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CHUN-PYO HONG

Series in Materials Science and Engineering

Computer Modelling of Heat and Fluid Flow in Materials Processing

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Preface

The importance of transport phenomena (heat, mass and momentum transfer) in materials processing has been recently re-evaluated. In the majority of materials processing, transport phenomena play an important role in that one or more types of transfer will be closely related to the processing of materials from one state to another. The understanding and analysis of transport phenomena related to materials processes is crucial to the design and optimization of the processes involved. Since 'transport phenomena' was first introduced into materials science and engineering curricula in the 1970s, the teaching of this subject has focused primarily on qualitative understanding of the physical phenomena involved in materials processes. The role of transport phenomena in materials science and engineering has been presented at a very scientific level, with little emphasis on practical application. Consequently, it has been very difficult for researchers and engineers who have this academic background in transport phenomena to put their knowledge into practice in real applications in materials processing. Recently, owing to greatly enhanced computer power, and development of numerical models and computational modeling software, transport phenomena coupled with computer simulations, i.e., 'Computational Transport Phenomena' can bridge this gap between 'Science' and 'Practice'.

The aims of this book are to enhance the capability of the reader (i) to utilize commercially available software, (ii) to develop tailored simulation software suitable for the processes of interest, and (iii) to apply the concepts of transport phenomena in materials science and engineering research. The book is not intended to include a comprehensive review of computational algorithms related to transport phenomena appearing in materials science and engineering problems and examples of applications in the field, rather it includes fundamentals of transport phenomena, basics of the finite-difference/finite-volume methods, algorithms of fluid flow simulations, and a few examples of applications.

The book is essentially intended to be self-contained. However, in order to maximize the benefit of this book the reader needs to have some knowledge of mathematics, especially integral and differential calculus, elementary vector/matrix algebra, and basic numerical methods. This book is intended for final-year undergraduate or graduate students, and also researchers and engineers who work in the field of materials processing and manufacturing.

The book consists of 13 chapters. The first part, consisting of chapters 1–3, provides basic concepts of transport phenomena, conservation laws for energy, mass and momentum, and derivation of governing integral and differential equations. The second part of this book, chapters 4–7, presents fundamentals of finite-difference/finite-volume methods, applications of finite volume methods to steady and transient potential flow problems, and heat transfer problems with phase change. The third part, chapters 8 and 9, deals with discretization schemes for convection and diffusion terms, and solution algorithms for solving fluid flow problems. The fourth part, chapters 10 and 11, describes basics of the SIMPLE methods for simulating fluid flow which include the discretization of governing equations and solution schemes, based on the Cartesian-coordinate and body-fitted-coordinate systems. The treatment of free surfaces in fluid flow is also included. The final part of this book, chapters 12 and 13, is devoted to applications of heat, mass and momentum transfer in materials processing, such as modelings of mould filling of molten metals in a die cavity and microstructure evolution in solidification of metals. The computer programs used in chapters 5–7 and 10–13 are available free online at www.bookmarkphysics.iop.org/.

Finally, the author would like to express his sincere thanks to many friends and colleagues who contributed to this textbook. First, I would like to thank Professor B Cantor, Professor T Umeda and Professor C S Choi for their kind suggestion and encouragement to write this book, and the team at Institute of Physics Publishing for their patience and support throughout the writing process. I especially thank my post-doc researchers, Dr S Y Lee, Dr J H Mok and Dr M F Zhu for their contributions to this book. I continue to be indebted to my students, W J Cho and H N Nam for their efforts in preparing the figures.

I would like to acknowledge my colleagues at Yonsei University, Professor C S Yoon, Professor T S Paik, Professor I W Paik, Professor J H Kim, and Professor C S Shin, for their continuous encouragement. I am also grateful to Dr M Itamura of Nano-Cast Corp. for his kind comments. Finally, I would like to thank my wife and two sons, Jung-Woo and Jin-Hyuk, for their patience and continued encouragement during the compilation of this book.

C P Hong
Yonsei University

'Your beginnings are humble, so prosperous will your future be' (Job 8:7)

Contents

Chapter 1

Mechanisms of transport phenomena

Transport phenomena in engineering fields involve three types of transfer: (1) energy or heat transport, (2) mass transport and (3) momentum transport or fluid dynamics. In this chapter, physical mechanisms of three types of transport phenomena will be briefly described.

1.1 Heat transfer

The irreversible phenomenon known as *heat transfer* occurs when there exists a temperature difference in a medium or between media. In order to understand the mechanisms of heat transfer, let us consider the cooling process of a heated carbon steel plate in a furnace, as shown in figure 1.1. Heat is transported from the steel plate to its surroundings by the three modes of heat transfer, which are generally recognized as *conduction*, *convection* and *radiation*.

1.1.1 Conduction—Fourier's Law of Conduction

The term *conduction* is used to refer to the transport of heat from high temperature to low temperature in a stationary medium, which may be a solid or a fluid, by the motion of molecules or electrons. In engineering applications, it is important to quantify heat transfer processes in terms of appropriate rate equations.

Consider the one-dimensional wall shown in figure 1.2, having a temperature distribution of $T(x)$. The temperature at $x = 0$ is higher than that at $x = L$, so heat is conducted from left to right, according to the rate equation known as *Fourier's law of conduction* expressed by

$$q_x = -\lambda \frac{\mathrm{d}T}{\mathrm{d}x}. \tag{1.1.1}$$

The heat flux q_x, which is the heat transfer rate in the x direction per unit area, is proportional to the temperature gradient, $\mathrm{d}T/\mathrm{d}x$. The cgs and mks

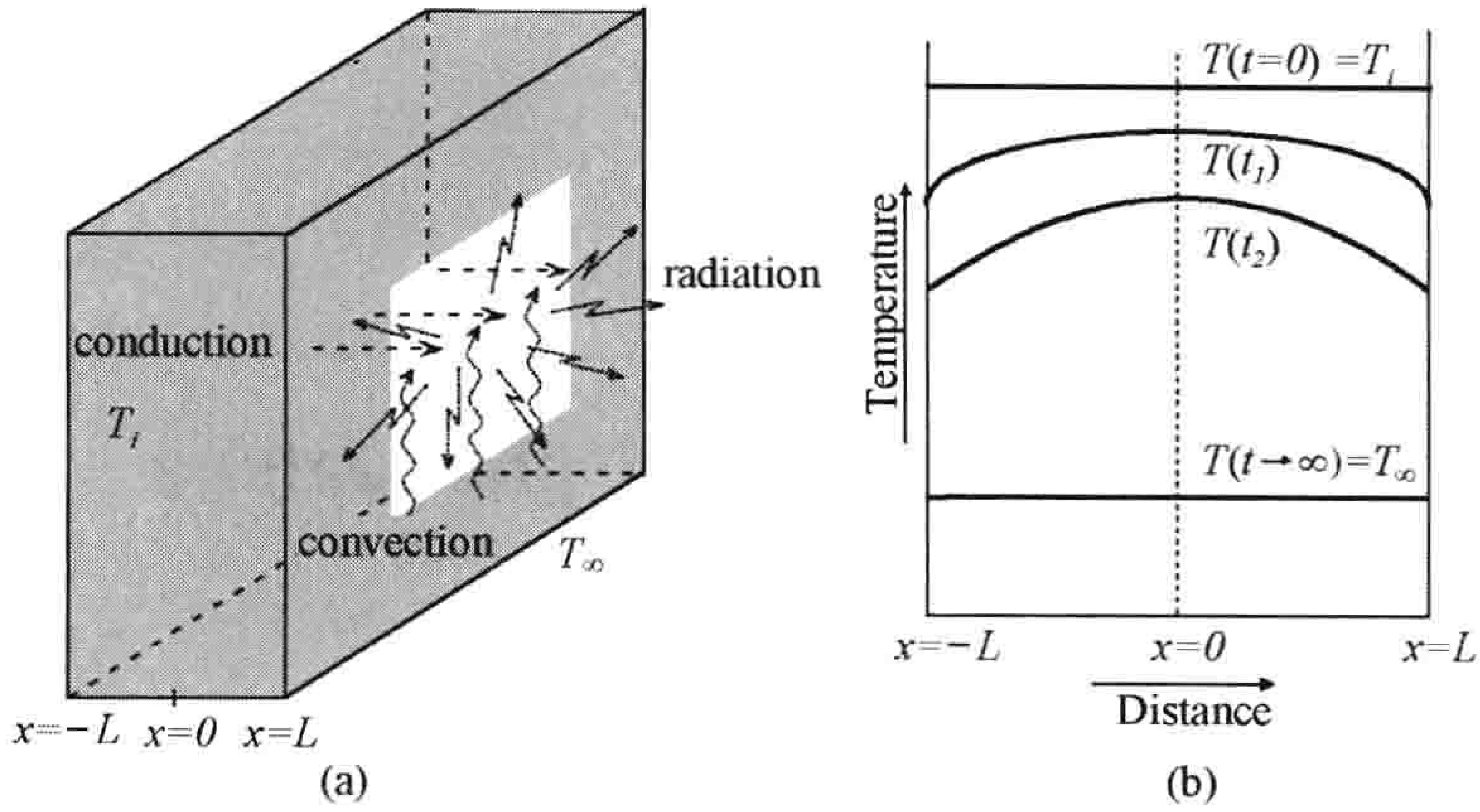

Figure 1.1. (a) Heat transfer mechanisms: conduction, convection and radiation, and (b) variation of temperature profiles with time.

units of the heat flux are $W \cdot cm^{-2}$ and $W \cdot m^{-2}$, respectively. Here the proportional constant λ is the *thermal conductivity* ($W \cdot cm^{-1} \cdot K^{-1}$ and $W \cdot m^{-1} \cdot K^{-1}$ in the cgs and mks units, respectively) and is a characteristic of the wall material. The negative sign in equation (1.1.1) indicates that heat is transferred in the direction of decreasing temperature.

1.1.2 Convection

Energy can be transported not only due to thermal gradient, but also due to bulk fluid flow. In order to estimate the heat transfer related to bulk fluid flow, let us consider a simple example, consisting of a fluid at a bulk temperature of T_∞ flowing with a bulk flow velocity of u_∞ through a circular channel

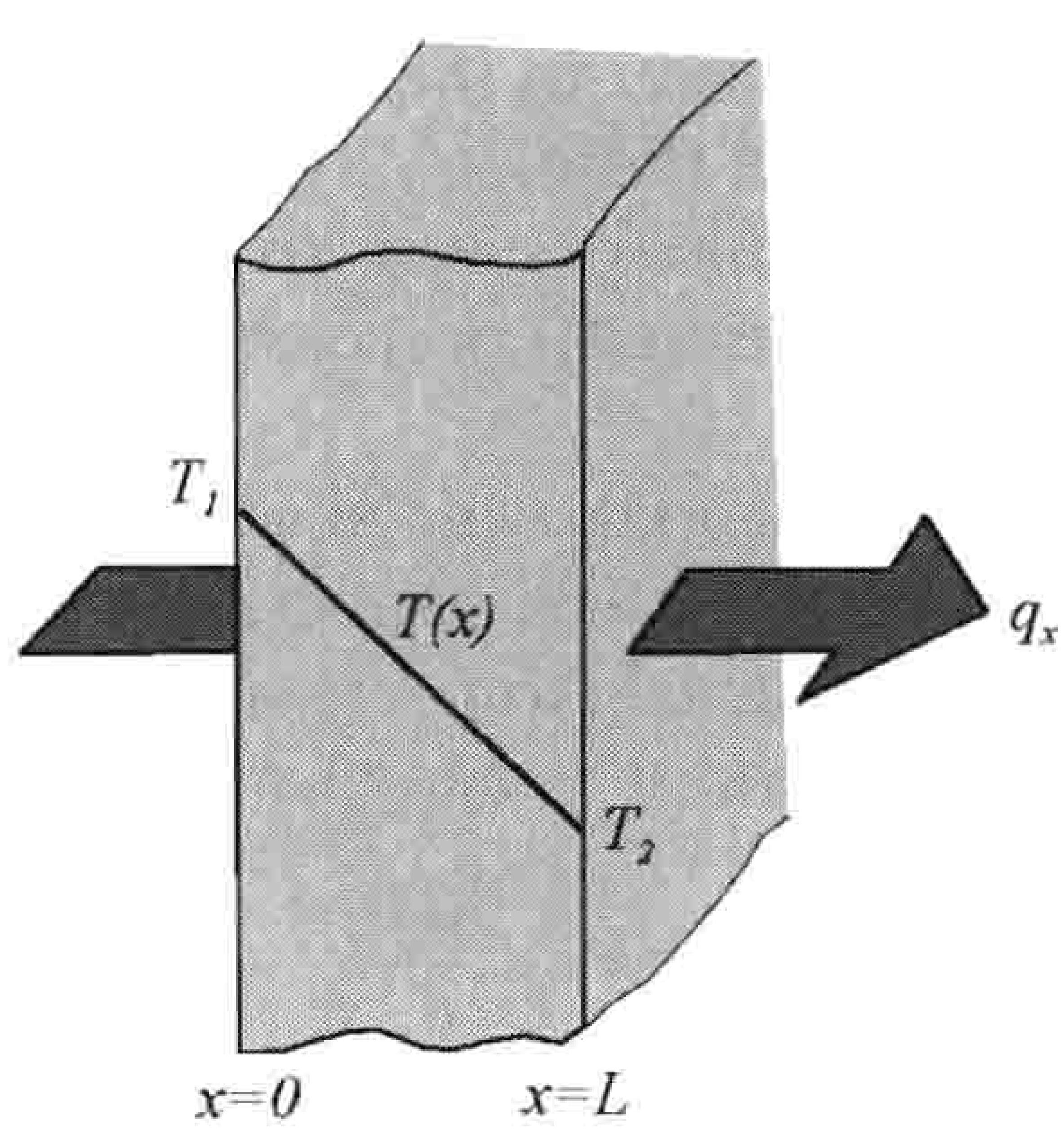

Figure 1.2. One-dimensional heat conduction through a plane wall.

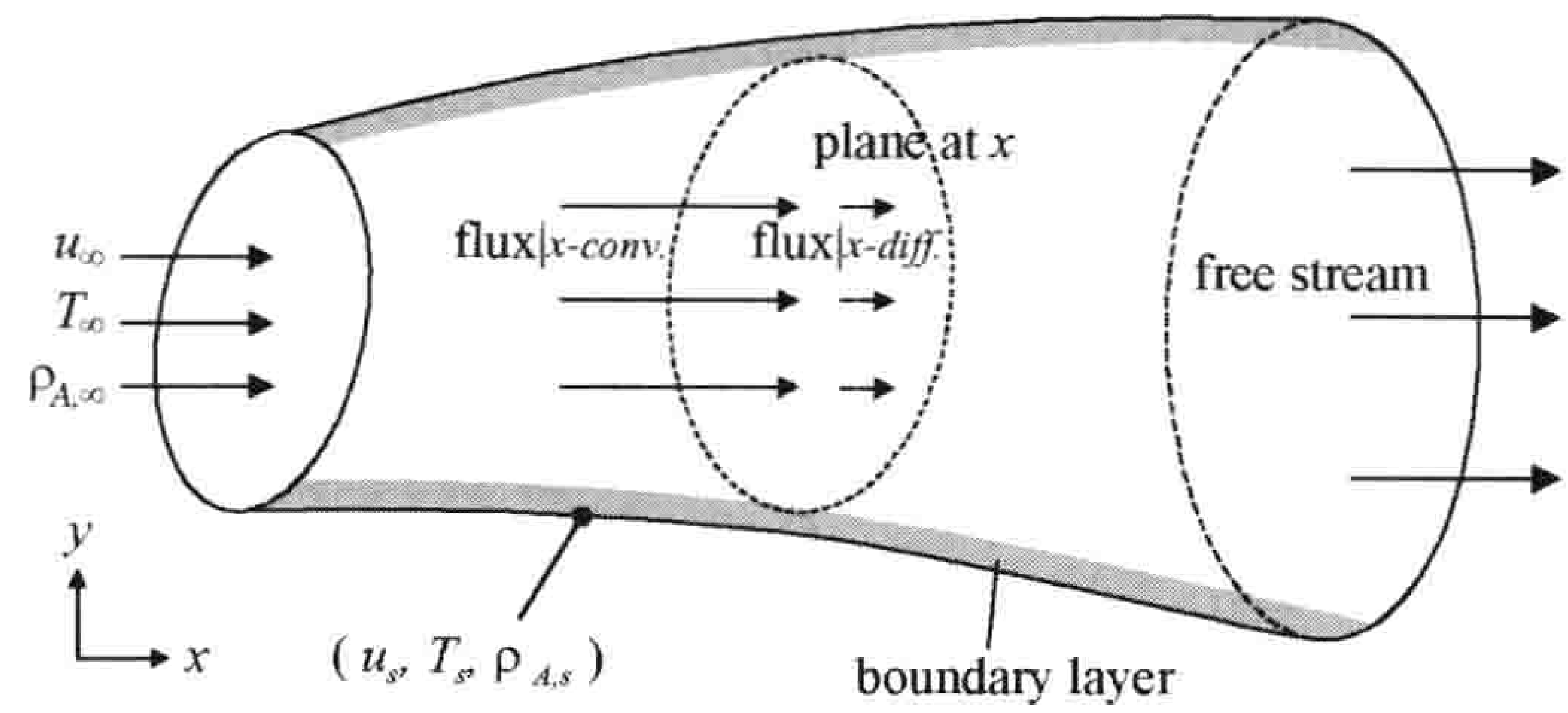

Figure 1.3. Bulk flow of fluids through a circular tube showing two components in heat, mass and momentum transport: conductive (diffusive or viscous) and convective flux terms.

whose inside surface is at temperature T_s, as shown in figure 1.3. If there is a temperature gradient in the fluid in the direction of bulk flow and T_∞ is different from T_s, two kinds of heat transfer can be considered in this system: one is the heat transfer in the direction of flow caused by the bulk fluid motion, and the other is the heat transfer which occurs between a fluid in motion and a bounding surface because of the temperature difference.

1.1.2.1 Energy flux by bulk flow

Consider first the heat transfer term in the direction of flow caused by the bulk fluid motion. This term consists of two components: the conductive (or diffusive) and convective components. The conductive heat flux per unit area across the plane at x is given by $q_{x_{\text{cond}}} = -\lambda(\mathrm{d}T/\mathrm{d}x)$, while the convective heat flux (or bulk heat flux) caused by bulk flow per unit area is given by $(\rho C_v T)u_\infty$, which is defined as the heat transferred across the plane at x resulting from the motion of the fluid itself. Here ρ is the density of the fluid and C_v is the specific heat capacity. Thus, the total heat flux $q_{x_{\text{total}}}$ is given by

$$q_{x_{\text{total}}} = -\lambda\frac{\mathrm{d}T}{\mathrm{d}x} + (\rho C_v T)u_\infty. \tag{1.1.2}$$

Convection heat transfer can be classified according to the nature of the flow. If a fluid motion is induced externally by a pump or a fan, the heat transfer is said to be *forced convection*. If the fluid motion is set up by the buoyancy effect resulting from the density difference caused by the difference of temperature or solute concentration in the fluid, the heat transfer is said to be *free* (or *natural*) *convection*.

1.1.2.2 Thermal boundary layer

Let us now consider heat transfer, which occurs between a fluid in motion and a bounding surface because of the temperature difference. This

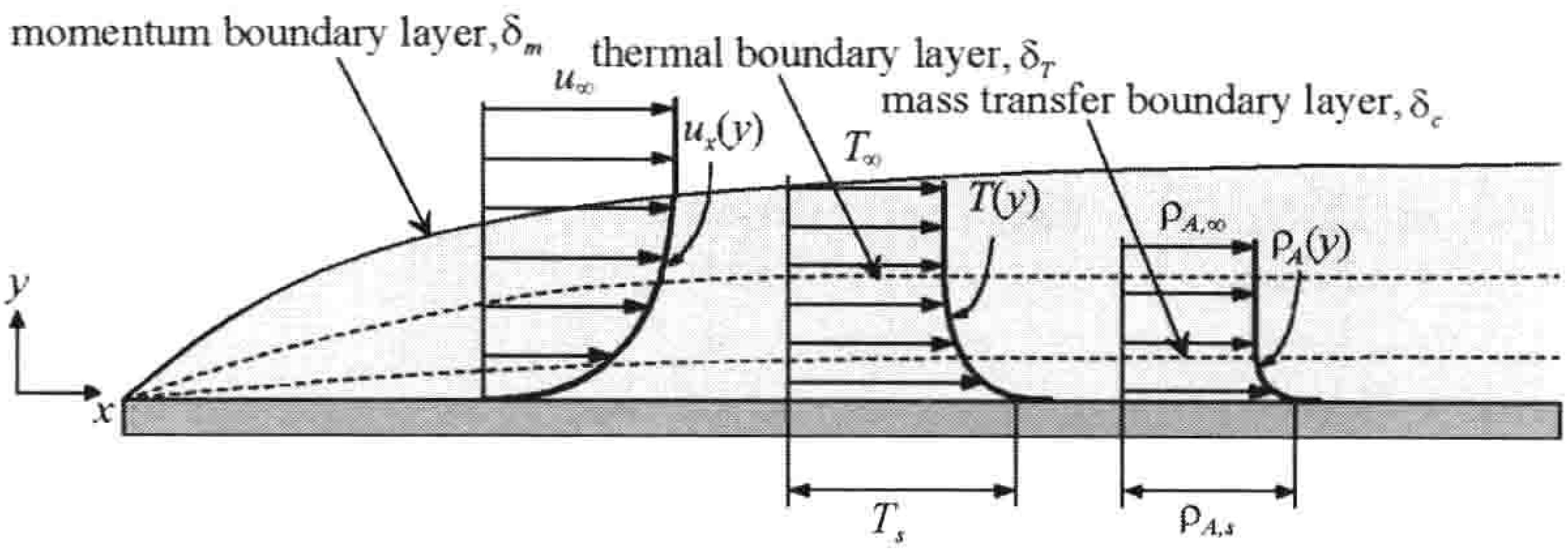

Figure 1.4. Development of momentum, thermal and mass transfer boundary layers in fluid flow over a solid surface.

mechanism of heat transfer, which is frequently encountered in materials processing, is also-called *convection*, since the motion of fluid plays an important role in determining the rate of heat transfer. As illustrated in figure 1.4, because of the interaction between a fluid and a solid surface and the effect of viscosity, there will be a region of fluid through which the fluid velocity varies from zero at the solid surface to u_∞ in the bulk flow. The velocity-affected region of flow is known as the *momentum* (or *velocity*) *boundary layer* δ_{m}, which is defined as the region where flow velocities are 99% or less of the bulk flow velocity u_∞, i.e., $(u_x(y) - u_{\mathrm{s}})/(u_\infty - u_{\mathrm{s}}) \le 0.99$. When u_{s} is equal to zero, $u_x(y)/u_\infty \le 0.99$. Similarly, there will be a region of the fluid through which the temperature of the fluid varies from T_{s} at the solid surface to T_∞ in the free stream. The *thermal boundary layer* δ_{T} can also be defined as the distance from the solid surface at which the dimensionless temperature $(T(y) - T_{\mathrm{s}})/(T_\infty - T_{\mathrm{s}})$ reaches 0.99. As the flow rate increases, both the thicknesses of the velocity and thermal boundary layers decrease, resulting in the increase in both the velocity and temperature gradients.

The convection heat transfer between the fluid and the solid surface consists of two components: one is the contribution due to random molecular motion (diffusion or conduction) which dominates near the solid surface where the fluid velocity is zero, and the other is the contribution due to the bulk fluid motion within the boundary layer. It is, therefore, essential to understand boundary layer phenomena in treating convection heat transfer.

In engineering applications, in order to calculate the convective heat transfer between a fluid and a solid surface, the appropriate rate equation is considered as follow.

$$q_{y_{\mathrm{conv}}} = h(T_\infty - T_{\mathrm{s}}) \tag{1.1.3}$$

where $q_{y_{\mathrm{conv}}}$ is the convective heat flux between the solid surface and the fluid, which is proportional to the temperature difference between them, and the proportional constant h is referred to as the *convection heat transfer*