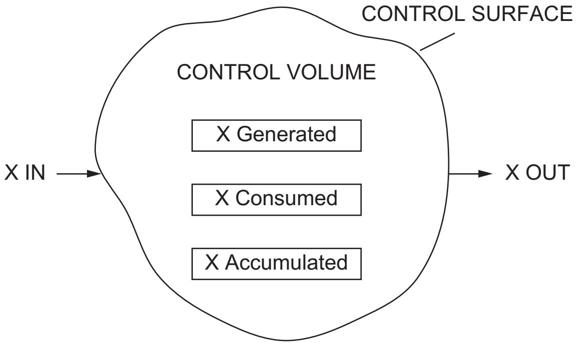

Figure 1.4 A schematic sketch of the conservation principle applied to a control volume.

Consider any quantity X of interest. Then the law of conservation of this quantity can be stated in words as follows:

$$\boxed{\textit{Input} + \textit{Generation} = \textit{Output} + \textit{Depletion} + \textit{Accumulation}}$$

The simple-minded statement written above is of fundamental importance and will be used extensively in this book. The statement is shown pictorially in Fig. 1.4.

The input and output terms represent the interaction of the control volume and the surroundings. Thus heat, mass, or momentum can flow in or out of the control volume or "diffuse" across the control surface boundary. Transport due to flow across a control surface boundary is called convective transport, and the rate of transport is readily calculated if the velocity at that point is known. This will be elaborated on later. Transport can also take place at a molecular level, and this is referred to as diffusive transport. Additional equations are needed in order to calculate the rate of transport by this mechanism. These laws are called constitutive laws. Commonly encountered transport laws are now enunciated, and the need for such laws is indicated.

1.1.5 The need for constitutive models

If there is a temperature difference between the two points on either side of a control surface, it is a common observation that heat moves in or out of the control surface depending on the direction of the temperature gradient. In addition, if there are concentration differences in the system then it is observed that the matter tends to move from regions of higher concentration to those of lower concentration. Finally, if two fluid layers are moving at different velocities, the faster-moving layer tends to drag the slower-moving layer; in other words, there is a drag force on the slower-moving layer (and *vice versa* on the faster-moving layer due to Newton's third law). This force can be viewed as an exchange of momentum between the two points where a velocity difference exists.

Equations describing the rate of transport indicated in the preceding paragraph are called the constitutive laws or simply transport laws. These laws have to be included in the basic model of the system to describe the rate of heat/mass/momentum crossing the control surface. Hence a system model can be developed by combining the constitutive equations and the conservation laws as indicated earlier in Fig. 1.3.

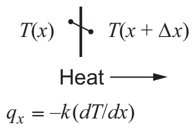

Figure 1.5 An illustration of Fourier's law of heat conduction: a temperature gradient drives heat transport.

1.1.6 Common constitutive models

Fourier's law

Consider the situation shown in Fig. 1.5, where there exists a temperature difference between two points separated by a distance Δx (on the adjacent side of a control surface for instance). Then there will be a heat flow across surfaces, which can be modeled by Fourier's law of heat conduction. This law states that the heat flux is proportional to the negative of the temperature gradient:

$$\boxed{q_x = -k\frac{dT}{dx}} \tag{1.1}$$

Here q_x is the heat flux, which is defined as the heat transported per unit time per unit transfer area in the x-direction. The units would then be $\mathrm{J/s \cdot m^2}$ or $\mathrm{W/m^2}$ in the SI system. The parameter k is a constant of proportionality, which relates the heat flux to the temperature gradient and is called the thermal conductivity. By matching the units on both sides we find that k has the units of $\mathrm{W/K \cdot m}$.

The magnitude of k varies widely for different materials and is dependent on the molecular structure of the system. This shows that the transport properties are closely linked to the molecular nature of the matter.

Later we will extend Fourier's law to the case of heat flow in all three coordinate directions, and this will require the definition of the gradient of a scalar field and the notion of a directional derivative.

> **Historical vignette.** The law was proposed by Fourier in 1807 in a landmark paper entitled "On the propagation of heat in solid bodies". His name is included on the list of 72 names inscribed on the Eiffel tower, and students of transport phenomena will recognize many of these luminaries.

Fick's law

In 1862 Fick developed a similar law for mass transport. The mass flux of a species A is the mass of A transported per unit time per unit transfer area in a specified direction. This can be measured in either mass units or mole units. If $J_{\mathrm{A}x}$ is then the moles of species A transported in the x-direction (per unit area of transport per unit time) then this is found to be proportional to the concentration gradient of A. Fick's law then states that

$$\boxed{J_{\mathrm{A}x} = -D_{\mathrm{A}}\frac{dC_{\mathrm{A}}}{dx}} \tag{1.2}$$

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Fick's law holds, strictly speaking, for binary systems, and more refined models are needed for multicomponent systems. Also Fick's law needs a definition of the system velocity and is applied to a system moving with a mixture velocity. These details are not important at this stage. Later we will study these in detail. At this point we simply note the similarity between Fourier's law and Fick's law, and also note that the diffusion coefficient D_A has units of m^2/s. The magnitude of D_A is vastly different for mass transport in gases, liquids, and solids, and depends on the molecular structure of matter. As an abbreviation we will often use D for diffusivity instead of D_A if we are focusing on the mass transport of just one species.

Newton's law of viscosity

In a similar manner, if there is a velocity difference between two points, i.e., if two fluid layers are moving at different velocities, then there is a force acting tangential to the surface. The magnitude of this force per unit area is called the shear stress. Newton proposed a law that related the stress to the velocity gradient:

$$\boxed{\tau = \frac{F_x}{A} = \mu \frac{dv_x}{dy}} \tag{1.3}$$

This is known as Newton's law of viscosity. Here τ is the shear stress. For the purpose of Chapters 1 and 2 the above definition of shear stress is sufficient. However, stress is a tensor type of quantity, as will be addressed in more detail in Chapter 4.

The schematic drawing in Fig. 1.6 makes the concept somewhat clearer. Let two fluid layers on adjacent sides of a control surface have different velocities. This velocity gradient causes a tangential force on the control surface as shown in Fig. 1.6. The force divided by area is the shear stress.

On comparing the units in Eq. (1.3). we find that viscosity has the units of $\mathrm{Pa \cdot s}$ or, in expanded terms, $\mathrm{kg/m \cdot s}$.

A remark on the sign convention is in order. The stress or the corresponding force is the force exerted by the $y+$ layer (the top layer in Fig. 1.6) on the $y-$ (bottom) layer. This will have a positive numerical value if the top layer is moving somewhat faster than the bottom layer and *vice versa.* It may also be noted that some books use the opposite sign convention to define the stress.

What is the force exerted by the $y-$ layer on the $y+$ layer?

Note that the extension to a case in which the velocity varies in all directions is deferred to a later chapter. This requires the notion of the gradient of a vector, which is a tensor

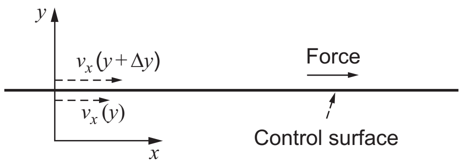

Figure 1.6 A schematic diagram to explain Newton's law of viscosity; the force on the surface divided by the surface area is the shear stress, denoted as τ.

quantity. Also many fluids do not obey such a simple linear behavior, and are called non-Newtonian fluids. Common fluids such as air, water, etc., with simple molecular structures do indeed obey Newton's law of viscosity.

The three modes of transport described above arise due to molecular-level interaction, and are therefore called molecular transport.

1.2 Typical transport property values

From the above discussion we find that the basic properties needed are therefore μ, k, and D. The molecular transport arises due to interaction of the molecules comprising the system and hence we would expect that molecular models would be useful to predict these properties. This link to molecular properties of matter is discussed briefly in Section 1.8

From a modeling point of view on a continuum basis (discussed in Section 1.3), we need only typical property values, and how the property changes as a function of temperature and pressure. Such information is briefly summarized below. It is also important to know how the property can be estimated for mixtures if no experimental data are available. Some information is provided in this section. The book by Reid, Prausnitz, and Poling (1987) provides further information on physical property values and prediction methods. The website http://www.engineeringtoolbox.com is a useful resource as well.

1.2.1 Viscosity: pure gases and vapors

Values of viscosity for air are given in the Table 1.1.

Note that the values in Table 1.1 must be multiplied by 10^{-5} to get the μ values. Thus the viscosity at 300 K is 1.846×10^{-5} Pa · s. Students often make such mistakes when looking at tabulated values of the physical properties from books or web sources. It is also important to have an appreciation of the range of values for typical compounds.

Viscosity values for steam are given in Table 1.2. It may be noted that the viscosity values for steam are about five times larger than those for air.

Table 1.1. Viscosity values for air at 1 atm pressure

	Temperature (K)					
	280	300	320	340	360	400
μ (10^5 Pa · s)	1.7503	1.846	1.9391	2.0300	2.1175	2.2857

Table 1.2. Viscosity values for steam at 1 atm pressure

	Temperature (K)					
	380	400	450	500	600	800
μ (10^5 Pa · s)	12.75	13.42	15.23	17.03	20.64	27.86