

$$\left( \begin{array}{c} \text{Rate of} \\ \text{Input of } \varphi \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{Output of } \varphi \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{Generation of } \varphi \end{array} \right) = \left( \begin{array}{c} \text{Rate of} \\ \text{Accumulation of } \varphi \end{array} \right)$$

# MODELLING IN TRANSPORT PHENOMENA

A Conceptual Approach

İSMAİL TOSUN

ELSEVIER

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## A Conceptual Approach

İSMAİL TOSUN

Professor of Chemical Engineering

Middle East Technical University

Ankara, Turkey

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To Ayşe

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# Preface

During their undergraduate education, students take various courses on fluid flow, heat transfer, mass transfer, chemical reaction engineering and thermodynamics. Most of the students, however, are unable to understand the links between the concepts covered in these courses and have difficulty in formulating equations, even of the simplest nature. This is a typical example of not seeing the forest for the trees.

The pathway from the real problem to the mathematical problem has two stages: perception and formulation. The difficulties encountered in both of these stages can be easily resolved if students recognize the forest first. Examination of trees one by one comes at a later stage.

In science and engineering, the forest is represented by the **basic concepts**, i.e., conservation of chemical species, conservation of mass, conservation of momentum, and conservation of energy. For each one of these conserved quantities, the following inventory rate equation can be written to describe the transformation of the particular conserved quantity  $\varphi$  :

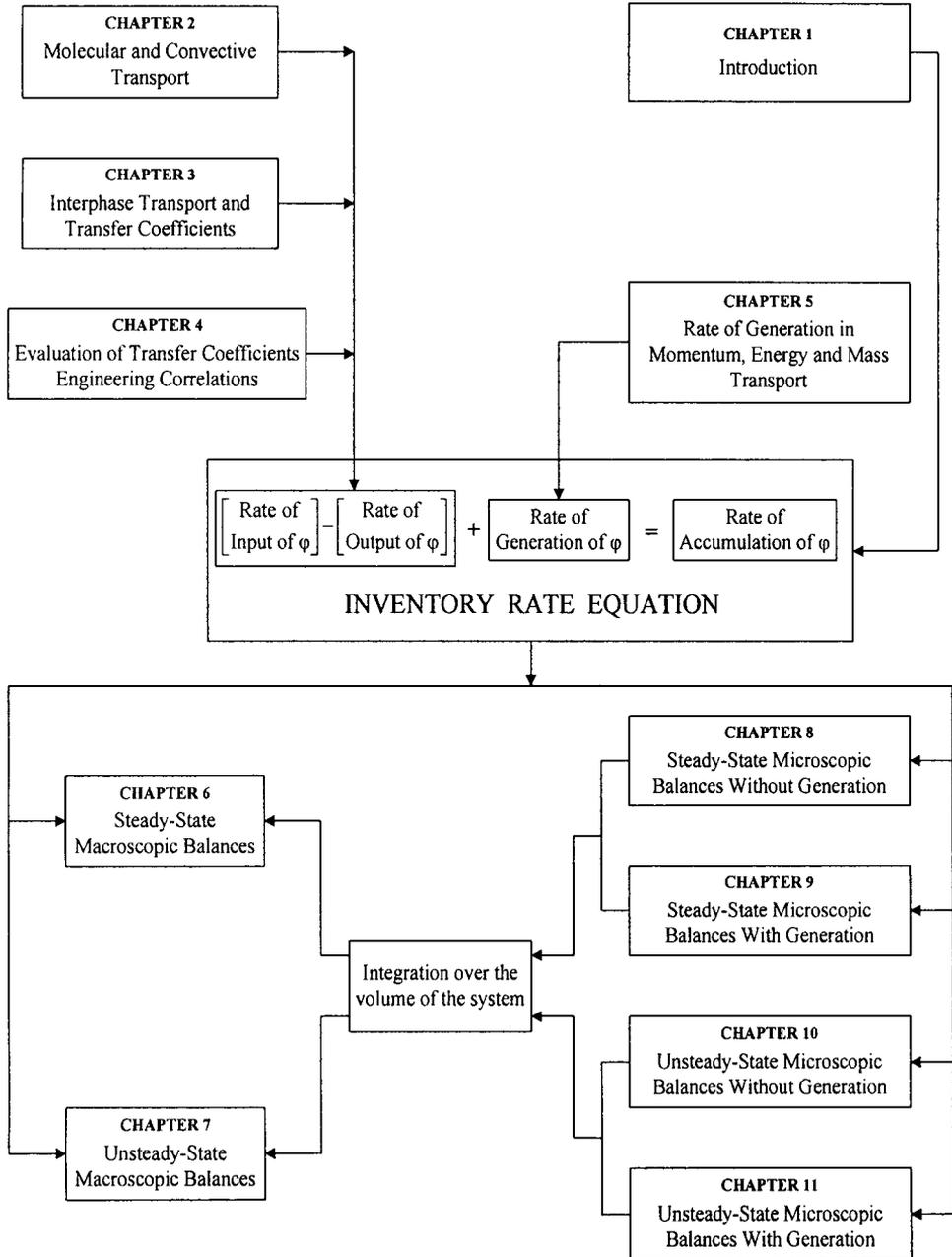
$$\left( \begin{array}{c} \text{Rate of} \\ \varphi \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \varphi \text{ out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of } \varphi \\ \text{generation} \end{array} \right) = \left( \begin{array}{c} \text{Rate of } \varphi \\ \text{accumulation} \end{array} \right)$$

in which the term  $\varphi$  may stand for chemical species, mass, momentum or energy.

My main purpose in writing this textbook is to show students how to translate the inventory rate equation into mathematical terms at both the macroscopic and microscopic levels. It is not my intention to exploit various numerical techniques to solve the governing equations in momentum, energy and mass transport. The emphasis is on obtaining the equation representing a physical phenomenon and its interpretation.

I have been using the draft chapters of this text in my third year *Mathematical Modelling in Chemical Engineering* course for the last two years. It is intended as an undergraduate textbook to be used in an (Introduction to) Transport Phenomena course in the junior year. This book can also be used in unit operations courses in conjunction with standard textbooks. Although it is written for students majoring in chemical engineering, it can also be used as a reference or supplementary text in environmental, mechanical, petroleum and civil engineering courses.

The overview of the manuscript is shown schematically in the figure below.



Chapter 1 covers the basic concepts and their characteristics. The terms appearing in the inventory rate equation are discussed qualitatively. Mathematical formulations of “rate of input” and “rate of output” terms are explained in Chapters 2, 3 and 4. Chapter 2 indicates that the total flux of any quantity is the sum of its molecular and convective fluxes. Chapter 3 deals with the formulation of the inlet and outlet terms when the transfer of matter takes place through the boundaries of the system by making use of the transfer coefficients, i.e., friction factor, heat transfer coefficient and mass transfer coefficient. The correlations available in the literature to evaluate these transfer coefficients are given in Chapter 4. Chapter 5 briefly talks about the rate of generation in transport of mass, momentum and energy.

Traditionally, the development of the microscopic balances precedes the macroscopic balances. However, it is my experience that students grasp the ideas better if the reverse pattern is followed. Chapters 6 and 7 deal with the application of the inventory rate equations at the macroscopic level.

The last four chapters cover the inventory rate equations at the microscopic level. Once the velocity, temperature or concentration distributions are determined, the resulting equations are integrated over the volume of the system to get the macroscopic equations covered in Chapters 6 and 7.

I had the privilege of having Professor Max S. Willis of the University of Akron as my Ph.D supervisor who introduced me to the real nature of transport phenomena. All that I profess to know about transport phenomena is based on the discussions with him as a student, a colleague, a friend and a mentor. His influence can be easily noticed throughout this book. Two of my colleagues, Güniz Gürüz and Zeynep Hiçşazmaz Katnaş, kindly read the entire manuscript and made many helpful suggestions. My thanks are also extended to the members of the Chemical Engineering Department for their many discussions with me and especially to Timur Doğu, Türker Gürkan, Gürkan Karakaş, Önder Özbelge, Canan Özgen, Deniz Üner, Levent Yılmaz and Hayrettin Yücel. I appreciate the help provided by my students, Gülden Camçı, Yeşim Güçbilmez and Özge Oğuzer, for proofreading and checking the numerical calculations.

Finally, without the continuous understanding, encouragement and tolerance of my wife Ayşe and our children, Çiğdem and Burcu, this book could not have been completed and I am grateful indeed.

Suggestions and criticisms from instructors and students using this book will be appreciated.

İSMAİL TOSUN (itosun@metu.edu.tr)

Ankara, Turkey  
March 2002

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# Chapter 1

## Introduction

### 1.1 BASIC CONCEPTS

A concept is a unit of thought. Any part of experience that we can organize into an idea is a concept. For example, man's concept of cancer is changing all the time as new medical information is gained as a result of experiments.

Concepts or ideas that are the basis of science and engineering are *chemical species, mass, momentum, and energy*. These are all conserved quantities. A *conserved* quantity is one which can be transformed. However, transformation does not alter the total amount of the quantity. For example, money can be transferred from a checking account to a savings account but the transfer does not affect the total assets.

For any quantity that is conserved, an *inventory rate equation* can be written to describe the transformation of the conserved quantity. Inventory of the conserved quantity is based on a specified unit of time, which is reflected in the term, *rate*. In words, this rate equation for any conserved quantity  $\varphi$  takes the form

$$\begin{aligned} \left( \begin{array}{c} \text{Rate of} \\ \text{input of } \varphi \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{output of } \varphi \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{generation of } \varphi \end{array} \right) \\ = \left( \begin{array}{c} \text{Rate of} \\ \text{accumulation of } \varphi \end{array} \right) \quad (1.1-1) \end{aligned}$$

Basic concepts, upon which the technique for solving engineering problems is based, are the rate equations for the

- Conservation of chemical species,
- Conservation of mass,
- Conservation of momentum,
- Conservation of energy.

The entropy inequality is also a basic concept but it only indicates the feasibility of a process and, as such, is not expressed as an inventory rate equation.

A rate equation based on the conservation of the value of money can also be considered as a basic concept, i.e., economics. Economics, however, is outside the scope of this text.

### 1.1.1 Characteristics of the Basic Concepts

The basic concepts have certain characteristics that are always taken for granted but seldom stated explicitly. The basic concepts are

- Independent of the level of application,
- Independent of the coordinate system to which they are applied,
- Independent of the substance to which they are applied.

The basic concepts are applied both at the microscopic and the macroscopic levels as shown in Table 1.1.

**Table 1.1** Levels of application of the basic concepts.

Level	Theory	Experiment
Microscopic	Equations of Change	Constitutive Equations
Macroscopic	Design Equations	Process Correlations

At the microscopic level, the basic concepts appear as partial differential equations in three independent space variables and time. Basic concepts at the microscopic level are called the *equations of change*, i.e., conservation of chemical species, mass, momentum and energy.

Any mathematical description of the response of a material to spatial gradients is called a *constitutive equation*. Just as the reaction of different people to the same joke may vary, the response of materials to the variable condition in a process differs. Constitutive equations are postulated and cannot be derived from the fundamental principles<sup>1</sup>. The coefficients appearing in the constitutive equations are obtained from experiments.

Integration of the equations of change over an arbitrary engineering volume which exchanges mass and energy with the surroundings gives the basic concepts at the macroscopic level. The resulting equations appear as ordinary differential equations with time as the only independent variable. The basic concepts at this level are called the *design equations* or *macroscopic balances*. For example, when the microscopic level mechanical energy balance is integrated over an arbitrary

<sup>1</sup>The mathematical form of a constitutive equation is constrained by the *second law of thermodynamics* so as to yield a positive entropy generation.

engineering volume, the result is the macroscopic level engineering Bernoulli equation.

Constitutive equations, when combined with the equations of change, may or may not comprise a determinate mathematical system. For a determinate mathematical system, i.e., number of unknowns = number of independent equations, the solutions of the equations of change together with the constitutive equations result in the velocity, temperature, pressure, and concentration profiles within the system of interest. These profiles are called *theoretical* (or, *analytical*) *solutions*. A theoretical solution enables one to design and operate a process without resorting to experiments or scale-up. Unfortunately, the number of such theoretical solutions is small relative to the number of engineering problems which must be solved.

If the required number of constitutive equations is not available, i.e., number of unknowns > number of independent equations, then the mathematical description at the microscopic level is indeterminate. In this case, the design procedure appeals to an experimental information called *process correlation* to replace the theoretical solution. All process correlations are limited to a specific geometry, equipment configuration, boundary conditions, and substance.

## 1.2 DEFINITIONS

The functional notation

$$\varphi = \varphi(t, x, y, z) \quad (1.2-1)$$

indicates that there are three *independent space variables*,  $x$ ,  $y$ ,  $z$ , and one *independent time variable*,  $t$ . The  $\varphi$  on the right side of Eq. (1.2-1) represents the functional form, and the  $\varphi$  on the left side represents the value of the dependent variable,  $\varphi$ .

### 1.2.1 Steady-State

The term steady-state means that at a particular location in space, the dependent variable does not change as a function of time. If the dependent variable is  $\varphi$ , then

$$\left( \frac{\partial \varphi}{\partial t} \right)_{x,y,z} = 0 \quad (1.2-2)$$

The partial derivative notation indicates that the dependent variable is a function of more than one independent variable. In this particular case, the independent variables are  $(x, y, z)$  and  $t$ . The specified location in space is indicated by the subscripts  $(x, y, z)$  and Eq. (1.2-2) implies that  $\varphi$  is not a function of time,  $t$ . When an ordinary derivative is used, i.e.,  $d\varphi/dt = 0$ , then this implies that  $\varphi$  is a constant. It is important to distinguish between partial and ordinary derivatives because the conclusions are very different.

**Example 1.1** A Newtonian fluid with constant viscosity,  $\mu$ , and density,  $\rho$ , is initially at rest in a very long horizontal pipe of length  $L$  and radius  $R$ . At  $t = 0$ , a pressure gradient  $|\Delta P|/L$  is imposed on the system and the volumetric flow rate,  $Q$ , is expressed as

$$Q = \frac{\pi R^4 |\Delta P|}{8 \mu L} \left[ 1 - 32 \sum_{n=1}^{\infty} \frac{\exp(-\lambda_n^2 \tau)}{\lambda_n^4} \right]$$

where  $\tau$  is the dimensionless time defined by

$$\tau = \frac{\mu t}{\rho R^2}$$

and  $\lambda_1 = 2.405$ ,  $\lambda_2 = 5.520$ ,  $\lambda_3 = 8.654$ , etc. Determine the volumetric flow rate under steady conditions.

### Solution

Steady-state solutions are independent of time. To eliminate the time from the unsteady-state solution, we have to let  $t \rightarrow \infty$ . In that case, the exponential term approaches zero and the resulting steady-state solution is

$$Q = \frac{\pi R^4 |\Delta P|}{8 \mu L}$$

which is known as the Hagen-Poiseuille law.

**Comment:** If time appears in the exponential term, then the term must have a negative sign to assure that the solution does not blow as  $t \rightarrow \infty$ .

**Example 1.2** A cylindrical tank is initially half full with water. The water is fed into the tank from the top and it leaves the tank from the bottom. The volumetric flow rates are different from each other. The differential equation describing the time rate of change of the height of water in the tank is given by

$$\frac{dh}{dt} = 6 - 8\sqrt{h}$$

where  $h$  is the height of water in meters. Calculate the height of water in the tank under steady conditions.

### Solution

Under steady conditions  $dh/dt$  must be zero. Then

$$0 = 6 - 8\sqrt{h}$$

or,

$$h = 0.56 \text{ m}$$

### 1.2.2 Uniform

The term *uniform* means that at a particular instant in time, the dependent variable is not a function of position. This requires that all three of the partial derivatives with respect to position be zero, i.e.,

$$\left(\frac{\partial\varphi}{\partial x}\right)_{y,z,t} = \left(\frac{\partial\varphi}{\partial y}\right)_{x,z,t} = \left(\frac{\partial\varphi}{\partial z}\right)_{x,y,t} = 0 \quad (1.2-3)$$

The variation of a physical quantity with respect to position is called *gradient*. Therefore, the gradient of a quantity must be zero for a uniform condition to exist with respect to that quantity.

### 1.2.3 Equilibrium

A system is in *equilibrium* if both steady-state and uniform conditions are met simultaneously. An equilibrium system does not exhibit any variations with respect to position or time. The state of an equilibrium system is specified completely by the non-Euclidean coordinates<sup>2</sup> ( $P, V, T$ ). The response of a material under equilibrium conditions is called *property correlation*. The ideal gas law is an example of a thermodynamic property correlation that is called an *equation of state*.

### 1.2.4 Flux

The flux of a certain quantity is defined by

$$\text{Flux} = \frac{\text{Flow of a quantity/Time}}{\text{Area}} = \frac{\text{Flow rate}}{\text{Area}} \quad (1.2-4)$$

where area is normal to the direction of flow. The units of momentum, energy, mass and molar fluxes are Pa ( $\text{N}/\text{m}^2$ , or  $\text{kg}/\text{m}\cdot\text{s}^2$ ),  $\text{W}/\text{m}^2$  ( $\text{J}/\text{m}^2\cdot\text{s}$ ),  $\text{kg}/\text{m}^2\cdot\text{s}$ , and  $\text{kmol}/\text{m}^2\cdot\text{s}$ , respectively.

## 1.3 MATHEMATICAL FORMULATION OF THE BASIC CONCEPTS

In order to obtain the mathematical description of a process, the general inventory rate equation given by Eq. (1.1-1) should be translated into mathematical terms.

### 1.3.1 Inlet and Outlet Terms

A quantity may enter or leave the system by two means: (i) by inlet and/or outlet streams, (ii) by exchange of a particular quantity between the system and its

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<sup>2</sup>A *Euclidean* coordinate system is one in which length can be defined. The coordinate system ( $P, V, T$ ) is *non-Euclidean*.

surroundings through the boundaries of the system. In either case, the rate of input and/or output of a quantity is expressed by using the flux of that particular quantity. The flux of a quantity may be either constant or dependent on position. Thus, the rate of a quantity can be determined as

$$\text{Inlet/Outlet rate} = \begin{cases} (\text{Flux})(\text{Area}) & \text{if flux is constant} \\ \iint_A \text{Flux } dA & \text{if flux is position dependent} \end{cases} \quad (1.3-1)$$

where  $A$  is the area perpendicular to the direction of the flux. The differential areas in cylindrical and spherical coordinate systems are given in Section A.1 in Appendix A.

**Example 1.3** *Note that the velocity can be interpreted as the volumetric flux ( $\text{m}^3/\text{m}^2 \cdot \text{s}$ ). Therefore, volumetric flow rate can be calculated by the integration of velocity distribution over the cross-sectional area that is perpendicular to the flow direction. Consider the flow of a very viscous fluid in the space between two concentric spheres as shown in Figure 1.1. The velocity distribution is given by Bird et al. (1960) as*

$$v_\theta = \frac{R|\Delta P|}{2\mu E(\varepsilon)\sin\theta} \left[ \left(1 - \frac{r}{R}\right) + \kappa \left(1 - \frac{R}{r}\right) \right]$$

where

$$E(\varepsilon) = \ln \left( \frac{1 + \cos\varepsilon}{1 - \cos\varepsilon} \right)$$

Use the velocity profile to find the volumetric flow rate,  $\mathcal{Q}$ .

### Solution

*Since the velocity is in the  $\theta$ -direction, the differential area that is perpendicular to the flow direction is given by Eq. (A.1-9) in Appendix A as*

$$dA = r \sin\theta \, dr d\phi \quad (1)$$

*Therefore, the volumetric flow rate is*

$$\mathcal{Q} = \int_0^{2\pi} \int_{\kappa R}^R v_\theta r \sin\theta \, dr d\phi \quad (2)$$

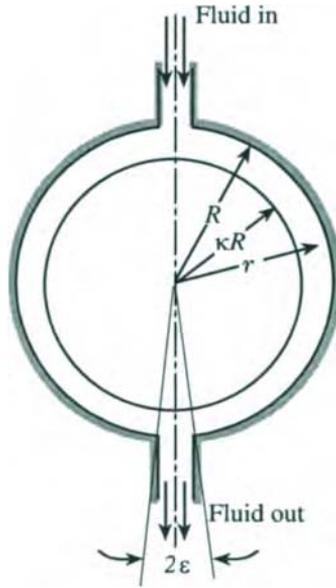


Figure 1.1 Flow between concentric spheres.

Substitution of the velocity distribution into Eq. (2) and integration gives

$$Q = \frac{\pi R^3 (1 - \kappa)^3}{6 \mu E(\epsilon)} |\Delta P| \quad (3)$$

### 1.3.2 Rate of Generation Term

The generation rate per unit volume is denoted by  $\mathfrak{R}$  and it may be either constant or dependent on position. Thus, the generation rate is expressed as

$$\text{Generation rate} = \begin{cases} (\mathfrak{R})(\text{Volume}) & \text{if } \mathfrak{R} \text{ is constant} \\ \iiint_V \mathfrak{R} dV & \text{if } \mathfrak{R} \text{ is position dependent} \end{cases} \quad (1.3-2)$$

where  $V$  is the volume of the system in question. It is also possible to have the depletion of a quantity. In that case, the plus sign in front of the generation term must be replaced by the minus sign, i.e.,

$$\text{Depletion rate} = - \text{Generation rate} \quad (1.3-3)$$

**Example 1.4** Energy generation rate per unit volume as a result of an electric current passing through a rectangular plate of cross-sectional area  $A$  and thickness  $L$  is given by

$$\mathfrak{R} = \mathfrak{R}_o \sin\left(\frac{\pi x}{L}\right)$$

where  $\mathfrak{R}$  is in  $\text{W}/\text{m}^3$ . Calculate the total energy generation rate within the plate.

### Solution

Since  $\mathfrak{R}$  is dependent on position, energy generation rate is calculated by integration of  $\mathfrak{R}$  over the volume of the plate, i.e.,

$$\begin{aligned} \text{Energy generation rate} &= A \mathfrak{R}_o \int_0^L \sin\left(\frac{\pi x}{L}\right) dx \\ &= \frac{2AL \mathfrak{R}_o}{\pi} \end{aligned}$$

### 1.3.3 Rate of Accumulation Term

The rate of accumulation of any quantity  $\varphi$  is the time rate of change of that particular quantity within the volume of the system. Let  $\rho$  be the mass density and  $\hat{\varphi}$  be the quantity per unit mass. Thus,

$$\text{Total quantity of } \varphi = \iiint_V \rho \hat{\varphi} dV \quad (1.3-4)$$

and the rate of accumulation is given by

$$\text{Accumulation rate} = \frac{d}{dt} \left( \iiint_V \rho \hat{\varphi} dV \right) \quad (1.3-5)$$

If  $\hat{\varphi}$  is independent of position, then Eq. (1.3-5) simplifies to

$$\text{Accumulation rate} = \frac{d}{dt} (m \hat{\varphi}) \quad (1.3-6)$$

where  $m$  is the total mass within the system.

The accumulation rate may be either positive or negative depending on whether the quantity is increasing or decreasing with time within the volume of the system.

## 1.4 SIMPLIFICATION OF THE RATE EQUATION

In this section, the general rate equation given by Eq. (1.1-1) will be simplified for two special cases: (i) steady-state transport without generation, (ii) steady-state transport with generation.

### 1.4.1 Steady-State Transport Without Generation

For this case Eq. (1.1-1) reduces to

$$\text{Rate of input of } \varphi = \text{Rate of output of } \varphi \quad (1.4-1)$$

Equation (1.4-1) can also be expressed in terms of flux as

$$\iint_{A_{in}} (\text{Inlet flux of } \varphi) dA = \iint_{A_{out}} (\text{Outlet flux of } \varphi) dA \quad (1.4-2)$$

For constant inlet and outlet fluxes Eq. (1.4-2) reduces to

$$\left( \begin{array}{c} \text{Inlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Inlet} \\ \text{area} \end{array} \right) = \left( \begin{array}{c} \text{Outlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Outlet} \\ \text{area} \end{array} \right) \quad (1.4-3)$$

If the inlet and outlet areas are equal, then Eq. (1.4-3) becomes

$$\text{Inlet flux of } \varphi = \text{Outlet flux of } \varphi \quad (1.4-4)$$

It is important to note that Eq. (1.4-4) is valid as long as the areas perpendicular to the direction of flow at the inlet and outlet of the system are equal to each other. The variation of the area in between does not affect this conclusion. Equation (1.4-4) obviously is not valid for the transfer processes taking place in the radial direction in cylindrical and spherical coordinate systems. In this case either Eq. (1.4-2) or Eq. (1.4-3) should be used.

**Example 1.5** Consider a solid cone of circular cross-section whose lateral surface is well insulated as shown in Figure 1.2. The diameters at  $x = 0$  and  $x = L$  are 25 cm and 5 cm, respectively. If the heat flux at  $x = 0$  is  $45 \text{ W/m}^2$  under steady conditions, determine the heat transfer rate and the value of the heat flux at  $x = L$ .

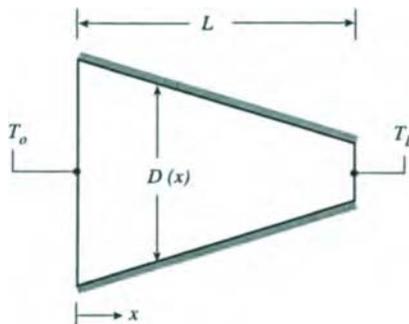


Figure 1.2 Heat transfer through a solid circular cone.

**Solution**

For steady-state conditions without generation, the heat transfer rate is constant and can be determined from Eq. (1.3-1) as

$$\text{Heat transfer rate} = (\text{Heat flux})_{x=0} (\text{Area})_{x=0}$$

Since the cross-sectional area of the cone is  $\pi D^2/4$ , then

$$\text{Heat transfer rate} = (45) \left[ \frac{\pi (0.25)^2}{4} \right] = 2.21 \text{ W}$$

The value of the heat transfer rate is also 2.21 W at  $x = L$ . However, the heat flux does depend on position and its value at  $x = L$  is

$$(\text{Heat flux})_{x=L} = \frac{2.21}{\left[ \pi (0.05)^2 / 4 \right]} = 1126 \text{ W/m}^2$$

**Comment:** Heat flux values are different from each other even though the heat flow rate is constant. Therefore, it is important to specify the area upon which a given heat flux is based when the area changes as a function of position.

**1.4.2 Steady-State Transport With Generation**

For this case Eq. (1.1-1) reduces to

$$\left( \begin{array}{c} \text{Rate of} \\ \text{input of } \varphi \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{generation of } \varphi \end{array} \right) = \left( \begin{array}{c} \text{Rate of} \\ \text{output of } \varphi \end{array} \right) \quad (1.4-5)$$

Equation (1.4-5) can also be written in the form

$$\iint_{A_{in}} (\text{Inlet flux of } \varphi) dA + \iiint_{V_{sys}} \mathfrak{R} dV = \iint_{A_{out}} (\text{Outlet flux of } \varphi) dA \quad (1.4-6)$$

where  $\mathfrak{R}$  is the generation rate per unit volume. If the inlet and outlet fluxes together with the generation rate are constant, then Eq. (1.4-6) reduces to

$$\left( \begin{array}{c} \text{Inlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Inlet} \\ \text{area} \end{array} \right) + \mathfrak{R} \left( \begin{array}{c} \text{System} \\ \text{volume} \end{array} \right) = \left( \begin{array}{c} \text{Outlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Outlet} \\ \text{area} \end{array} \right) \quad (1.4-7)$$

**Example 1.6** An exothermic chemical reaction takes place in a 20 cm thick slab and the energy generation rate per unit volume is  $1 \times 10^6 \text{ W/m}^3$ . The steady-state heat transfer rate into the slab at the left-hand side, i.e., at  $x = 0$ , is 280 W. Calculate the heat transfer rate to the surroundings from the right-hand side of the slab, i.e., at  $x = L$ . The surface area of each face is  $40 \text{ cm}^2$ .

**Solution**

At steady-state, there is no accumulation of energy and the use of Eq. (1.4-5) gives

$$\begin{aligned}(\text{Heat transfer rate})_{x=L} &= (\text{Heat transfer rate})_{x=0} + \mathfrak{R}(\text{Volume}) \\ &= 280 + (1 \times 10^6)(40 \times 10^{-4})(20 \times 10^{-2}) = 1080 \text{ W}\end{aligned}$$

The values of the heat fluxes at  $x = 0$  and  $x = L$  are

$$\begin{aligned}(\text{Heat flux})_{x=0} &= \frac{280}{40 \times 10^{-4}} = 70 \times 10^3 \text{ W/m}^2 \\ (\text{Heat flux})_{x=L} &= \frac{1080}{40 \times 10^{-4}} = 270 \times 10^3 \text{ W/m}^2\end{aligned}$$

**Comment:** *Even though the steady-state conditions prevail, both the heat transfer rate and the heat flux are not constant. This is due to the generation of energy within the slab.*

**REFERENCE**

Bird, R.B., W.C. Stewart and E.N. Lightfoot, 1960, Transport Phenomena, Wiley, New York.

**SUGGESTED REFERENCES FOR FURTHER STUDY**

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Felder, R.M. and R.W. Rousseau, 2000, Elementary Principles of Chemical Processes, 3<sup>rd</sup> Ed., Wiley, New York.

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## PROBLEMS

1.1 One of your friends writes down the inventory rate equation for money as

$$\left( \begin{array}{c} \text{Change in amount} \\ \text{of dollars} \end{array} \right) = (\text{Interest}) - \left( \begin{array}{c} \text{Service} \\ \text{charge} \end{array} \right) + \left( \begin{array}{c} \text{Dollars} \\ \text{deposited} \end{array} \right) - \left( \begin{array}{c} \text{Checks} \\ \text{written} \end{array} \right)$$

Identify the terms in the above equation.

1.2 Determine whether steady- or unsteady-state conditions prevail for the following cases:

- The height of water in a dam during a heavy rain,
- The weight of an athlete during a marathon,
- The temperature of an ice cube as it melts.

1.3 What is the form of the function  $\varphi(x, y)$  if  $\partial^2 \varphi / \partial x \partial y = 0$ ?

(Answer:  $\varphi(x, y) = f(x) + h(y) + C$ , where  $C$  is a constant)

1.4 Steam at a temperature of 200 °C flows through a pipe of 5 cm inside diameter and 6 cm outside diameter. The length of the pipe is 30 m. If the steady rate of heat loss per unit length of the pipe is 2 W/m, calculate the heat fluxes at the inner and outer surfaces of the pipe.

(Answer: 12.7 W/m<sup>2</sup> and 10.6 W/m<sup>2</sup>)

1.5 Dust evolves at a rate of 0.3 kg/h in a foundry which has the dimensions of 20 m × 8 m × 4 m. According to ILO (International Labor Organization) standards, the dust concentration should not exceed 20 mg/m<sup>3</sup> to protect workers' health. Determine the volumetric flow rate of ventilating air to meet the standards of ILO.

(Answer: 15,000 m<sup>3</sup>/h)

1.6 An incompressible Newtonian fluid flows in the  $z$ -direction in space between two parallel plates that are separated by a distance  $2B$  as shown in Figure 1.3 (a). The length and the width of each plate are  $L$  and  $W$ , respectively. The velocity distribution under steady conditions is given by

$$v_z = \frac{|\Delta P| B^2}{2 \mu L} \left[ 1 - \left( \frac{x}{B} \right)^2 \right]$$

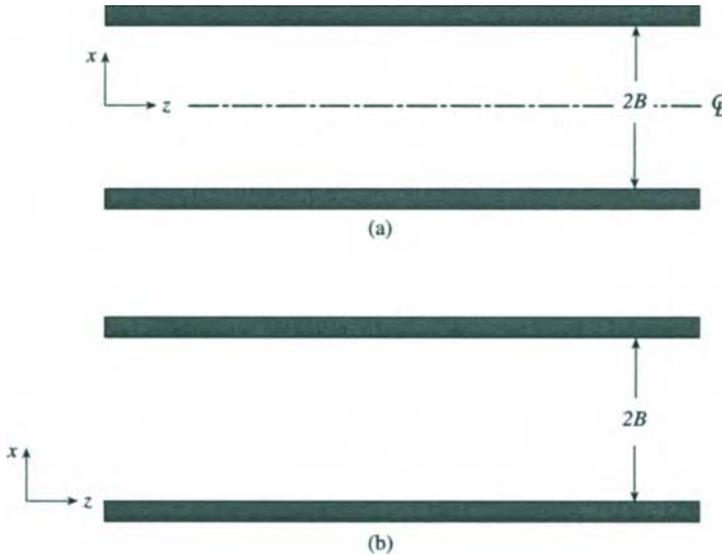


Figure 1.3 Flow between parallel plates.

a) For the coordinate system shown in Figure 1.3 (b), show that the velocity distribution takes the form

$$v_z = \frac{|\Delta P| B^2}{2 \mu L} \left[ 2 \left( \frac{x}{B} \right) - \left( \frac{x}{B} \right)^2 \right]$$

b) Calculate the volumetric flow rate by using the velocity distributions given above. What is your conclusion?

(Answer: b) For both cases  $Q = \frac{2 |\Delta P| B^3 W}{3 \mu L}$ )

1.7 An incompressible Newtonian fluid flows in the  $z$ -direction through a straight duct of triangular cross-sectional area, bounded by the plane surfaces  $y = H$ ,  $y = \sqrt{3} x$  and  $y = -\sqrt{3} x$ . The velocity distribution under steady conditions is given by

$$v_z = \frac{|\Delta P|}{4 \mu L H} (y - H) (3 x^2 - y^2)$$

Calculate the volumetric flow rate.

(Answer:  $Q = \frac{\sqrt{3} H^4 |\Delta P|}{180 \mu L}$ )

1.8 For radial flow of an incompressible Newtonian fluid between two parallel circular disks of radius  $R_2$  as shown in Figure 1.4, the steady-state velocity distribution is (Bird *et al.*, 1960)

$$v_r = \frac{b^2 |\Delta P|}{2 \mu r \ln(R_2/R_1)} \left[ 1 - \left( \frac{z}{b} \right)^2 \right]$$

where  $R_1$  is the radius of the entrance hole. Determine the volumetric flow rate.

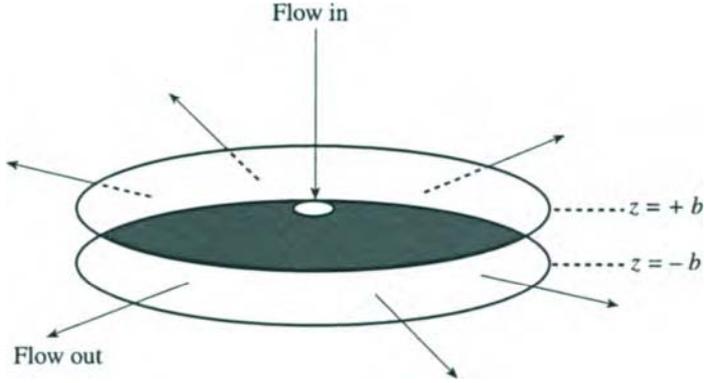


Figure 1.4 Flow between circular disks.

$$\left( \text{Answer: } Q = \frac{4}{3} \frac{\pi b^3 |\Delta P|}{\ln(R_2/R_1)} \right)$$

## Chapter 2

# Molecular and Convective Transport

The total flux of any quantity is the sum of the molecular and convective fluxes. The fluxes arising from potential gradients or driving forces are called *molecular fluxes*. Molecular fluxes are expressed in the form of *constitutive* (or, *phenomenological*) *equations* for momentum, energy, and mass transport. Momentum, energy, and mass can also be transported by bulk fluid motion or bulk flow and the resulting flux is called *convective flux*. This chapter deals with the formulation of molecular and convective fluxes in momentum, energy and mass transport.

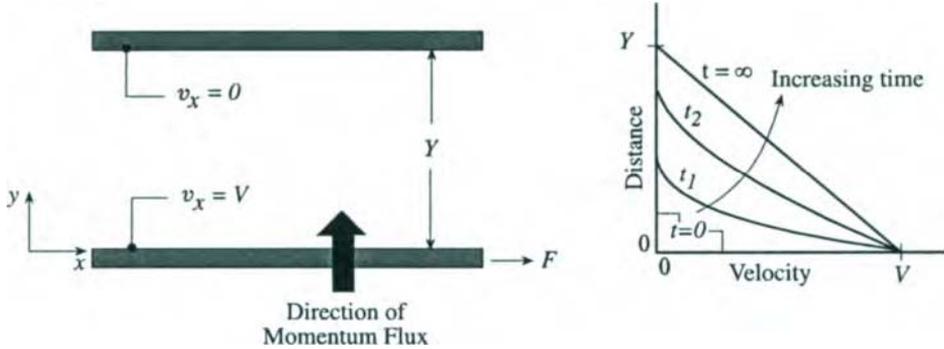
## 2.1 MOLECULAR TRANSPORT

Substances may behave differently when subjected to the same gradients. *Constitutive equations* identify the characteristics of a particular substance. For example, if the gradient is momentum, then the viscosity is defined by the constitutive equation called *Newton's law of viscosity*. If the gradient is energy, then the thermal conductivity is defined by *Fourier's law of heat conduction*. If the gradient is concentration, then the diffusion coefficient is defined by *Fick's first law of diffusion*. Viscosity, thermal conductivity and diffusion coefficient are called *transport properties*.

### 2.1.1 Newton's Law of Viscosity

Consider a fluid contained between two large parallel plates of area  $A$ , separated by a very small distance  $Y$ . The system is initially at rest but at time  $t = 0$ , the lower plate is set in motion in the  $x$ -direction at a constant velocity  $V$  by applying a force  $F$  in the  $x$ -direction while the upper plate is kept stationary. The resulting velocity profiles are shown in Figure 2.1 for various times. At  $t = 0$ ,

the velocity is zero everywhere except at the lower plate which has a velocity  $V$ . Then the velocity distribution starts to develop as a function of time. Finally, at steady-state, a linear velocity distribution is obtained.



**Figure 2.1** Velocity profile development in flow between parallel plates.

Experimental results show that the force required to maintain the motion of the lower plate per unit area (or, momentum flux) is proportional to the velocity gradient, i.e.,

$$\underbrace{\frac{F}{A}}_{\text{Momentum flux}} = \underbrace{\mu}_{\text{Transport property}} \underbrace{\frac{V}{Y}}_{\text{Velocity gradient}} \quad (2.1-1)$$

and the proportionality constant,  $\mu$ , is the *viscosity*. Equation (2.1-1) is a macroscopic equation. Microscopic form of this equation is given by

$$\tau_{yx} = -\mu \frac{dv_x}{dy} = -\mu \dot{\gamma}_{yx} \quad (2.1-2)$$

which is known as *Newton's law of viscosity* and any fluid obeying Eq. (2.1-2) is called a *Newtonian fluid*. The term  $\dot{\gamma}_{yx}$  is called *rate of strain*<sup>1</sup> or *rate of deformation* or *shear rate*. The term  $\tau_{yx}$  is called *shear stress*. It contains two subscripts,  $x$  which represents the direction of force, and  $y$  which represents the direction of the normal to the surface on which the force is acting. Therefore, it is possible to interpret  $\tau_{yx}$  as the flux of  $x$ -momentum in the  $y$ -direction.

Since the velocity gradient is negative, i.e.,  $v_x$  decreases with increasing  $y$ , a negative sign is introduced on the right-hand side of Eq. (2.1-2) so that the stress in tension is positive.

<sup>1</sup>Strain is defined as deformation per unit length. For example, if a spring of original length  $L_o$  is stretched to a length  $L$ , then the strain is  $(L - L_o)/L_o$ .

In SI units, shear stress is expressed in  $\text{N}/\text{m}^2$  (Pa) and velocity gradient in  $(\text{m}/\text{s})/\text{m}$ . Thus, the examination of Eq. (2.1-1) indicates that the units of viscosity in SI units are

$$\mu = \frac{\text{N}/\text{m}^2}{(\text{m}/\text{s})/\text{m}} = \text{Pa} \cdot \text{s} = \frac{\text{N} \cdot \text{s}}{\text{m}^2} = \frac{(\text{kg} \cdot \text{m}/\text{s}^2) \cdot \text{s}}{\text{m}^2} = \frac{\text{kg}}{\text{m} \cdot \text{s}}$$

Most viscosity data in the cgs system are usually reported in  $\text{g}/(\text{cm} \cdot \text{s})$ , known as a poise (P), or in centipoise ( $1 \text{ cP} = 0.01 \text{ P}$ ) where

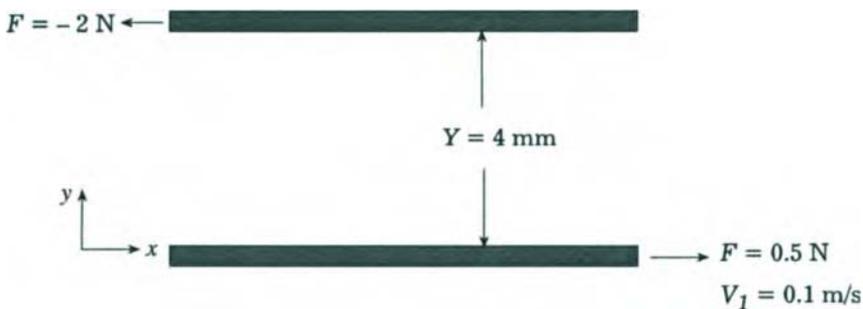
$$1 \text{ Pa} \cdot \text{s} = 10 \text{ P} = 10^3 \text{ cP}$$

Viscosity varies with temperature. While liquid viscosity decreases with increasing temperature, gas viscosity increases with increasing temperature. Concentration also affects viscosity for solutions or suspensions. Viscosity values of various substances are given in Table D.1 in Appendix D.

**Example 2.1** A Newtonian fluid with a viscosity of 10 cP is placed between two large parallel plates. The distance between the plates is 4 mm. The lower plate is pulled in the positive  $x$ -direction with a force of 0.5 N, while the upper plate is pulled in the negative  $x$ -direction with a force of 2 N. Each plate has an area of  $2.5 \text{ m}^2$ . If the velocity of the lower plate is 0.1 m/s, calculate:

- The steady-state momentum flux,
- The velocity of the upper plate,
- Parts (a) and (b) for a Newtonian fluid with  $\mu = 1 \text{ cP}$ .

**Solution**



- The momentum flux (or, force per unit area) is

$$\begin{aligned} \tau_{yx} &= \frac{F}{A} \\ &= \frac{0.5 + 2}{2.5} = 1 \text{ Pa} \end{aligned}$$

b) From Eq. (2.1-2)

$$\tau_{yx} \int_0^Y dy = -\mu \int_{V_1}^{V_2} dv_x \quad \Rightarrow \quad V_2 = V_1 - \frac{\tau_{yx} Y}{\mu} \quad (1)$$

Substitution of the values into Eq. (1) gives

$$V_2 = 0.1 - \frac{(1)(4 \times 10^{-3})}{10 \times 10^{-3}} = -0.3 \text{ m/s} \quad (2)$$

The minus sign indicates that the upper plate moves in the negative  $x$ -direction. Note that the velocity gradient is  $dv_x/dy = -100 \text{ s}^{-1}$ .

c) Since the momentum flux is the same irrespective of the fluid,  $\tau_{yx} = 1 \text{ Pa}$ .

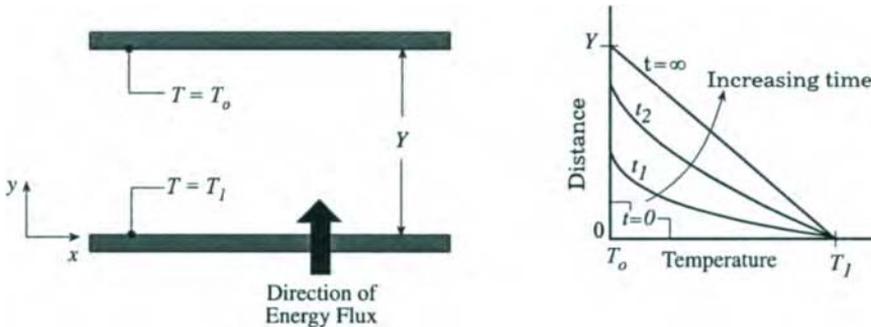
$$\begin{aligned} V_2 &= V_1 - \frac{\tau_{yx} Y}{\mu} \\ &= 0.1 - \frac{(1)(4 \times 10^{-3})}{1 \times 10^{-3}} = -3.9 \text{ m/s} \end{aligned} \quad (3)$$

The velocity gradient in this case is  $dv_x/dy = -1000 \text{ s}^{-1}$ .

**Comment:** Viscosity is a measure of the ability of the fluid to transfer momentum. Therefore, the decrease in viscosity causes a steeper velocity gradient.

### 2.1.2 Fourier's Law of Heat Conduction

Consider a slab of solid material of area  $A$  between two large parallel plates of a distance  $Y$  apart. Initially the solid material is at a temperature  $T_o$  throughout. Then the lower plate is suddenly brought to a slightly higher temperature  $T_1$  and maintained at that temperature. The second law of thermodynamics states that heat flows spontaneously from the higher temperature  $T_1$  to the lower temperature  $T_o$ . As time proceeds, the temperature profile in the slab changes, and ultimately a linear steady-state temperature is attained as shown in Figure 2.3.



**Figure 2.3** Temperature profile development in a solid slab between two plates.

Experimental measurements made at steady-state indicate that the rate of heat flow per unit area is proportional to the temperature gradient, i.e.,

$$\underbrace{\frac{\dot{Q}}{A}}_{\text{Energy flux}} = \underbrace{k}_{\text{Transport property}} \underbrace{\frac{T_1 - T_o}{Y}}_{\text{Temperature gradient}} \quad (2.1-3)$$

The proportionality constant,  $k$ , between the energy flux and the temperature gradient is called *thermal conductivity*. In SI units,  $\dot{Q}$  is in W(J/s),  $A$  in  $\text{m}^2$ ,  $dT/dx$  in K/m, and  $k$  in W/(m.K). The thermal conductivity of a material is, in general, a function of temperature. However, in many engineering applications the variation is sufficiently small to be neglected. Thermal conductivity values for various substances are given in Table D.2 in Appendix D.

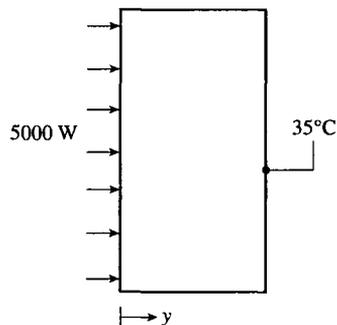
The microscopic form of Eq. (2.1-3) is known as *Fourier's law of heat conduction* and is given by

$$\boxed{q_y = -k \frac{dT}{dy}} \quad (2.1-4)$$

in which the subscript  $y$  indicates the direction of the energy flux. The negative sign in Eq. (2.1-4) indicates that heat flows in the direction of decreasing temperature.

**Example 2.2** *One side of a copper slab receives a net heat input at a rate of 5000 W due to radiation. The other face is held at a temperature of 35°C. If steady-state conditions prevail, calculate the surface temperature of the side receiving radiant energy. The surface area of each face is 0.05  $\text{m}^2$ , and the slab thickness is 4 cm.*

**Solution**



**Physical properties**

*For copper:*  $k = 398 \text{ W/m.K}$

### Analysis

*System: Copper slab*

*Under steady conditions with no internal generation, conservation statement for energy reduces to*

$$\text{Rate of energy in} = \text{Rate of energy out} = 5000 \text{ W}$$

*Since the slab area across which heat transfer takes place is constant, the heat flux through the slab is also constant and is given by*

$$q_y = \frac{5000}{0.05} = 100,000 \text{ W/m}^2$$

*Therefore, the use of Fourier's law of heat conduction, Eq. (2.1-4), gives*

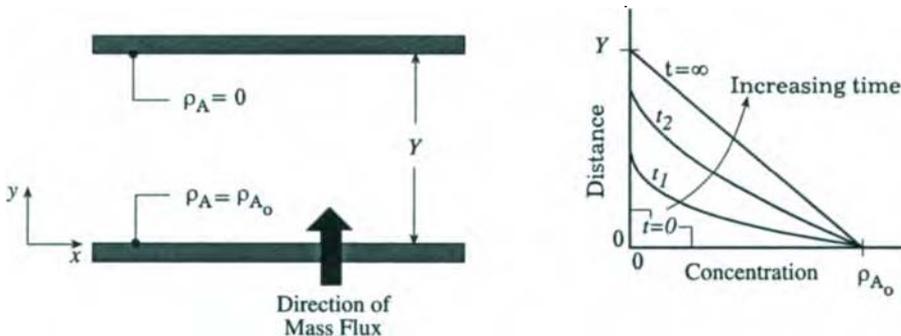
$$100,000 \int_0^{0.04} dy = -398 \int_{T_o}^{35} dT$$

*or,*

$$T_o = 45.1^\circ\text{C}$$

### 2.1.3 Fick's First Law of Diffusion

Consider two large parallel plates of area  $A$ . The lower one is coated with a material  $A$  which has a very low solubility in the stagnant fluid  $B$  filling the space between the plates. Suppose that the saturation concentration of  $A$  is  $\rho_{A_o}$  and  $A$  undergoes a rapid chemical reaction at the surface of the upper plate and its concentration is zero at that surface. At  $t = 0$  the lower plate is exposed to the fluid  $B$  and as time proceeds, the concentration profile develops as shown in Figure 2.4. Since the solubility of  $A$  is low, an almost a linear distribution is reached under steady conditions.



**Figure 2.4** Concentration profile development between parallel plates.

Experimental measurements indicate that the mass flux of  $\mathcal{A}$  is proportional to the concentration gradient, i.e.,

$$\underbrace{\frac{\dot{m}_A}{A}}_{\text{Mass flux of } \mathcal{A}} = \underbrace{D_{AB}}_{\text{Transport property}} \underbrace{\frac{\rho_{A_0}}{Y}}_{\text{Concentration gradient}} \quad (2.1-5)$$

where the proportionality constant,  $D_{AB}$ , is called the *binary molecular mass diffusivity* (or, *diffusion coefficient*) of species  $\mathcal{A}$  through  $\mathcal{B}$ . The microscopic form of Eq. (2.1-5) is known as *Fick's first law of diffusion* and is given by

$$j_{A_y} = -D_{AB} \rho \frac{d\omega_A}{dy} \quad (2.1-6)$$

where  $j_{A_y}$  and  $\omega_A$  represent the molecular mass flux of species  $\mathcal{A}$  in the  $y$ -direction and mass fraction of species  $\mathcal{A}$ , respectively. If the total density,  $\rho$ , is constant, then the term  $\rho(d\omega_A/dy)$  can be replaced by  $d\rho_A/dy$  and Eq. (2.1-6) becomes

$$j_{A_y} = -D_{AB} \frac{d\rho_A}{dy} \quad \rho = \text{constant} \quad (2.1-7)$$

To measure  $D_{AB}$  experimentally, it is necessary to design an experiment (like the one given above) in which the convective mass flux is almost zero.

In mass transfer calculations, it is sometimes more convenient to express concentrations in molar units rather than mass units. In terms of molar concentration, Fick's first law of diffusion is written as

$$J_{A_y}^* = -D_{AB} c \frac{dx_A}{dy} \quad (2.1-8)$$

where  $J_{A_y}^*$  and  $x_A$  represent the molecular molar flux of species  $\mathcal{A}$  in the  $y$ -direction and mole fraction of species  $\mathcal{A}$ , respectively. If the total molar concentration,  $c$ , is constant, then the term  $c(dx_A/dy)$  can be replaced by  $dc_A/dy$  and Eq. (2.1-8) becomes

$$J_{A_y}^* = -D_{AB} \frac{dc_A}{dy} \quad c = \text{constant} \quad (2.1-9)$$

Diffusion coefficient has the dimensions of  $\text{m}^2/\text{s}$  in SI units. Typical values of  $D_{AB}$  are given in Appendix D. Examination of these values indicates that the diffusion coefficient of gases has an order of magnitude of  $10^{-5} \text{m}^2/\text{s}$  under atmospheric conditions. Assuming ideal gas behavior, the pressure and temperature dependence of the diffusion coefficient of gases may be estimated from the relation

$$D_{AB} \propto \frac{T^{3/2}}{P} \quad (2.1-10)$$

Diffusion coefficients for liquids are usually in the order of  $10^{-9}$  m<sup>2</sup>/s. On the other hand,  $\mathcal{D}_{AB}$  values for solids vary from  $10^{-10}$  to  $10^{-14}$  m<sup>2</sup>/s.

**Example 2.3** Air at atmospheric pressure and 95 °C flows at 20 m/s over a flat plate of naphthalene 80 cm long in the direction of flow and 60 cm wide. Experimental measurements report the molar concentration of naphthalene in the air,  $c_A$ , as a function of distance  $x$  from the plate as follows:

$x$ (cm)	$c_A$ (mol/m <sup>3</sup> )
0	0.117
10	0.093
20	0.076
30	0.063
40	0.051
50	0.043

Determine the molar flux of naphthalene from the plate surface under steady conditions.

### Solution

#### Physical properties

Diffusion coefficient of naphthalene (A) in air (B) at 95 °C (368 K) :

$$\begin{aligned} (\mathcal{D}_{AB})_{368} &= (\mathcal{D}_{AB})_{300} \left( \frac{368}{300} \right)^{3/2} = (0.62 \times 10^{-5}) \left( \frac{368}{300} \right)^{3/2} \\ &= 0.84 \times 10^{-5} \text{ m}^2/\text{s} \end{aligned}$$

#### Assumptions

1. The total molar concentration,  $c$ , is constant.
2. Naphthalene plate is also at a temperature of 95 °C.

#### Analysis

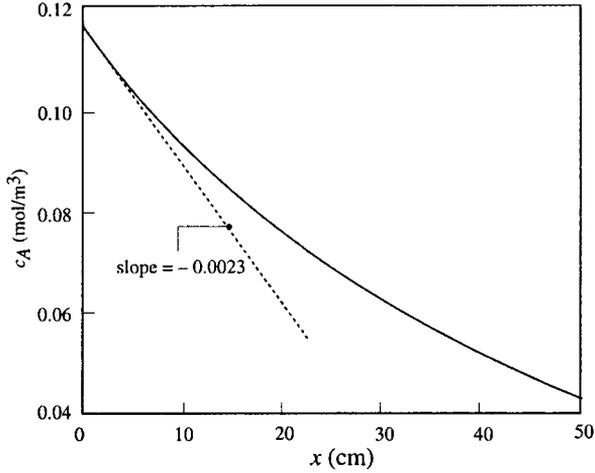
The molar flux of naphthalene transferred from the plate surface to the flowing stream is determined from

$$J_{A_x}^* \Big|_{x=0} = -\mathcal{D}_{AB} \left( \frac{dc_A}{dx} \right)_{x=0} \quad (1)$$

It is possible to calculate the concentration gradient on the surface of the plate by using one of the several methods explained in Section A.5 in Appendix A.

**Graphical method**

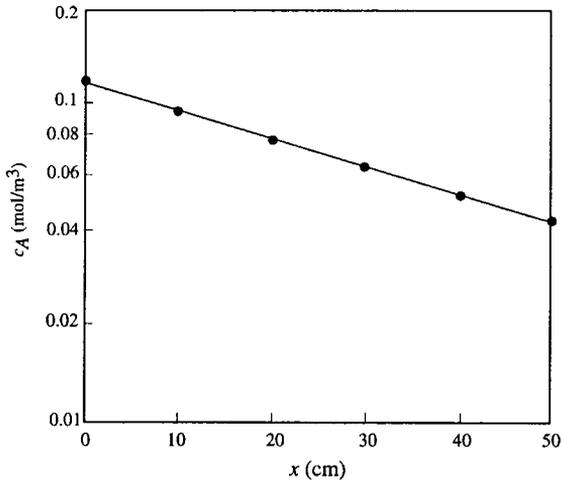
The plot of  $c_A$  versus  $x$  is given in Figure 2.5. The slope of the tangent to the curve at  $x = 0$  is  $-0.0023 \text{ (mol/m}^3\text{)/cm}$ .



**Figure 2.5** Concentration of species  $A$  as a function of position.

**Curve fitting method**

Semi-log plot of  $c_A$  versus  $x$  is shown in Figure 2.6.



**Figure 2.6** Concentration of species  $A$  as a function of position.

It appears from Figure 2.6 that a straight line represents the data fairly well. The equation of this line can be determined by the method of least squares in the form

$$y = mx + b \quad (2)$$

where

$$y = \log c_A \quad (3)$$

To determine the values of  $m$  and  $b$  from Eqs. (A.6-10) and (A.6-11) in Appendix A, the required values are calculated as follows:

$y_i$	$x_i$	$x_i y_i$	$x_i^2$
-0.932	0	0	0
-1.032	10	-10.32	100
-1.119	20	-22.38	400
-1.201	30	-36.03	900
-1.292	40	-51.68	1600
-1.367	50	-68.35	2500
<hr/>			
$\sum y_i = -6.943$	$\sum x_i = 150$	$\sum x_i y_i = -188.76$	$\sum x_i^2 = 5500$

The values of  $m$  and  $b$  are

$$m = \frac{(6)(-188.76) - (150)(-6.943)}{(6)(5500) - (150)^2} = -0.0087$$

$$b = \frac{(-6.943)(5500) - (150)(-188.76)}{(6)(5500) - (150)^2} = -0.94$$

Therefore, Eq. (2) takes the form

$$\log c_A = -0.087x - 0.94 \quad (4)$$

or,

$$c_A = 0.115 e^{-0.02x} \quad (5)$$

Differentiation of Eq. (5) gives the concentration gradient on the surface of the plate as

$$\left( \frac{dc_A}{dx} \right)_{x=0} = -(0.115)(0.02) = -0.0023 \text{ (mol/m}^3\text{)}/\text{cm} = -0.23 \text{ mol/m}^4 \quad (6)$$

Substitution of the numerical values into Eq. (1) gives the molar flux of naphthalene from the surface as

$$J_{A_x}^* \Big|_{x=0} = (0.84 \times 10^{-5})(0.23) = 19.32 \times 10^{-7} \text{ mol/m}^2 \cdot \text{s}$$

## 2.2 DIMENSIONLESS NUMBERS

Newton's "law" of viscosity, Fourier's "law" of heat conduction, and Fick's first "law" of diffusion, in reality, **are not laws** but defining equations for viscosity,  $\mu$ , thermal conductivity,  $k$ , and diffusion coefficient,  $\mathcal{D}_{AB}$ . The fluxes ( $\tau_{yx}$ ,  $q_y$ ,  $j_{A_y}$ ) and the gradients ( $dv_x/dy$ ,  $dT/dy$ ,  $d\rho_A/dy$ ) must be known or measurable for the experimental determination of  $\mu$ ,  $k$ , and  $\mathcal{D}_{AB}$ .

Newton's law of viscosity, Eq. (2.1-2), Fourier's law of heat conduction, Eq. (2.1-4), and Fick's first law of diffusion, Eqs. (2.1-7) and (2.1-9), can be generalized as

$$\boxed{\left( \begin{array}{c} \text{Molecular} \\ \text{flux} \end{array} \right) = \left( \begin{array}{c} \text{Transport} \\ \text{property} \end{array} \right) \left( \begin{array}{c} \text{Gradient of} \\ \text{driving force} \end{array} \right)} \quad (2.2-1)$$

Although the constitutive equations are similar, they are not completely analogous because the transport properties ( $\mu$ ,  $k$ ,  $\mathcal{D}_{AB}$ ) have different units. These equations can also be expressed in the following forms:

$$\tau_{yx} = -\frac{\mu}{\rho} \frac{d}{dy}(\rho v_x) \quad \rho = \text{constant} \quad \rho v_x = \text{momentum/volume} \quad (2.2-2)$$

$$q_y = -\frac{k}{\rho \hat{C}_P} \frac{d}{dy}(\rho \hat{C}_P T) \quad \rho \hat{C}_P = \text{constant} \quad \rho \hat{C}_P T = \text{energy/volume} \quad (2.2-3)$$

$$j_{A_y} = -\mathcal{D}_{AB} \frac{d\rho_A}{dy} \quad \rho = \text{constant} \quad \rho_A = \text{mass of } A/\text{volume} \quad (2.2-4)$$

The term  $\mu/\rho$  in Eq. (2.2-2) is called *momentum diffusivity* or *kinematic viscosity*, and the term  $k/\rho\hat{C}_P$  in Eq. (2.2-3) is called *thermal diffusivity*. Momentum and thermal diffusivities are designated by  $\nu$  and  $\alpha$ , respectively. Note that the terms  $\nu$ ,  $\alpha$ , and  $\mathcal{D}_{AB}$  all have the same units,  $\text{m}^2/\text{s}$ , and Eqs. (2.2-2)-(2.2-4) can be expressed in the general form as

$$\boxed{\left( \begin{array}{c} \text{Molecular} \\ \text{flux} \end{array} \right) = (\text{Diffusivity}) \left( \begin{array}{c} \text{Gradient of} \\ \text{Quantity/Volume} \end{array} \right)} \quad (2.2-5)$$

The quantities that appear in Eqs. (2.2-1) and (2.2-5) are summarized in Table 2.1. Since the terms  $\nu$ ,  $\alpha$ , and  $\mathcal{D}_{AB}$  all have the same units, the ratio of any two of these diffusivities results in a dimensionless number. For example, the ratio of momentum diffusivity to thermal diffusivity gives the *Prandtl number*,  $\text{Pr}$ :

$$\text{Prandtl number} = \text{Pr} = \frac{\nu}{\alpha} = \frac{\hat{C}_P \mu}{k} \quad (2.2-6)$$

The Prandtl number is a function of temperature and pressure. However, its dependence on temperature, at least for liquids, is much stronger. The order of magnitude of the Prandtl number for gases and liquids can be estimated as

**Table 2.1** Analogous terms in constitutive equations for momentum, energy, and mass (or, mole) transfer in one-dimension.

	Momentum	Energy	Mass	Mole
Molecular flux	$\tau_{yx}$	$q_y$	$j_{A_v}$	$J_{A_v}^*$
Transport property	$\mu$	$k$	$\mathcal{D}_{AB}$	$\mathcal{D}_{AB}$
Gradient of driving force	$\frac{dv_x}{dy}$	$\frac{dT}{dy}$	$\frac{d\rho_A}{dy}$	$\frac{dc_A}{dy}$
Diffusivity	$\nu$	$\alpha$	$\mathcal{D}_{AB}$	$\mathcal{D}_{AB}$
Quantity/Volume	$\rho v_x$	$\rho \hat{C}_P T$	$\rho_A$	$c_A$
Gradient of Quantity/Volume	$\frac{d(\rho v_x)}{dy}$	$\frac{d(\rho \hat{C}_P T)}{dy}$	$\frac{d\rho_A}{dy}$	$\frac{dc_A}{dy}$

$$\text{Pr} = \frac{(10^3)(10^{-5})}{10^{-2}} = 1 \quad \text{for gases}$$

$$\text{Pr} = \frac{(10^3)(10^{-3})}{10^{-1}} = 10 \quad \text{for liquids}$$

The *Schmidt number* is defined as the ratio of the momentum to mass diffusivities:

$$\text{Schmidt number} = \text{Sc} = \frac{\nu}{\mathcal{D}_{AB}} = \frac{\mu}{\rho \mathcal{D}_{AB}} \quad (2.2-7)$$

The order of magnitude of the Schmidt number for gases and liquids can be estimated as

$$\text{Sc} = \frac{10^{-5}}{(1)(10^{-5})} = 1 \quad \text{for gases}$$

$$\text{Sc} = \frac{10^{-3}}{(10^3)(10^{-9})} = 10^3 \quad \text{for liquids}$$

Finally, the ratio of  $\alpha$  to  $\mathcal{D}_{AB}$  gives the *Lewis number*, *Le*:

$$\text{Lewis number} = \text{Le} = \frac{\alpha}{\mathcal{D}_{AB}} = \frac{k}{\rho \hat{C}_P \mathcal{D}_{AB}} = \frac{\text{Sc}}{\text{Pr}} \quad (2.2-8)$$

## 2.3 CONVECTIVE TRANSPORT

Convective flux or bulk flux of a quantity is expressed as

$$\left( \begin{array}{c} \text{Convective} \\ \text{flux} \end{array} \right) = (\text{Quantity/Volume}) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right) \quad (2.3-1)$$

When air is pumped through a pipe, it is considered to be a single phase and a single component system. In this case, there is no ambiguity in defining the characteristic velocity. However, if the oxygen in the air were reacting, then the fact that air is composed predominantly of two species,  $O_2$  and  $N_2$ , had to be taken into account. Hence, air should be considered a single phase, binary component system. For a single phase system composed of  $n$  components, the general definition of a characteristic velocity is given by

$$v_{ch} = \sum_i^n \beta_i v_i \quad (2.3-2)$$

where  $\beta_i$  is the weighting factor and  $v_i$  is the velocity of a constituent. The three most common characteristic velocities are listed in Table 2.2. The term  $\bar{V}_i$  in the definition of the volume average velocity represents the partial molar volume of a constituent. The molar average velocity is equal to the volume average velocity when the total molar concentration,  $c$ , is constant. On the other hand, the mass average velocity is equal to the volume average velocity when the total mass density,  $\rho$ , is constant.

**Table 2.2** Common characteristic velocities.

Characteristic Velocity	Weighting Factor	Formulation
Mass average	Mass fraction ( $\omega_i$ )	$v = \sum_i \omega_i v_i$
Molar average	Mole fraction ( $x_i$ )	$v^* = \sum_i x_i v_i$
Volume average	Volume fraction ( $c_i \bar{V}_i$ )	$v^\square = \sum_i c_i \bar{V}_i v_i$

The choice of a characteristic velocity is arbitrary. For a given problem, it is more convenient to select a characteristic velocity which will make the convective flux zero and thus yield a simpler problem. In the literature, it is common practice to use the molar average velocity for dilute gases, i.e.,  $c = \text{constant}$ , and the mass average velocity for liquids, i.e.,  $\rho = \text{constant}$ .

It should be noted that the molecular mass flux expression given by Eq. (2.1-6) represents the molecular mass flux with respect to the mass average velocity. Therefore, in the equation representing the total mass flux, the characteristic velocity in the convective mass flux term is taken as the mass average velocity. On the other hand, Eq. (2.1-8) is the molecular molar flux with respect to the molar average velocity. Therefore, the molar average velocity is considered to be the characteristic velocity in the convective molar flux term.

## 2.4 TOTAL FLUX

Since the total flux of any quantity is the sum of its molecular and convective fluxes, then

$$\left( \begin{array}{c} \text{Total} \\ \text{flux} \end{array} \right) = \underbrace{\left( \begin{array}{c} \text{Transport} \\ \text{property} \end{array} \right) \left( \begin{array}{c} \text{Gradient of} \\ \text{driving force} \end{array} \right)}_{\text{Molecular flux}} + \underbrace{\left( \frac{\text{Quantity}}{\text{Volume}} \right) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right)}_{\text{Convective flux}} \quad (2.4-1)$$

or,

$$\left( \begin{array}{c} \text{Total} \\ \text{flux} \end{array} \right) = \underbrace{(\text{Diffusivity}) \left( \begin{array}{c} \text{Gradient of} \\ \text{Quantity/Volume} \end{array} \right)}_{\text{Molecular flux}} + \underbrace{\left( \frac{\text{Quantity}}{\text{Volume}} \right) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right)}_{\text{Convective flux}} \quad (2.4-2)$$

The quantities that appear in Eqs. (2.4-1) and (2.4-2) are given in Table 2.3.

**Table 2.3** Analogous terms in flux expressions for various types of transport in one-dimension.

Type of Transport	Total Flux	Molecular Flux	Convective Flux	Constraint
Momentum	$\pi_{yx}$	$-\mu \frac{dv_x}{dy}$	$(\rho v_x) v_y$	None
		$-\nu \frac{d(\rho v_x)}{dy}$		$\rho = \text{const.}$
Energy	$e_y$	$-k \frac{dT}{dy}$	$(\rho \hat{C}_P T) v_y$	None
		$-\alpha \frac{d(\rho \hat{C}_P T)}{dy}$		$\rho \hat{C}_P = \text{const.}$
Mass	$\mathcal{W}_{A_y}$	$-\rho \mathcal{D}_{AB} \frac{d\omega_A}{dy}$	$\rho_A v_y$	None
		$-\mathcal{D}_{AB} \frac{d\rho_A}{dy}$		$\rho = \text{const.}$
Mole	$N_{A_y}$	$-c \mathcal{D}_{AB} \frac{dx_A}{dy}$	$c_A v_y^*$	None
		$-\mathcal{D}_{AB} \frac{dc_A}{dy}$		$c = \text{const.}$

The general flux expressions for momentum, energy and mass transport in different coordinate systems are given in Appendix C.

From Eq. (2.4-2), the ratio of the convective flux to the molecular flux is given by

$$\frac{\text{Convective flux}}{\text{Molecular flux}} = \frac{(\text{Quantity/Volume})(\text{Characteristic velocity})}{(\text{Diffusivity})(\text{Gradient of Quantity/Volume})} \quad (2.4-3)$$

Since the gradient of a quantity represents the variation of that particular quantity over a characteristic length, the "Gradient of Quantity/Volume" can be expressed as

$$\text{Gradient of Quantity/Volume} = \frac{\text{Difference in Quantity/Volume}}{\text{Characteristic length}} \quad (2.4-4)$$

The use of Eq. (2.4-4) in Eq. (2.4-3) gives

$$\frac{\text{Convective flux}}{\text{Molecular flux}} = \frac{(\text{Characteristic velocity})(\text{Characteristic length})}{\text{Diffusivity}} \quad (2.4-5)$$

The ratio of the convective flux to the molecular flux is known as the *Peclet number*,  $Pe$ . Therefore, Peclet numbers for heat and mass transfers are

$$Pe_H = \frac{v_{ch}L_{ch}}{\alpha} \quad (2.4-6)$$

$$Pe_M = \frac{v_{ch}L_{ch}}{D_{AB}} \quad (2.4-7)$$

Hence, the total flux of any quantity is given by

$$\text{Total flux} = \begin{cases} \text{Molecular flux} & Pe \ll 1 \\ \text{Molecular flux} + \text{Convective flux} & Pe \simeq 1 \\ \text{Convective flux} & Pe \gg 1 \end{cases} \quad (2.4-8)$$

### 2.4.1 Rate of Mass Entering and/or Leaving the System

The mass flow rate of species  $i$  entering and/or leaving the system,  $\dot{m}_i$ , is expressed as

$$\dot{m}_i = \left[ \underbrace{\left( \frac{\text{Mass}}{\text{Diffusivity}} \right) \left( \frac{\text{Gradient of Mass of } i/\text{Volume}}{\text{Molecular mass flux of species } i} \right)}_{\text{Molecular mass flux of species } i} + \underbrace{\left( \frac{\text{Mass of } i}{\text{Volume}} \right) \left( \frac{\text{Characteristic velocity}}{\text{Convective mass flux of species } i} \right)}_{\text{Convective mass flux of species } i} \right] \left( \text{Flow area} \right) \quad (2.4-9)$$

In general, the mass of species  $i$  may enter and/or leave the system by two means:

- Entering and/or leaving conduits,
- Exchange of mass between the system and its surroundings through the boundaries of the system, i.e., interphase transport.

When a mass of species  $i$  enters and/or leaves the system by a conduit(s), the characteristic velocity is taken as the average velocity of the flowing stream and it is usually large enough to neglect the molecular flux compared to the convective flux, i.e.,  $Pe_M \gg 1$ . Therefore, Eq. (2.4-9) simplifies to

$$\dot{m}_i = \left( \frac{\text{Mass of } i}{\text{Volume}} \right) \left( \text{Average velocity} \right) \left( \text{Flow area} \right) \quad (2.4-10)$$

or,

$$\dot{m}_i = \rho_i \langle v \rangle A = \rho_i Q \quad (2.4-11)$$

Summation of Eq. (2.4-11) over all species leads to the total mass flow rate,  $\dot{m}$ , entering and/or leaving the system by a conduit in the form

$$\dot{m} = \rho \langle v \rangle A = \rho Q \quad (2.4-12)$$

In terms of molar basis, Eqs. (2.4-11) and (2.4-12) take the form

$$\dot{n}_i = c_i \langle v \rangle A = c_i Q \quad (2.4-13)$$

$$\dot{n} = c \langle v \rangle A = c Q \quad (2.4-14)$$

On the other hand, when a mass of species  $i$  enters and/or leaves the system as a result of interphase transport, the flux expression to be used is dictated by the value of the Peclet number as shown in Eq. (2.4-8).

**Example 2.4** *Liquid B is flowing over a vertical plate as shown in Figure 2.7. The surface of the plate is coated with a material A which has a very low solubility in liquid B. The concentration distribution of species A in the liquid is given by Bird et al. (1960) as*

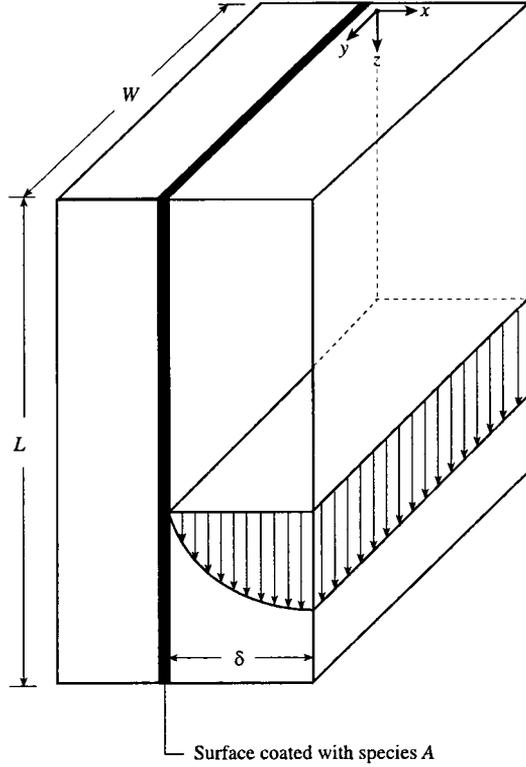
$$\frac{c_A}{c_{A_o}} = \frac{1}{\Gamma(4/3)} \int_{\eta}^{\infty} e^{-u^3} du$$

where  $c_{A_o}$  is the solubility of A in B,  $\eta$  is the dimensionless parameter defined by

$$\eta = x \left( \frac{\rho g \delta}{9 \mu D_{AB} z} \right)^{1/3}$$

and  $\Gamma(4/3)$  is the gamma function defined by

$$\Gamma(n) = \int_0^{\infty} \beta^{n-1} e^{-\beta} d\beta \quad n > 0$$



**Figure 2.7** Solid dissolution into a falling film.

*Calculate the rate of transfer of species A into the flowing liquid.*

**Solution**

**Assumptions**

1. The total molar concentration in the liquid phase is constant.
2. In the  $x$ -direction, the convective flux is small compared to the molecular flux.

**Analysis**

The molar rate of transfer of species A can be calculated from the expression

$$\dot{n}_A = \int_0^W \int_0^L N_{A_x}|_{x=0} dz dy \quad (1)$$

where the total molar flux of species  $A$  at the interface,  $N_{A_x}|_{x=0}$ , is given by

$$N_{A_x}|_{x=0} = J_{A_x}^*|_{x=0} = -D_{AB} \left( \frac{\partial c_A}{\partial x} \right)_{x=0} \quad (2)$$

By the application of the chain rule, Eq. (2) takes the form

$$N_{A_x}|_{x=0} = -D_{AB} \frac{\partial \eta}{\partial x} \left( \frac{dc_A}{d\eta} \right)_{\eta=0} \quad (3)$$

The term  $\partial \eta / \partial x$  is

$$\frac{\partial \eta}{\partial x} = \left( \frac{\rho g \delta}{9 \mu D_{AB} z} \right)^{1/3} \quad (4)$$

On the other hand, the term  $dc_A/d\eta$  can be calculated by the application of the Leibnitz formula, i.e., Eq. (A.4-3) in Appendix A, as

$$\frac{dc_A}{d\eta} = -\frac{c_{A_o}}{\Gamma(4/3)} e^{-\eta^3} \quad (5)$$

Substitution of Eqs. (4) and (5) into Eq. (3) yields

$$N_{A_x}|_{x=0} = \frac{D_{AB} c_{A_o}}{\Gamma(4/3)} \left( \frac{\rho g \delta}{9 \mu D_{AB} z} \right)^{1/3} \quad (6)$$

Finally, the use of Eq. (6) in Eq. (1) gives the molar rate of transfer of species  $A$  as

$$\dot{n}_A = \frac{1}{2} \frac{W c_{A_o}}{\Gamma(4/3)} \left( \frac{3 \rho g \delta}{\mu} \right)^{1/3} (D_{ABL})^{2/3} \quad (7)$$

## 2.4.2 Rate of Energy Entering and/or Leaving the System

The rate of energy entering and/or leaving the system,  $\dot{E}$ , is expressed as

$$\dot{E} = \left[ \underbrace{\left( \begin{array}{c} \text{Thermal} \\ \text{diffusivity} \end{array} \right) \left( \begin{array}{c} \text{Gradient of} \\ \text{Energy/Volume} \end{array} \right)}_{\text{Molecular energy flux}} + \underbrace{\left( \begin{array}{c} \text{Energy} \\ \text{Volume} \end{array} \right) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right)}_{\text{Convective energy flux}} \right] \left( \begin{array}{c} \text{Flow} \\ \text{area} \end{array} \right) \quad (2.4-15)$$

As in the case of mass, energy may enter or leave the system by two means:

- By inlet and/or outlet streams,
- By exchange of energy between the system and its surroundings through the boundaries of the system in the form of heat and work.

When energy enters and/or leaves the system by a conduit(s), the characteristic velocity is taken as the average velocity of the flowing stream and it is usually large enough to neglect the molecular flux compared to the convective flux, i.e.,  $Pe_H \gg 1$ . Therefore, Eq. (2.4-15) simplifies to

$$\dot{E} = \left( \frac{\text{Energy}}{\text{Volume}} \right) \left( \text{Average velocity} \right) \left( \frac{\text{Flow}}{\text{area}} \right) \quad (2.4-16)$$

Energy per unit volume, on the other hand, is expressed as the product of energy per unit mass,  $\hat{E}$ , and mass per unit volume, i.e., density, such that Eq. (2.4-16) becomes

$$\dot{E} = \left( \frac{\text{Energy}}{\text{Mass}} \right) \underbrace{\left( \frac{\text{Mass}}{\text{Volume}} \right) \left( \text{Average velocity} \right) \left( \frac{\text{Flow}}{\text{area}} \right)}_{\text{Mass flow rate}} = \hat{E} \dot{m} \quad (2.4-17)$$

## NOTATION

$A$	area, $m^2$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ}/\text{kg}\cdot\text{K}$
$c$	total concentration, $\text{kmol}/m^3$
$c_i$	concentration of species $i$ , $\text{kmol}/m^3$
$D_{AB}$	diffusion coefficient for system $A-B$ , $m^2/s$
$\dot{E}$	rate of energy, $W$
$e$	total energy flux, $W/m^2$
$F$	force, $N$
$J^*$	molecular molar flux, $\text{kmol}/m^2\cdot s$
$j$	molecular mass flux, $\text{kg}/m^2\cdot s$
$k$	thermal conductivity, $W/m\cdot K$
$\dot{m}$	total mass flow rate, $\text{kg}/s$
$\dot{m}_i$	mass flow rate of species $i$ , $\text{kg}/s$
$N$	total molar flux, $\text{kmol}/m^2\cdot s$
$\dot{n}$	total molar flow rate, $\text{kmol}/s$
$\dot{n}_i$	molar flow rate of species $i$ , $\text{kmol}/s$
$P$	pressure, $Pa$
$\dot{Q}$	heat transfer rate, $W$
$\mathcal{Q}$	volumetric flow rate, $m^3/s$
$q$	heat flux, $W/m^2$
$T$	temperature, $^{\circ}C$ or $K$

$t$	time, s
$V$	volume, $\text{m}^3$
$\bar{V}_i$	partial molar volume of species $i$ , $\text{m}^3/\text{kmol}$
$v$	velocity, $\text{m}/\text{s}$
$v^*$	molar average velocity, $\text{m}/\text{s}$
$v^\blacksquare$	volume average velocity, $\text{m}/\text{s}$
$\mathcal{W}$	total mass flux, $\text{kg}/\text{m}^2 \cdot \text{s}$
$x$	rectangular coordinate, m
$x_i$	mole fraction of species $i$
$y$	rectangular coordinate, m
$\alpha$	thermal diffusivity, $\text{m}^2/\text{s}$
$\dot{\gamma}$	rate of strain, $1/\text{s}$
$\mu$	viscosity, $\text{kg}/\text{m} \cdot \text{s}$
$\nu$	kinematic viscosity (or, momentum diffusivity), $\text{m}^2/\text{s}$
$\pi$	total momentum flux, $\text{N}/\text{m}^2$
$\rho$	total density, $\text{kg}/\text{m}^3$
$\rho_i$	density of species $i$ , $\text{kg}/\text{m}^3$
$\tau_{yx}$	flux of $x$ – momentum in the $y$ – direction, $\text{N}/\text{m}^2$
$\omega_i$	mass fraction of species $i$

**Overlines**

$\hat{\quad}$	per unit mass
$\bar{\quad}$	partial molar

**Bracket**

$\langle a \rangle$	average value of $a$
---------------------	----------------------

**Superscript**

$_{sat}$	saturation
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**Subscripts**

$A, B$	species in binary systems
$ch$	characteristic
$i$	species in multicomponent systems

**Dimensionless Numbers**

Le	Lewis number
$Pe_H$	Peclet number for heat transfer
$Pe_M$	Peclet number for mass transfer
Pr	Prandtl number
Sc	Schmidt number

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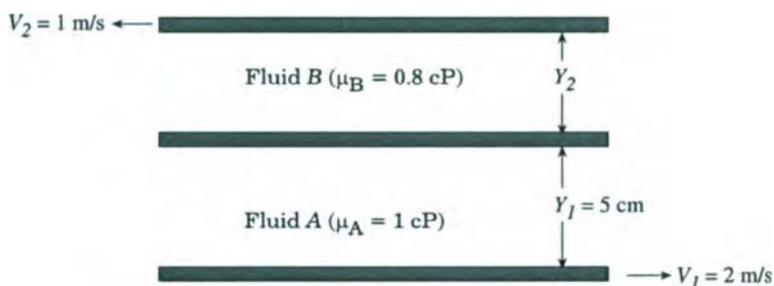
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## PROBLEMS

**2.1** Three parallel flat plates are separated by two fluids as shown in the figure below. What should be the value of  $Y_2$  so as to keep the plate in the middle stationary?



(Answer: 2 cm)

**2.2** The steady rate of heat loss through a plane slab, which has a surface area of  $3 \text{ m}^2$  and is  $7 \text{ cm}$  thick, is  $72 \text{ W}$ . Determine the thermal conductivity of the slab if the temperature distribution in the slab is given as

$$T = 5x + 10$$

where  $T$  is temperature in  $^{\circ}\text{C}$  and  $x$  is the distance measured from one side of the slab in  $\text{cm}$ .

(Answer:  $0.048 \text{ W/m}\cdot\text{K}$ )

**2.3** The inner and outer surface temperatures of a  $20 \text{ cm}$  thick brick wall are  $30^{\circ}\text{C}$  and  $-5^{\circ}\text{C}$ , respectively. The surface area of the wall is  $25 \text{ m}^2$ . Determine the steady rate of heat loss through the wall if the thermal conductivity is  $0.72 \text{ W/m}\cdot\text{K}$ .

(Answer:  $3150 \text{ W}$ )

**2.4** Energy is generated uniformly in a  $6 \text{ cm}$  thick wall. The steady-state temperature distribution is

$$T = 145 + 3000z - 1500z^2$$

where  $T$  is temperature in  $^{\circ}\text{C}$  and  $z$  is the distance measured from one side of the wall in meters. Determine the rate of heat generation per unit volume if the thermal conductivity of the wall is  $15 \text{ W/m}\cdot\text{K}$ .

(Answer:  $45 \text{ kW/m}^3$ )

**2.5** The temperature distribution in a one-dimensional wall of thermal conductivity  $20 \text{ W/m}\cdot\text{K}$  and thickness  $60 \text{ cm}$  is

$$T = 80 + 10e^{-0.09t} \sin(\pi\xi)$$

where  $T$  is temperature in  $^{\circ}\text{C}$ ,  $t$  is time in hours,  $\xi = z/L$  is the dimensionless distance with  $z$  being a coordinate measured from one side of the wall and  $L$  is the wall thickness in meters. Calculate the total amount of heat transferred in half an hour if the surface area of the wall is  $15 \text{ m}^2$ .

(Answer:  $15,360 \text{ J}$ )

**2.6** The steady-state temperature distribution within a plane wall of  $1 \text{ m}$  thick with a thermal conductivity of  $8 \text{ W/m}\cdot\text{K}$  is measured as a function of position as follows:

$z$ (m)	$T$ (°C)
0	30
0.1	46
0.2	59
0.3	70
0.4	79
0.5	85
0.6	89
0.7	90
0.8	89
0.9	86
1.0	80

where  $z$  is the distance measured from one side of the wall. Determine the uniform rate of energy generation per unit volume within the wall.

(Answer: 1920 W/m<sup>3</sup>)

**2.7** The *geothermal gradient* is the rate of increase of temperature with depth in the earth's crust.

a) If the average geothermal gradient of the earth is about 25 °C/km, estimate the steady rate of heat loss from the surface of the earth.

b) One of your friends claims that the amount of heat escaping from 1 m<sup>2</sup> in 4 days is enough to heat a cup of coffee. Do you agree? Justify your answer.

Take the diameter and the thermal conductivity of the earth as  $1.27 \times 10^4$  km and 3 W/m.K, respectively.

(Answer: a)  $38 \times 10^9$  kW)

**2.8** Estimate the earth's age by making use of the following assumptions:

(i) Neglecting the curvature, the earth may be assumed to be semi-infinite plane that began to cool from an initial molten state of  $T_o = 1200$  °C. Taking the interface temperature at  $z = 0$  to be equal to zero, the corresponding temperature distribution takes the form

$$T = T_o \operatorname{erf} \left( \frac{z}{2\sqrt{\alpha t}} \right) \quad (1)$$

where  $\operatorname{erf}(x)$  is the *error function* defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du \quad (2)$$

(ii) The temperature gradient at  $z = 0$  is equal to the geothermal gradient of the earth, i.e.,  $25^\circ\text{C}/\text{km}$ .

(iii) The thermal conductivity, the density and the heat capacity of the earth are  $3\text{ W/m}\cdot\text{K}$ ,  $5500\text{ kg/m}^3$  and  $2000\text{ J/kg}\cdot\text{K}$ , respectively.

Estimation of the age of the earth, based on the above model, is first used by Lord Kelvin (1864). However, he knew nothing about radioactivity and heating of the earth's crust by radioactive decay at that time. As a result, his estimates, ranging from 20 to 200 million years, were completely wrong. Today, the geologists generally accept the age of the earth as 4.55 billion years.

(Answer:  $85.3 \times 10^6$  year)

**2.9** A slab is initially at a uniform temperature  $T_o$  and occupies the space from  $z = 0$  to  $z = \infty$ . At time  $t = 0$ , the temperature of the surface at  $z = 0$  is suddenly changed to  $T_1$  ( $T_1 > T_o$ ) and maintained at that temperature for  $t > 0$ . Under these conditions the temperature distribution is given by

$$\frac{T_1 - T}{T_1 - T_o} = \text{erf}\left(\frac{z}{2\sqrt{\alpha t}}\right) \quad (1)$$

If the surface area of the slab is  $A$ , determine the amount of heat transferred into the slab as a function of time.

(Answer:  $Q = \frac{2kA(T_1 - T_o)}{\sqrt{\pi\alpha}} \sqrt{t}$ )

**2.10** Air at  $20^\circ\text{C}$  and 1 atm pressure flows over a porous plate that is soaked in ethanol. The molar concentration of ethanol in the air,  $c_A$ , is given by

$$c_A = 4e^{-1.5z}$$

where  $c_A$  is in  $\text{kmol/m}^3$  and  $z$  is the distance measured from the surface of the plate in meters. Calculate the molar flux of ethanol from the plate.

(Answer:  $0.283\text{ kmol/m}^2\cdot\text{h}$ )

**2.11** The formal definition of the partial molar volume is given by

$$\bar{V}_i = \left(\frac{\partial V}{\partial n_i}\right)_{T,P,n_{j \neq i}} \quad (1)$$

Substitute

$$V = \frac{n}{c} \quad (2)$$

into Eq. (1) and show that the volume fraction is equal to the mole fraction for constant total molar concentration,  $c$ , i.e.,

$$c_i \bar{V}_i = x_i \quad (3)$$

This further implies that the molar average velocity is equal to the volume average velocity when the total molar concentration is constant.

**2.12** For a gas at constant pressure, why does the Schmidt number usually remain fairly constant over a large temperature range, whereas the diffusion coefficient changes markedly?

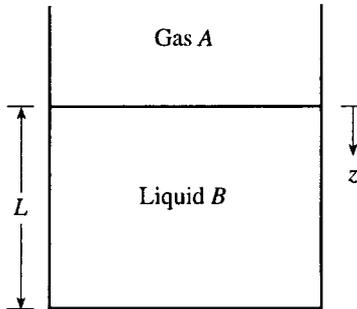
**2.13** Gas  $\mathcal{A}$  dissolves in liquid  $\mathcal{B}$  and diffuses into the liquid phase. As it diffuses, species  $\mathcal{A}$  undergoes an irreversible chemical reaction as shown in the figure below. Under steady conditions, the resulting concentration distribution in the liquid phase is given by

$$\frac{c_A}{c_{A_0}} = \frac{\cosh \{ \Lambda [1 - (z/L)] \}}{\cosh \Lambda}$$

in which

$$\Lambda = \sqrt{\frac{kL^2}{D_{AB}}}$$

where  $c_{A_0}$  is the surface concentration,  $k$  is the reaction rate constant and  $D_{AB}$  is the diffusion coefficient.



- a) Determine the rate of moles of  $\mathcal{A}$  entering into the liquid phase if the cross-sectional area of the tank is  $A$ .
- b) Determine the molar flux at  $z = L$ . What is the physical significance of this result?

(Answer: a)  $\dot{n}_A = \frac{AD_{AB}c_{A_0}\Lambda \tanh \Lambda}{L}$     b) 0)

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# Chapter 3

## Interphase Transport and Transfer Coefficients

In engineering calculations, we are interested in the determination of the rate of momentum, heat and mass transfer from one phase to another across the phase interface. This can be achieved by integrating the flux expression over the interfacial area. Equation (2.4-2) gives the value of the flux at the interface as

$$\left( \begin{array}{c} \text{Interphase} \\ \text{flux} \end{array} \right) = \left[ (\text{Diffusivity}) \left( \begin{array}{c} \text{Gradient of} \\ \text{Quantity/Volume} \end{array} \right) + \left( \frac{\text{Quantity}}{\text{Volume}} \right) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right) \right]_{\text{interface}}$$

Note that the determination of the interphase flux requires the values of the *quantity/volume* and its gradient to be known at the interface. Therefore, equations of change must be solved to obtain the distribution of *quantity/volume* as a function of position. These analytical solutions, however, are not possible most of the time. In that case we resort to experimental data and correlate the results by the transfer coefficients, namely, the friction factor, the heat transfer coefficient, and the mass transfer coefficient. The resulting correlations are then used in designing equipment.

This chapter deals with the physical significance of these three transfer coefficients. In addition, the relationships between these transfer coefficients will be explained by using dimensionless numbers and analogies.

### 3.1 FRICTION FACTOR

Let us consider a flat plate of length  $L$  and width  $W$  suspended in a uniform stream having an approach velocity  $v_\infty$  as shown in Figure 3.1.



Figure 3.1 Flow on a flat plate.

As an engineer we are interested in the determination of the total drag force, i.e., the component of the force in the direction of flow, exerted by the flowing stream on the plate. This force can be calculated by integrating the total momentum flux at the wall over the surface area. The total momentum flux at the wall,  $\pi_{yx}|_{y=0}$ , is

$$\pi_{yx}|_{y=0} = \tau_{yx}|_{y=0} + (\rho v_x v_y)|_{y=0} \quad (3.1-1)$$

where  $\tau_{yx}|_{y=0}$  is the value of the shear stress at the wall. Since the plate is stationary, the fluid which is in contact with the plate is also stagnant<sup>1</sup> and both  $v_x$  and  $v_y$  are zero at  $y = 0$ . Therefore, Eq. (3.1-1) reduces to

$$\pi_{yx}|_{y=0} = \tau_{yx}|_{y=0} = \tau_w \quad (3.1-2)$$

and the drag force,  $F_D$ , on one side of the plate can be calculated from

$$F_D = \int_0^W \int_0^L \tau_w dx dz \quad (3.1-3)$$

Evaluation of the integral in Eq. (3.1-3) requires the value of the velocity gradient at the wall, which can be obtained from the solution of the equations of change. Since this is almost an impossible task in most cases, it is customary in engineering practice to replace  $\tau_w$  by a dimensionless term called the *friction factor*,  $f$ , such that

$$\tau_w = \frac{1}{2} \rho v_\infty^2 f \quad (3.1-4)$$

Substitution of Eq. (3.1-4) into Eq. (3.1-3) gives

$$F_D = \frac{1}{2} \rho v_\infty^2 \int_0^W \int_0^L f dx dz = (WL) \left( \frac{1}{2} \rho v_\infty^2 \right) \langle f \rangle \quad (3.1-5)$$

where  $\langle f \rangle$  is the friction factor averaged over the area of the plate<sup>2</sup>, i.e.,

$$\langle f \rangle = \frac{\int_0^W \int_0^L f dx dz}{\int_0^W \int_0^L dx dz} = \frac{1}{WL} \int_0^W \int_0^L f dx dz \quad (3.1-6)$$

<sup>1</sup>This is known as the *no-slip boundary condition*.

<sup>2</sup>See Section A.2 in Appendix A.

Equation (3.1-5) can be generalized in the form

$$\boxed{F_D = A_{ch} K_{ch} (f)} \quad (3.1-7)$$

in which the terms  $A_{ch}$ , characteristic area, and  $K_{ch}$ , characteristic kinetic energy, are defined by

$$A_{ch} = \begin{cases} \text{Wetted surface area} & \text{for flow in conduits} \\ \text{Projected area} & \text{for flow around submerged objects} \end{cases} \quad (3.1-8)$$

$$K_{ch} = \frac{1}{2} \rho v_{ch}^2 \quad (3.1-9)$$

where  $v_{ch}$  is the characteristic velocity.

Power,  $\dot{W}$ , is defined as the rate at which work is done. Therefore,

$$\text{Power} = \frac{\text{Work}}{\text{Time}} = \frac{(\text{Force})(\text{Distance})}{\text{Time}} = (\text{Force})(\text{Velocity}) \quad (3.1-10)$$

or,

$$\boxed{\dot{W} = F_D v_{ch}} \quad (3.1-11)$$

**Example 3.1** *Advertisements for cars in the magazines give the complete list of their features, one of which is the friction factor (or, drag coefficient) based on the frontal area. Sports cars, such as Toyota Celica, usually have a friction factor of around 0.24. If the car has a width of 2 m and a height of 1.5 m,*

- Determine the power consumed by the car when it is going at 100 km/h.*
- Repeat part (a) if the wind blows at a velocity of 30 km/h opposite to the direction of the car.*
- Repeat part (a) if the wind blows at a velocity of 30 km/h in the direction of the car.*

### Solution

#### Physical properties

*For air at 20°C (293 K) :  $\rho = 1.2 \text{ kg/m}^3$*

#### Assumption

- Air is at 20°C.*

#### Analysis

- The characteristic velocity is*

$$v_{ch} = (100) \left( \frac{1000}{3600} \right) = 27.78 \text{ m/s}$$

The drag force can be calculated from Eq. (3.1-7) as

$$\begin{aligned} F_D &= A_{ch} \left( \frac{1}{2} \rho v_{ch}^2 \right) \langle f \rangle \\ &= (2 \times 1.5) \left[ \frac{1}{2} (1.2)(27.78)^2 \right] (0.24) = 333.4 \text{ N} \end{aligned}$$

The use of Eq. (3.1-11) gives the power consumed as

$$\begin{aligned} \dot{W} &= F_D v_{ch} \\ &= (333.4)(27.78) = 9262 \text{ W} \end{aligned}$$

b) In this case the characteristic velocity is

$$v_{ch} = (100 + 30) \left( \frac{1000}{3600} \right) = 36.11 \text{ m/s}$$

Therefore, the drag force and the power consumed are

$$\begin{aligned} F_D &= (2 \times 1.5) \left[ \frac{1}{2} (1.2)(36.11)^2 \right] (0.24) = 563.3 \text{ N} \\ \dot{W} &= (563.3)(36.11) = 20,341 \text{ W} \end{aligned}$$

c) In this case the characteristic velocity is

$$v_{ch} = (100 - 30) \left( \frac{1000}{3600} \right) = 19.44 \text{ m/s}$$

Therefore, the drag force and the power consumed are

$$\begin{aligned} F_D &= (2 \times 1.5) \left[ \frac{1}{2} (1.2)(19.44)^2 \right] (0.24) = 163.3 \text{ N} \\ \dot{W} &= (163.3)(19.44) = 3175 \text{ W} \end{aligned}$$

### 3.1.1 Physical Interpretation of Friction Factor

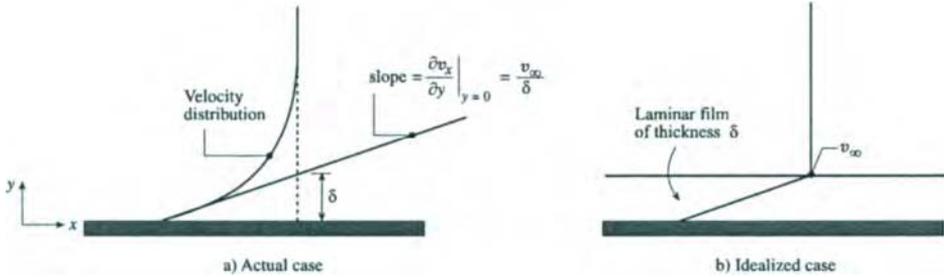
According to Newton's law of viscosity, Eq. (2.1-2), the shear stress at the wall is expressed as

$$\tau_w = \mu \left. \frac{\partial v_x}{\partial y} \right|_{y=0} \quad (3.1-12)$$

The minus sign is omitted in Eq. (3.1-12) because the value of  $v_x$  increases as the distance  $y$  increases. Substitution of Eq. (3.1-12) into Eq. (3.1-4) gives

$$\frac{1}{2} f = \frac{\mu}{\rho v_\infty^2} \left. \frac{\partial v_x}{\partial y} \right|_{y=0} \quad (3.1-13)$$

The friction factor can be determined from Eq. (3.1-13) if the physical properties of the fluid (viscosity and density), the approach velocity of the fluid, and the velocity gradient at the wall are known. Since the calculation of the velocity gradient requires determination of the velocity distribution in the fluid phase, the actual case is idealized as shown in Figure 3.2. The entire resistance to momentum transport is assumed to be due to a laminar film of thickness  $\delta$  next to the wall.



**Figure 3.2** The film model for momentum transfer.

The velocity gradient in the film is constant and is equal to

$$\left. \frac{\partial v_x}{\partial y} \right|_{y=0} = \frac{v_\infty}{\delta} \quad (3.1-14)$$

Substitution of Eq. (3.1-14) into Eq. (3.1-13) and multiplication of the resulting equation by the characteristic length,  $L_{ch}$ , yields

$$\boxed{\frac{1}{2} f \text{Re} = \frac{L_{ch}}{\delta}} \quad (3.1-15)$$

where the dimensionless term  $\text{Re}$  is the *Reynolds number* defined by

$$\text{Re} = \frac{L_{ch} v_\infty \rho}{\mu} \quad (3.1-16)$$

Equation (3.1-15) indicates that the product of the friction factor with the Reynolds number is directly proportional to the characteristic length and inversely proportional to the thickness of the momentum boundary layer.

## 3.2 HEAT TRANSFER COEFFICIENT

### 3.2.1 Convection Heat Transfer Coefficient

Let us consider a flat plate suspended in a uniform stream of velocity  $v_\infty$  and temperature  $T_\infty$  as shown in Figure 3.3. The temperature at the surface of the plate is kept constant at  $T_w$ .

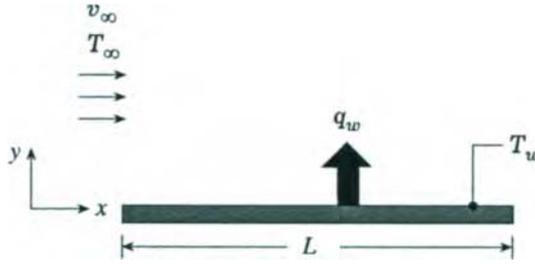


Figure 3.3 Flow over a flat plate.

As an engineer we are interested in the total rate of heat transfer from the plate to the flowing stream. This can be calculated by integrating the total energy flux at the wall over the surface area. The total energy flux at the wall,  $e_y|_{y=0}$ , is

$$e_y|_{y=0} = q_y|_{y=0} + (\rho \hat{C}_P T v_y)|_{y=0} \quad (3.2-1)$$

where  $q_y|_{y=0}$  is the molecular (or, conductive) energy flux at the wall. As a result of the no-slip boundary condition at the wall, the fluid in contact with the plate is stagnant and heat is transferred by pure conduction through the fluid layer immediately adjacent to the plate. Therefore, Eq. (3.2-1) reduces to

$$e_y|_{y=0} = q_y|_{y=0} = q_w \quad (3.2-2)$$

and the rate of heat transfer,  $\dot{Q}$ , from one side of the plate to the flowing stream is

$$\dot{Q} = \int_0^W \int_0^L q_w \, dx dz \quad (3.2-3)$$

Evaluation of the integral in Eq. (3.2-3) requires the determination of the temperature gradient at the wall. However, the fluid motion makes the analytical solution of the temperature distribution impossible to obtain in most cases. Hence, we usually resort to experimentally determined values of the energy flux at a solid-fluid boundary in terms of the *convection heat transfer coefficient*,  $h$ , as

$$\boxed{q_w = h(T_w - T_\infty)} \quad (3.2-4)$$

which is known as *Newton's law of cooling*. The convection heat transfer coefficient,  $h$ , has the units of  $W/m^2 \cdot K$ . It depends on the fluid flow mechanism, fluid properties (density, viscosity, thermal conductivity, heat capacity) and flow geometry.

Substitution of Eq. (3.2-4) into Eq. (3.2-3) gives the rate of heat transfer as

$$\dot{Q} = (T_w - T_\infty) \int_0^W \int_0^L h \, dx dz = (WL) \langle h \rangle (T_w - T_\infty) \quad (3.2-5)$$

where  $\langle h \rangle$  is the heat transfer coefficient averaged over the area of the plate and is defined by

$$\langle h \rangle = \frac{\int_0^W \int_0^L h \, dx dz}{\int_0^W \int_0^L dx dz} = \frac{1}{WL} \int_0^W \int_0^L h \, dx dz \quad (3.2-6)$$

Equation (3.2-5) can be generalized in the form

$$\dot{Q} = A_H \langle h \rangle (\Delta T)_{ch} \quad (3.2-7)$$

where  $A_H$  is the heat transfer area and  $(\Delta T)_{ch}$  is the characteristic temperature difference.

### 3.2.1.1 Physical interpretation of heat transfer coefficient

According to Fourier's law of heat conduction, Eq. (2.1-4), the molecular energy flux at the wall is expressed as

$$q_w = -k \left. \frac{\partial T}{\partial y} \right|_{y=0} \quad (3.2-8)$$

Combination of Eqs. (3.2-4) and (3.2-8) gives

$$h = - \frac{k}{T_w - T_\infty} \left. \frac{\partial T}{\partial y} \right|_{y=0} \quad (3.2-9)$$

The convection heat transfer coefficient can be determined from Eq. (3.2-9) if the thermal conductivity of the fluid, the overall temperature difference, and the temperature gradient at the wall are known. Since the calculation of the temperature gradient at the wall requires the determination of the temperature distribution in the fluid phase, the actual case is idealized as shown in Figure 3.4.

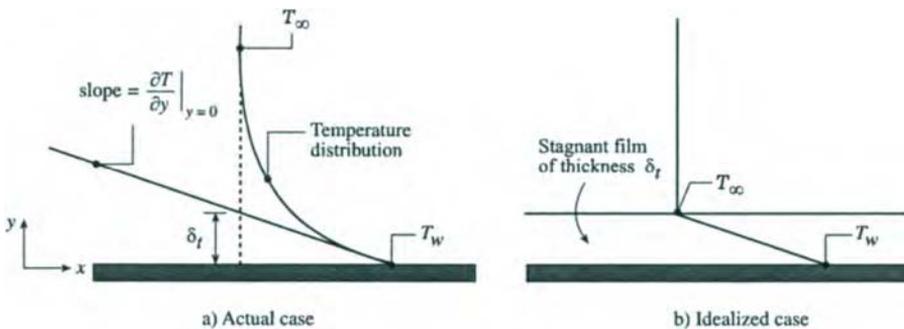


Figure 3.4 The film model for energy transfer.

The entire resistance to heat transfer is assumed to be due to a stagnant film in the fluid next to the wall. The thickness of the film,  $\delta_t$ , is such that it provides the same resistance to heat transfer as the resistance that exists for the actual convection process. The temperature gradient in the film is constant and is equal to

$$\left. \frac{\partial T}{\partial y} \right|_{y=0} = \frac{T_\infty - T_w}{\delta_t} \quad (3.2-10)$$

Substitution of Eq. (3.2-10) into Eq. (3.2-9) gives

$$\boxed{h = \frac{k}{\delta_t}} \quad (3.2-11)$$

Equation (3.2-11) indicates that the thickness of the film,  $\delta_t$ , determines the value of  $h$ . For this reason the term  $h$  is frequently referred to as the *film heat transfer coefficient*.

**Example 3.2** *Energy generation rate per unit volume as a result of fission within a spherical reactor of radius  $R$  is given as a function of position as*

$$\mathfrak{R} = \mathfrak{R}_o \left[ 1 - \left( \frac{r}{R} \right)^2 \right]$$

where  $r$  is the radial distance measured from the center of the sphere. Cooling fluid at a temperature of  $T_\infty$  flows over the reactor. If the average heat transfer coefficient  $\langle h \rangle$  at the surface of the reactor is known, determine the surface temperature of the reactor at steady-state.

### Solution

*System: Reactor*

### Analysis

The inventory rate equation for energy becomes

$$\text{Rate of energy out} = \text{Rate of energy generation} \quad (1)$$

The rate at which energy leaves the sphere by convection is given by Newton's law of cooling as

$$\text{Rate of energy out} = (4\pi R^2) \langle h \rangle (T_w - T_\infty) \quad (2)$$

where  $T_w$  is the surface temperature of the sphere.

The rate of energy generation can be determined by integrating  $\mathfrak{R}$  over the volume of the sphere. The result is

$$\begin{aligned} \text{Rate of energy generation} &= \int_0^{2\pi} \int_0^\pi \int_0^R \mathfrak{R}_o \left[ 1 - \left( \frac{r}{R} \right)^2 \right] r^2 \sin \theta \, dr \, d\theta \, d\phi \\ &= \frac{8\pi}{15} \mathfrak{R}_o R^3 \end{aligned} \quad (3)$$

Substitution of Eqs. (2) and (3) into Eq. (1) gives the surface temperature as

$$T_w = T_\infty + \frac{2}{15} \frac{\Re_o R}{\langle h \rangle} \quad (4)$$

### 3.2.2 Radiation Heat Transfer Coefficient

The heat flux due to radiation,  $q^R$ , from a small object to the surroundings wall is given as

$$q^R = \varepsilon \sigma (T_1^4 - T_2^4) \quad (3.2-12)$$

where  $\varepsilon$  is the emissivity of the small object,  $\sigma$  is the *Stefan-Boltzmann constant* ( $5.67051 \times 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$ ),  $T_1$  and  $T_2$  are the temperatures of the small object and the wall in degrees Kelvin, respectively.

In engineering practice, Eq. (3.2-12) is written in an analogous fashion to Eq. (3.2-4) as

$$q^R = h^R (T_1 - T_2) \quad (3.2-13)$$

where  $h^R$  is the *radiation heat transfer coefficient*. Comparison of Eqs. (3.2-12) and (3.2-13) gives

$$h^R = \frac{\varepsilon \sigma (T_1^4 - T_2^4)}{T_1 - T_2} \simeq 4 \varepsilon \sigma \langle T \rangle^3 \quad (3.2-14)$$

provided that  $\langle T \rangle \gg (T_1 - T_2)/2$ , where  $\langle T \rangle = (T_1 + T_2)/2$ .

## 3.3 MASS TRANSFER COEFFICIENT

Let us consider a flat plate suspended in a uniform stream of fluid (species  $\mathcal{B}$ ) having a velocity  $v_\infty$  and species  $\mathcal{A}$  concentration  $c_{A_\infty}$  as shown in Figure 3.5. The surface of the plate is also coated with species  $\mathcal{A}$  with concentration  $c_{A_w}$ .

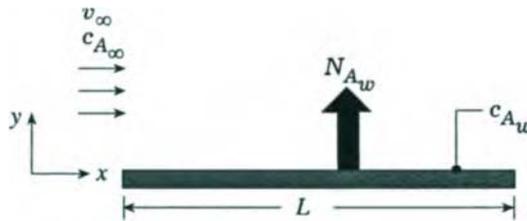


Figure 3.5 Flow over a flat plate.

As an engineer we are interested in the total number of moles of species  $\mathcal{A}$  transferred from the plate to the flowing stream. This can be calculated by integrating the total molar flux at the wall over the surface area. The total molar flux

at the wall,  $N_{A_y}|_{y=0}$ , is

$$N_{A_y}|_{y=0} = J_{A_y}^*|_{y=0} + (c_A v_y^*)|_{y=0} \quad (3.3-1)$$

where  $J_{A_y}^*|_{y=0}$  is the molecular (or, diffusive) molar flux at the wall. For low mass transfer rates Eq. (3.3-1) can be simplified to<sup>3</sup>

$$N_{A_y}|_{y=0} = N_{A_w} \simeq J_{A_y}^*|_{y=0} \quad (3.3-2)$$

and the rate of moles of species  $\mathcal{A}$  transferred,  $\dot{n}_A$ , from one side of the plate to the flowing stream is

$$\dot{n}_A = \int_0^W \int_0^L N_{A_w} dx dz \quad (3.3-3)$$

Evaluation of  $N_{A_w}$  requires the determination of the concentration gradient at the wall. Since this is almost impossible to obtain, in an analogous manner to the definition of the heat transfer coefficient, the *convection mass transfer coefficient*,  $k_c$ , is defined by<sup>4</sup>

$$\boxed{N_{A_w} = k_c (c_{A_w} - c_{A_\infty})} \quad (3.3-4)$$

The mass transfer coefficient has the units of m/s. It depends on the fluid flow mechanism, fluid properties (density, viscosity, diffusion coefficient) and flow geometry.

Substitution of Eq. (3.3-4) into Eq. (3.3-3) gives the rate of moles of species  $\mathcal{A}$  transferred as

$$\dot{n}_A = (c_{A_w} - c_{A_\infty}) \int_0^W \int_0^L k_c dx dz = (WL) \langle k_c \rangle (c_{A_w} - c_{A_\infty}) \quad (3.3-5)$$

where  $\langle k_c \rangle$  is the mass transfer coefficient averaged over the area of the plate and is defined by

$$\langle k_c \rangle = \frac{\int_0^W \int_0^L k_c dx dz}{\int_0^W \int_0^L dx dz} = \frac{1}{WL} \int_0^W \int_0^L k_c dx dz \quad (3.3-6)$$

<sup>3</sup>Note that  $v_y^*$  is the molar average velocity defined by

$$v_y^* = \frac{c_A v_{A_y} + c_B v_{B_y}}{c}$$

At the wall, i.e.,  $y = 0$ ,  $v_{B_y} = 0$  due to no-slip boundary condition. However,  $v_{A_y} \neq 0$  as a result of the transfer of species  $\mathcal{A}$  from the surface to the flowing stream. Therefore,  $v_y^*|_{y=0} \neq 0$ .

<sup>4</sup>Equation (3.3-4) may be called *Newton's law of mass transfer* as suggested by Slattery (1999).

Equation (3.3-5) can be generalized in the form

$$\dot{n}_A = A_M (k_c) (\Delta c_A)_{ch} \quad (3.3-7)$$

where  $A_M$  is the mass transfer area and  $(\Delta c_A)_{ch}$  is the characteristic concentration difference.

### 3.3.1 Physical Interpretation of Mass Transfer Coefficient

The use of Fick's first law of diffusion, Eq. (2.1-9), in Eq. (3.3-2) gives

$$N_{A_w} = -D_{AB} \left. \frac{\partial c_A}{\partial y} \right|_{y=0} \quad (3.3-8)$$

Combination of Eqs. (3.3-4) and (3.3-8) gives

$$k_c = - \frac{D_{AB}}{c_{A_w} - c_{A_\infty}} \left. \frac{\partial c_A}{\partial y} \right|_{y=0} \quad (3.3-9)$$

The convection mass transfer coefficient can be determined from Eq. (3.3-9) if the diffusion coefficient, the overall concentration difference, and the concentration gradient at the wall are known. Since the calculation of the concentration gradient requires the determination of the concentration distribution, the actual case is idealized as shown in Figure 3.6.

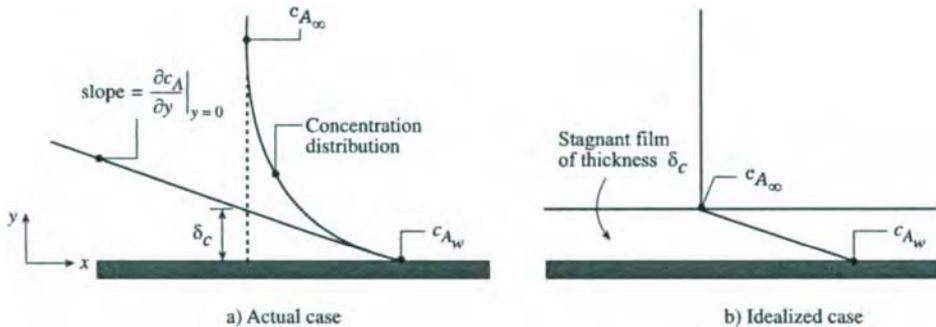


Figure 3.6 The film model for mass transfer.

The entire resistance to mass transfer is due to a stagnant film in the fluid next to the wall. The thickness of the film,  $\delta_c$ , is such that it provides the same resistance to mass transfer by molecular diffusion as the resistance that exists for the actual convection process. The concentration gradient in the film is constant and equal to

$$\left. \frac{\partial c_A}{\partial y} \right|_{y=0} = \frac{c_{A_\infty} - c_{A_w}}{\delta_c} \quad (3.3-10)$$

Substitution of Eq. (3.3-10) into Eq. (3.3-9) gives

$$k_c = \frac{D_{AB}}{\delta_c} \quad (3.3-11)$$

Equation (3.3-11) indicates that the mass transfer coefficient is directly proportional to the diffusion coefficient and inversely proportional to the thickness of the concentration boundary layer.

### 3.3.2 Concentration at the Phase Interface

Consider the transfer of species  $\mathcal{A}$  from the solid phase to the fluid phase through a flat interface as shown in Figure 3.7. The molar flux of species  $\mathcal{A}$  is expressed by Eq. (3.3-4). In the application of this equation to practical problems of interest, there is no difficulty in defining the concentration in the bulk fluid phase,  $c_{A\infty}$ , since this can be measured experimentally. However, to estimate the value of  $c_{A_w}$ , one has to make an assumption about the conditions at the interface. It is generally assumed that the two phases are in equilibrium with each other at the solid-fluid interface. If  $T_w$  represents the interface temperature, the value of  $c_{A_w}$  is given by

$$c_{A_w} = \begin{cases} P_A^{sat}/RT & \text{(Assuming ideal gas behavior)} & \text{fluid = gas} \\ \text{Solubility of solid in liquid at } T_w & & \text{fluid = liquid} \end{cases} \quad (3.3-12)$$

The *Antoine equation* is widely used to estimate vapor pressures and it is given in Appendix D.

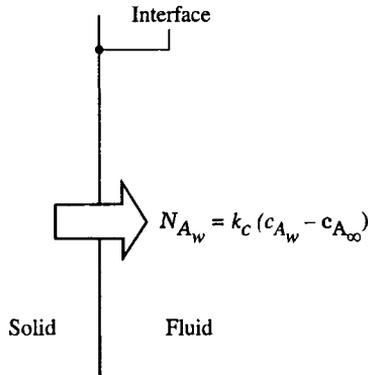


Figure 3.7 Transfer of species  $\mathcal{A}$  from the solid to the fluid phase.

**Example 3.3** 0.5 L of ethanol is poured into a cylindrical tank of 2 L capacity and the top is quickly sealed. The total height of the cylinder is 1 m. Calculate the mass transfer coefficient if the ethanol concentration in the air reaches 2% of its saturation value in 5 minutes. The cylinder temperature is kept constant at 20°C.

**Solution****Physical properties**

$$\text{For ethanol (A) at } 20^\circ\text{C (293 K): } \begin{cases} \rho = 789 \text{ kg/m}^3 \\ \mathcal{M} = 46 \\ P_A^{\text{sat}} = 43.6 \text{ mmHg} \end{cases}$$

**Assumption**

1. *Ideal gas behavior.*

**Analysis**

The mass transfer coefficient can be calculated from Eq. (3.3-4), i.e.,

$$N_{A_w} = k_c (c_{A_w} - c_{A_\infty}) \quad (1)$$

The concentration difference in Eq. (1) is given as the concentration of ethanol vapor at the surface of the liquid,  $c_{A_w}$ , minus that in the bulk solution,  $c_{A_\infty}$ . The concentration at the liquid surface is the saturation concentration while the concentration in the bulk is essentially zero at relatively short times so that  $c_{A_w} - c_{A_\infty} \simeq c_{A_w}$ . Therefore Eq. (1) simplifies to

$$N_{A_w} = k_c c_{A_w} \quad (2)$$

The saturation concentration of ethanol is

$$\begin{aligned} c_{A_w} &= \frac{P_A^{\text{sat}}}{RT} \\ &= \frac{43.6/760}{(0.08205)(20 + 273)} = 2.39 \times 10^{-3} \text{ kmol/m}^3 \end{aligned} \quad (3)$$

Since the ethanol concentration within the cylinder reaches 2% of its saturation value in 5 minutes, the moles of ethanol evaporated during this period is

$$n_A = (0.02)(2.39 \times 10^{-3})(1.5 \times 10^{-3}) = 7.17 \times 10^{-8} \text{ kmol} \quad (4)$$

where  $1.5 \times 10^{-3} \text{ m}^3$  is the volume of the air space in the tank. Therefore, the molar flux at 5 minutes can be calculated as

$$\begin{aligned} N_{A_w} &= \frac{n_A}{(\text{Area})(\text{Time})} \\ &= \frac{7.17 \times 10^{-8}}{(2 \times 10^{-3}/1)(5 \times 60)} = 1.2 \times 10^{-7} \text{ kmol/m}^2 \cdot \text{s} \end{aligned} \quad (5)$$

Substitution of Eqs. (3) and (5) into Eq. (2) gives the mass transfer coefficient as

$$k_c = \frac{1.2 \times 10^{-7}}{2.39 \times 10^{-3}} = 5 \times 10^{-5} \text{ m/s} \quad (6)$$

### 3.4 DIMENSIONLESS NUMBERS

Rearrangement of Eqs. (3.1-4), (3.2-4) and (3.3-4) gives

$$\tau_w = \frac{1}{2} f v_{ch} \Delta(\rho v_{ch}) \quad \Delta(\rho v_{ch}) = \rho v_{\infty} - 0 \quad (3.4-1)$$

$$q_w = \frac{h}{\rho \hat{C}_P} \Delta(\rho \hat{C}_P T) \quad \Delta(\rho \hat{C}_P T) = \rho \hat{C}_P T_w - \rho \hat{C}_P T_{\infty} \quad (3.4-2)$$

$$N_{A_w} = k_c \Delta c_A \quad \Delta c_A = c_{A_w} - c_{A_{\infty}} \quad (3.4-3)$$

Note that Eqs. (3.4-1)-(3.4-3) has the general form

$$\left( \begin{array}{c} \text{Interphase} \\ \text{flux} \end{array} \right) = \left( \begin{array}{c} \text{Transfer} \\ \text{coefficient} \end{array} \right) \left( \begin{array}{c} \text{Difference in} \\ \text{Quantity/Volume} \end{array} \right) \quad (3.4-4)$$

and the terms  $f v_{ch}/2$ ,  $h/\rho \hat{C}_P$ , and  $k_c$  all have the same units, m/s. Thus, the ratio of these quantities must yield dimensionless numbers:

$$\text{Heat transfer Stanton number} = \text{St}_H = \frac{h}{\rho \hat{C}_P v_{ch}} \quad (3.4-5)$$

$$\text{Mass transfer Stanton number} = \text{St}_M = \frac{k_c}{v_{ch}} \quad (3.4-6)$$

Since the term  $f/2$  is dimensionless itself, it is omitted in Eqs. (3.4-5) and (3.4-6).

Dimensionless numbers can also be obtained by taking the ratio of the fluxes. For example, when the concentration gradient is expressed in the form

$$\text{Gradient of Quantity/Volume} = \frac{\text{Difference in Quantity/Volume}}{\text{Characteristic length}} \quad (3.4-7)$$

the expression for the molecular flux, Eq. (2.2-5), becomes

$$\text{Molecular flux} = \frac{(\text{Diffusivity}) (\text{Difference in Quantity/Volume})}{\text{Characteristic length}} \quad (3.4-8)$$

Therefore, the ratio of the total interphase flux, Eq. (3.4-4), to the molecular flux, Eq. (3.4-8), is

$$\frac{\text{Interphase flux}}{\text{Molecular flux}} = \frac{(\text{Transfer coefficient}) (\text{Characteristic length})}{\text{Diffusivity}} \quad (3.4-9)$$

The quantities in Eq. (3.4-9) for various transport processes are given in Table 3.1.

**Table 3.1** Transfer coefficient, diffusivity and flux ratio for the transport of momentum, energy and mass.

Process	Transfer Coefficient	Diffusivity	$\frac{\text{Interphase Flux}}{\text{Molecular Flux}}$
Momentum	$\frac{1}{2} f v_{ch}$	$\frac{\mu}{\rho}$	$\frac{1}{2} f \frac{\rho v_{ch} L_{ch}}{\mu}$
Energy	$\frac{h}{\rho \hat{C}_P}$	$\frac{k}{\rho \hat{C}_P}$	$\frac{h L_{ch}}{k}$
Mass	$k_c$	$\mathcal{D}_{AB}$	$\frac{k_c L_{ch}}{\mathcal{D}_{AB}}$

The dimensionless terms representing the ratio of the interphase flux to the molecular flux in Table 3.1 are defined in terms of the dimensionless numbers as

$$\frac{1}{2} f \frac{\rho v_{ch} L_{ch}}{\mu} = \frac{1}{2} f \text{Re} \quad (3.4-10)$$

$$\frac{h L_{ch}}{k} = \text{Nu} \quad (3.4-11)$$

$$\frac{k_c L_{ch}}{\mathcal{D}_{AB}} = \text{Nu}_M = \text{Sh} \quad (3.4-12)$$

where Nu is the *heat transfer Nusselt number* and Nu<sub>M</sub> is the *mass transfer Nusselt number*. The mass transfer Nusselt number is generally called the *Sherwood number*, Sh. Equations (3.4-10)-(3.4-12) indicate that the product ( $f \text{Re}/2$ ) is more closely analogous to the Nusselt and Sherwood numbers than  $f$  itself. A summary of the analogous dimensionless numbers for energy and mass transfer covered so far is given in Table 3.2.

**Table 3.2** Analogous dimensionless numbers in energy and mass transfer.

Energy	Mass
$\text{Pr} = \frac{\nu}{\alpha} = \frac{\mu \hat{C}_P}{k}$	$\text{Sc} = \frac{\nu}{\mathcal{D}_{AB}} = \frac{\mu}{\rho \mathcal{D}_{AB}}$
$\text{Nu} = \frac{h L_{ch}}{k}$	$\text{Nu}_M = \text{Sh} = \frac{k_c L_{ch}}{\mathcal{D}_{AB}}$
$\text{St}_H = \frac{\text{Nu}}{\text{Re Pr}} = \frac{h}{\rho \hat{C}_P v_{ch}}$	$\text{St}_M = \frac{\text{Sh}}{\text{Re Sc}} = \frac{k_c}{v_{ch}}$

### 3.5 TRANSPORT ANALOGIES

Existing analogies in various transport processes depend on the relationship between the dimensionless numbers defined by Eqs. (3.4-10)-(3.4-12). In Section 3.1.1 we showed that

$$\frac{1}{2} f \text{Re} = \frac{L_{ch}}{\delta} \quad (3.5-1)$$

On the other hand, substitution of Eqs. (3.2-11) and (3.3-11) into Eqs. (3.4-11) and (3.4-12), respectively, gives

$$\text{Nu} = \frac{L_{ch}}{\delta_t} \quad (3.5-2)$$

and

$$\text{Sh} = \frac{L_{ch}}{\delta_c} \quad (3.5-3)$$

Examination of Eqs. (3.5-1)-(3.5-3) indicates that

$$\frac{\text{Interphase flux}}{\text{Molecular flux}} = \frac{\text{Characteristic length}}{\text{Effective film thickness}} \quad (3.5-4)$$

Comparison of Eqs. (3.4-9) and (3.5-4) implies that

$$\text{Effective film thickness} = \frac{\text{Diffusivity}}{\text{Transfer coefficient}} \quad (3.5-5)$$

Note that the *effective film thickness* is the thickness of a fictitious film which would be required to account for the entire resistance if only molecular transport were involved.

Using Eqs. (3.5-1)- (3.5-3), it is possible to express the characteristic length as

$$L_{ch} = \frac{1}{2} f \text{Re} \delta = \text{Nu} \delta_t = \text{Sh} \delta_c \quad (3.5-6)$$

Substitution of  $\text{Nu} = \text{St}_H \text{Re} \text{Pr}$  and  $\text{Sh} = \text{St}_M \text{Re} \text{Sc}$  into Eq. (3.5-6) gives

$$\frac{1}{2} f \delta = \text{St}_H \text{Pr} \delta_t = \text{St}_M \text{Sc} \delta_c \quad (3.5-7)$$

#### 3.5.1 The Reynolds Analogy

Similarities between the transport of momentum, energy and mass were first noted by Reynolds in 1874. He proposed that the effective film thicknesses for the transfer of momentum, energy and mass are equal, i.e.,

$$\delta = \delta_t = \delta_c \quad (3.5-8)$$

Therefore, Eq. (3.5-7) becomes

$$\frac{f}{2} = \text{St}_H \text{Pr} = \text{St}_M \text{Sc} \quad (3.5-9)$$

Reynolds further assumed that  $Pr = Sc = 1$ . Under these circumstances Eq. (3.5-9) reduces to

$$\boxed{\frac{f}{2} = St_H = St_M} \quad (3.5-10)$$

which is known as the *Reynolds analogy*. Physical properties in Eq. (3.5-10) must be evaluated at  $T = (T_w + T_\infty)/2$ .

The Reynolds analogy is reasonably valid for gas systems but should not be considered for liquid systems.

### 3.5.2 The Chilton-Colburn Analogy

In the Chilton-Colburn analogy the relationships between the effective film thicknesses are expressed as

$$\frac{\delta}{\delta_t} = Pr^{1/3} \quad \frac{\delta}{\delta_c} = Sc^{1/3} \quad (3.5-11)$$

Substitution of Eq. (3.5-11) into Eq. (3.5-7) yields

$$\boxed{\frac{f}{2} = St_H Pr^{2/3} \equiv j_H} \quad (3.5-12)$$

and

$$\boxed{\frac{f}{2} = St_M Sc^{2/3} \equiv j_M} \quad (3.5-13)$$

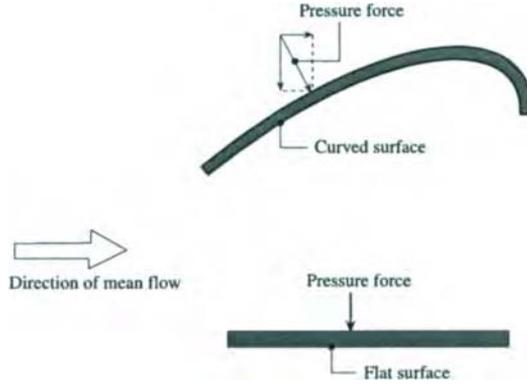
where  $j_H$  and  $j_M$  are the *Colburn  $j$ -factors* for heat and mass transfer, respectively.

Physical properties in Eqs. (3.5-12) and (3.5-13) must be evaluated at  $T = (T_w + T_\infty)/2$ . The Chilton-Colburn analogy is valid when  $0.6 \leq Pr \leq 60$  and  $0.6 \leq Sc \leq 3000$ . Note that Eqs. (3.5-12) and (3.5-13) reduce to Reynolds analogy, Eq. (3.5-10), for fluids with  $Pr = 1$  and  $Sc = 1$ .

As stated in Section 3.1, the drag force is the component of the force in the direction of mean flow. In general, both viscous and pressure forces contribute to this force<sup>5</sup>. In Eq. (3.1-3), only viscous force is considered in the evaluation of the drag force. The reason for this is that the pressure always acts normal to the surface of the flat plate and the component of this force in the direction of mean flow is zero. In the case of curved surfaces, however, the component of normal force to the surface in the direction of mean flow is not necessarily zero as shown in Figure 3.8. Therefore, the friction factor for flow over flat plates and for flow inside circular ducts includes only friction drag, whereas the friction factor for flow around cylinders, spheres, and other bluff objects includes both friction and form drags. As a result,  $f/2$  term for flow around cylinders and spheres is greater than

<sup>5</sup>The drag force arising from viscous and pressure forces are called *friction* (or, *skin*) *drag* and *form drag*, respectively.

the  $j$ -factors. The validity of the Chilton-Colburn analogy for flow in different geometries is given in Table 3.3.



**Figure 3.8** Pressure force acting on curved and flat surfaces.

**Table 3.3** Validity of the Chilton-Colburn analogy for various geometries.

Flow Geometry	Chilton-Colburn Analogy
Flow over a flat plate	$\frac{f}{2} = j_H = j_M$
Flow over a cylinder	$j_H = j_M$
Flow over a sphere	$j_H = j_M$ if $\begin{cases} \text{Nu} \gg 2 \\ \text{Sh} \gg 2 \end{cases}$
Flow in a pipe	$\frac{f}{2} = j_H = j_M$ if $\text{Re} > 10,000$ (Smooth pipe)

**Example 3.4** Water evaporates from a wetted surface of rectangular shape when air at 1 atm and 35°C is blown over the surface at a velocity of 15 m/s. Heat transfer measurements indicate that for air at 1 atm and 35°C the average heat transfer coefficient is given by the following empirical relation

$$\langle h \rangle = 21 v_\infty^{0.6}$$

where  $\langle h \rangle$  is in  $\text{W}/\text{m}^2\cdot\text{K}$  and  $v_\infty$ , air velocity, is in  $\text{m}/\text{s}$ . Estimate the mass transfer coefficient and the rate of evaporation of water from the surface if the area is  $1.5 \text{ m}^2$ .

**Solution****Physical properties**

For water at 35 °C (308 K) :  $P^{sat} = 0.0562$  bar

$$\text{For air at 35 °C (308 K) : } \begin{cases} \rho = 1.1460 \text{ kg/m}^3 \\ \nu = 16.47 \times 10^{-6} \text{ m}^2/\text{s} \\ \hat{C}_P = 1.005 \text{ kJ/kg.K} \\ \text{Pr} = 0.711 \end{cases}$$

Diffusion coefficient of water (A) in air (B) at 35 °C (308 K) :

$$\begin{aligned} (D_{AB})_{308} &= (D_{AB})_{313} \left( \frac{308}{313} \right)^{3/2} \\ &= (2.88 \times 10^{-5}) \left( \frac{308}{313} \right)^{3/2} = 2.81 \times 10^{-5} \text{ m}^2/\text{s} \end{aligned}$$

The Schmidt number is

$$\begin{aligned} \text{Sc} &= \frac{\nu}{D_{AB}} \\ &= \frac{16.47 \times 10^{-6}}{2.81 \times 10^{-5}} = 0.586 \end{aligned}$$

**Assumption**

1. Ideal gas behavior.

**Analysis**

The use of the Chilton-Colburn analogy,  $j_H = j_M$ , gives

$$\langle k_c \rangle = \frac{\langle h \rangle}{\rho \hat{C}_P} \left( \frac{\text{Pr}}{\text{Sc}} \right)^{2/3} = \frac{21 v_\infty^{0.6}}{\rho \hat{C}_P} \left( \frac{\text{Pr}}{\text{Sc}} \right)^{2/3} \quad (1)$$

Substitution of the values into Eq. (1) gives the average mass transfer coefficient as

$$\langle k_c \rangle = \frac{(21)(15)^{0.6}}{(1.1460)(1005)} \left( \frac{0.711}{0.586} \right)^{2/3} = 0.105 \text{ m/s}$$

Saturation concentration of water is

$$\begin{aligned} c_{A_w} &= \frac{P_A^{sat}}{\mathcal{R}T} \\ &= \frac{0.0562}{(8.314 \times 10^{-2})(35 + 273)} = 2.19 \times 10^{-3} \text{ kmol/m}^3 \end{aligned}$$

Therefore, the evaporation rate of water from the surface is

$$\begin{aligned}\dot{n}_A &= A(k_c)(c_{A_w} - c_{A_\infty}) \\ &= (1.5)(0.105)(2.19 \times 10^{-3} - 0) = 3.45 \times 10^{-4} \text{ kmol/s}\end{aligned}$$

## NOTATION

$A$	area, $\text{m}^2$
$A_H$	heat transfer area, $\text{m}^2$
$A_M$	mass transfer area, $\text{m}^2$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ/kg}\cdot\text{K}$
$c_i$	concentration of species $i$ , $\text{kmol/m}^3$
$D_{AB}$	diffusion coefficient for system $A$ - $B$ , $\text{m}^2/\text{s}$
$F_D$	drag force, $\text{N}$
$f$	friction factor
$h$	heat transfer coefficient, $\text{W/m}^2\cdot\text{K}$
$j_H$	Chilton-Colburn $j$ – factor for heat transfer
$j_M$	Chilton-Colburn $j$ – factor for mass transfer
$K$	kinetic energy per unit volume, $\text{J/m}^3$
$k$	thermal conductivity, $\text{W/m}\cdot\text{K}$
$k_c$	mass transfer coefficient, $\text{m/s}$
$L$	length, $\text{m}$
$\mathcal{M}$	molecular weight, $\text{kg/kmol}$
$N$	total molar flux, $\text{kmol/m}^2\cdot\text{s}$
$\dot{n}_i$	molar flow rate of species $i$ , $\text{kmol/s}$
$P$	pressure, $\text{Pa}$
$\dot{Q}$	heat transfer rate, $\text{W}$
$q$	heat flux, $\text{W/m}^2$
$q^R$	heat flux due to radiation, $\text{W/m}^2$
$\mathcal{R}$	gas constant, $\text{J/mol}\cdot\text{K}$
$\mathfrak{R}$	energy generation rate per unit volume, $\text{W/m}^3$
$T$	temperature, $^\circ\text{C}$ or $\text{K}$
$t$	time, $\text{s}$
$v$	velocity, $\text{m/s}$
$\dot{W}$	rate of work, $\text{W}$
$x$	rectangular coordinate, $\text{m}$
$y$	rectangular coordinate, $\text{m}$
$z$	rectangular coordinate, $\text{m}$

$\alpha$	thermal diffusivity, $\text{m}^2/\text{s}$
$\Delta$	difference
$\delta$	fictional film thickness for momentum transfer, m
$\delta_c$	fictional film thickness for mass transfer, m
$\delta_t$	fictional film thickness for heat transfer, m
$\varepsilon$	emissivity
$\mu$	viscosity, $\text{kg}/\text{m}\cdot\text{s}$
$\nu$	kinematic viscosity (or, momentum diffusivity), $\text{m}^2/\text{s}$
$\pi$	total momentum flux, $\text{N}/\text{m}^2$
$\rho$	density, $\text{kg}/\text{m}^3$
$\sigma$	Stefan-Boltzmann constant, $\text{W}/\text{m}^2\cdot\text{K}^4$
$\tau_{yx}$	flux of $x$ – momentum in the $y$ – direction, $\text{N}/\text{m}^2$

**Bracket**

$\langle a \rangle$	average value of $a$
---------------------	----------------------

**Superscript**

$sat$	saturation
-------	------------

**Subscripts**

$A, B$	species in binary systems
$ch$	characteristic
$i$	species in multicomponent systems
$w$	surface or wall
$\infty$	free-stream

**Dimensionless Numbers**

$Nu$	Nusselt number for heat transfer
$Nu_M$	Nusselt number for mass transfer
$Pr$	Prandtl number
$Re$	Reynolds number
$Sc$	Schmidt number
$Sh$	Sherwood number
$St_H$	Stanton number for heat transfer
$St_M$	Stanton number for mass transfer

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## SUGGESTED REFERENCES FOR FURTHER STUDY

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## PROBLEMS

**3.1** Your friend claims that humid air causes an increase in the gas consumption of cars. Do you agree?

**3.2** Air at 20 °C flows over a flat plate of dimensions 50 cm × 25 cm. If the average heat transfer coefficient is 250 W/m<sup>2</sup>.K, determine the steady rate of heat transfer from one side of the plate to air when the plate is maintained at 40 °C.

(Answer: 625 W)

**3.3** Air at 15 °C flows over a spherical LPG tank of radius 4 m. The outside surface temperature of the tank is 4 °C. If the steady rate of heat transfer from the air to the storage tank is 62,000 W, determine the average heat transfer coefficient.

(Answer: 28 W/m<sup>2</sup>.K)

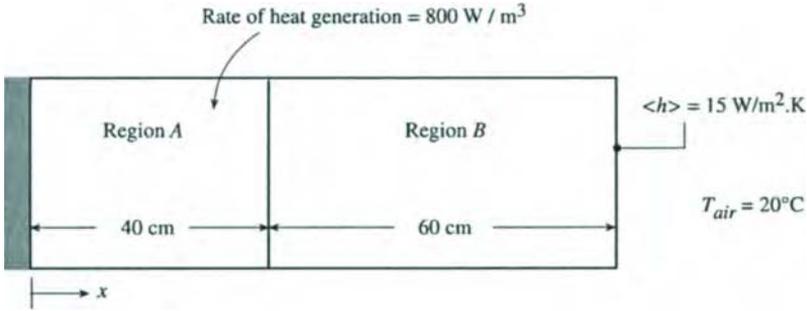
**3.4** The volumetric heat generation in a hollow aluminum sphere of inner and outer radii of 20 cm and 50 cm, respectively, is given by

$$\mathfrak{R} = 4.5 \times 10^4 (1 + 0.6 r^2)$$

in which  $\mathfrak{R}$  is in W/m<sup>3</sup> and  $r$  is the radial coordinate measured in meters. The inner surface of the sphere is subjected to a uniform heat flux of 15,000 W/m<sup>2</sup>, while heat is dissipated by convection to an ambient air at 25 °C through the outer surface with an average heat transfer coefficient of 150 W/m<sup>2</sup>.K. Determine the temperature of the outer surface under steady conditions.

(Answer: 92.3 °C)

3.5 In the system shown below, the rate of heat generation is  $800 \text{ W/m}^3$  in Region A which is perfectly insulated on the left-hand side. Given the conditions indicated in the figure, calculate the heat flux and temperature at the right-hand side, i.e., at  $x = 100 \text{ cm}$ , under steady-state conditions.



(Answer: 320 W, 41.3°C)

3.6 Uniform energy generation rate per unit volume at  $\mathfrak{R} = 2.4 \times 10^6 \text{ W/m}^3$  is occurring within a spherical nuclear fuel element of 20 cm diameter. Under steady conditions the temperature distribution is given by

$$T = 900 - 10,000 r^2$$

where  $T$  is in degrees Celsius and  $r$  is in meters.

- a) Determine the thermal conductivity of the nuclear fuel element.
- b) What is the average heat transfer coefficient at the surface of the sphere if the ambient temperature is 35°C?

(Answer: a) 40 W/m.K b) 104.6 W/m<sup>2</sup>.K)

3.7 A plane wall, with a surface area of 30 m<sup>2</sup> and a thickness of 20 cm, separates a hot fluid at a temperature of 170°C from a cold fluid at 15°C. Under steady-state conditions, the temperature distribution across a wall is given by

$$T = 150 - 600x - 50x^2$$

where  $x$  is the distance measured from the hot wall in meters and  $T$  is the temperature in degrees Celsius. If the thermal conductivity of the wall is 10 W/m.K :

- a) Calculate the average heat transfer coefficients at the hot and cold surfaces.
- b) Determine the rate of energy generation within the wall.

(Answer: a)  $\langle h \rangle_{hot} = 300 \text{ W/m}^2\cdot\text{K}$ ,  $\langle h \rangle_{cold} = 477 \text{ W/m}^2\cdot\text{K}$  b) 6000 W)

3.8 Derive Eq. (3.2-14).

(Hint: Express  $T_1$  and  $T_2$  in terms of  $\langle T \rangle$ .)

**3.9** It is also possible to interpret the Nusselt and Sherwood numbers as dimensionless temperature and concentration gradients, respectively. Show that the Nusselt and Sherwood numbers can be expressed as

$$\text{Nu} = \frac{-(\partial T / \partial y)_{y=0}}{(T_w - T_\infty) / L_{ch}}$$

and

$$\text{Sh} = \frac{-(\partial c_A / \partial y)_{y=0}}{(c_{A_w} - c_{A_\infty}) / L_{ch}}$$

## Chapter 4

# Evaluation of Transfer Coefficients: Engineering Correlations

Since most engineering problems do not have theoretical solutions, a large portion of engineering analysis is concerned with the experimental information which is usually expressed in terms of engineering correlations. These correlations, however, are limited to a specific geometry, equipment configuration, boundary conditions, and substance. As a result, the values obtained from correlations are not exact and it is possible to obtain two different answers from two different correlations for the same problem. Therefore, one should keep in mind that the use of a correlation introduces an error in the order of  $\pm 25\%$ .

Engineering correlations are given in terms of dimensionless numbers. For example, the correlations used to determine friction factor, heat transfer coefficient and mass transfer coefficient are generally expressed in the form

$$\begin{aligned}f &= f(\text{Re}) \\ \text{Nu} &= \text{Nu}(\text{Re}, \text{Pr}) \\ \text{Sh} &= \text{Sh}(\text{Re}, \text{Sc})\end{aligned}$$

In this chapter, some of the available correlations for momentum, energy, and mass transport in different geometries will be presented. Emphasis will be placed on the calculations of force (or, rate of work), heat transfer rate and mass transfer rate under steady conditions.

## 4.1 REFERENCE TEMPERATURE AND CONCENTRATION

The evaluation of the dimensionless numbers that appear in the correlation requires the physical properties of the fluid to be known or estimated. The physical properties, such as density and viscosity, depend on temperature and/or concentration. Temperature and concentration, on the other hand, vary as a function of position. Two commonly used reference temperatures and concentrations are the *bulk temperature* or *concentration* and the *film temperature* or *concentration*.

### 4.1.1 Bulk Temperature and Concentration

For flow inside pipes, the *bulk temperature* or *concentration* at a particular location in the pipe is the average temperature or concentration if the fluid were thoroughly mixed, sometimes called the *mixing-cup temperature* or *concentration*. The bulk temperature and the bulk concentration are denoted by  $T_b$  and  $c_b$ , respectively, and are defined by

$$T_b = \frac{\iint_A v_n T dA}{\iint_A v_n dA} \quad (4.1-1)$$

and

$$c_b = \frac{\iint_A v_n c dA}{\iint_A v_n dA} \quad (4.1-2)$$

where  $v_n$  is the component of velocity in the direction of mean flow.

For the case of flow past bodies immersed in an infinite fluid, the bulk temperature and bulk concentration become the free stream temperature and free stream concentration, respectively, i.e.,

$$\left. \begin{array}{l} T_b = T_\infty \\ c_b = c_\infty \end{array} \right\} \text{For flow over submerged objects} \quad (4.1-3)$$

### 4.1.2 Film Temperature and Concentration

The *film temperature*,  $T_f$ , and the *film concentration*,  $c_f$ , are defined as the arithmetic average of the bulk and surface values, i.e.,

$$T_f = \frac{T_b + T_w}{2} \quad (4.1-4)$$

and

$$c_f = \frac{c_b + c_w}{2} \quad (4.1-5)$$

where subscript  $w$  represents the conditions at the surface or the wall.

## 4.2 FLOW PAST A FLAT PLATE

Let us consider a flat plate suspended in a uniform stream of velocity  $v_\infty$  and temperature  $T_\infty$  as shown in Figure 3.3. The length of the plate in the direction of flow is  $L$  and its width is  $W$ . The local values of the friction factor, the Nusselt number and the Sherwood number are given in Table 4.1 for both laminar and turbulent flow conditions. The term  $Re_x$  is the Reynolds number based on the distance  $x$  and defined by

$$Re_x = \frac{x v_\infty \rho}{\mu} = \frac{x v_\infty}{\nu} \quad (4.2-1)$$

**Table 4.1** The local values of the friction factor, the Nusselt number and the Sherwood number for flow over a flat plate.

	Laminar		Turbulent	
$f_x$	$0.664 Re_x^{-1/2}$	(A)	$0.0592 Re_x^{-1/5}$	(D)
$Nu_x$	$0.332 Re_x^{1/2} Pr^{1/3}$	(B)	$0.0296 Re_x^{4/5} Pr^{1/3}$	(E)
$Sh_x$	$0.332 Re_x^{1/2} Sc^{1/3}$	(C)	$0.0296 Re_x^{4/5} Sc^{1/3}$	(F)
	$Re_x \leq 500,000$		$5 \times 10^5 < Re_x < 10^7$	
	$0.6 \leq Pr \leq 60$		$0.6 \leq Sc \leq 3000$	

The expression for the friction factor under laminar flow conditions, Eq. (A) in Table 4.1, can be obtained analytically from the solution of the equations of change. Blasius (1908) was the first to obtain this solution using a mathematical technique called the *similarity solution* or the *method of combination of variables*. Note that Eqs. (B) and (C) in Table 4.1 can be obtained from Eq. (A) by using the Chilton-Colburn analogy. Since analytical solutions are impossible for turbulent flow, Eq. (D) in Table 4.1 is obtained experimentally. The use of this equation in the Chilton-Colburn analogy yields Eqs. (E) and (F).

The average values of the friction factor, the Nusselt number and the Sherwood number can be obtained from the local values by the application of the mean value theorem. In many cases, however, the transition from laminar to turbulent flow will occur on the plate. In this case, both the laminar and turbulent flow regions must be taken into account in calculating the average values. For example, if the

transition takes place at  $x_c$ , where  $0 < x_c < L$ , then the average friction factor is given by

$$\langle f \rangle = \frac{1}{L} \left[ \int_0^{x_c} (f_x)_{lam} dx + \int_{x_c}^L (f_x)_{turb} dx \right] \quad (4.2-2)$$

Change of variable from  $x$  to  $Re_x$  reduces Eq. (4.2-2) to

$$\langle f \rangle = \frac{1}{Re_L} \left[ \int_0^{Re_c} (f_x)_{lam} dRe_x + \int_{Re_c}^{Re_L} (f_x)_{turb} dRe_x \right] \quad (4.2-3)$$

where  $Re_c$ , the Reynolds number at the point of transition, and  $Re_L$ , the Reynolds number based on the length of the plate, are defined by

$$Re_c = \frac{x_c v_\infty}{\nu} \quad (4.2-4)$$

$$Re_L = \frac{L v_\infty}{\nu} \quad (4.2-5)$$

Substitution of Eqs. (A) and (D) in Table 4.1 into Eq. (4.2-3) gives

$$\langle f \rangle = \frac{0.074}{Re_L^{1/5}} + \frac{1.328 Re_c^{1/2} - 0.074 Re_c^{4/5}}{Re_L} \quad (4.2-6)$$

Taking  $Re_c = 500,000$  results in

$$\langle f \rangle = \frac{0.074}{Re_L^{1/5}} - \frac{1743}{Re_L} \quad (4.2-7)$$

The average values of the friction factor, the Nusselt number and the Sherwood number can be calculated in a similar way for a variety of flow conditions. The results are given in Table 4.2. In these correlations all physical properties must be evaluated at the film temperature.

Note that once the average values of the Nusselt and Sherwood numbers are determined, the average values of the heat and mass transfer coefficients are calculated from

$$\langle h \rangle = \frac{\langle Nu \rangle k}{L} \quad (4.2-8)$$

$$\langle k_c \rangle = \frac{\langle Sh \rangle D_{AB}}{L} \quad (4.2-9)$$

On the other hand, the rate of momentum transfer, i.e., the drag force, the rate of heat transfer and the rate of mass transfer of species  $A$  from one side of the plate are calculated as

$$F_D = (WL) \left( \frac{1}{2} \rho v_\infty^2 \right) \langle f \rangle \quad (4.2-10)$$

Table 4.2 Correlations for flow past a flat plate.

	Laminar		Laminar and Turbulent		Turbulent	
$\langle f \rangle$	$1.328 \text{Re}_L^{-1/2}$	(A)	$0.074 \text{Re}_L^{-1/5} - 1743 \text{Re}_L^{-1}$	(D)	$0.074 \text{Re}_L^{-1/5}$	(G)
$\langle \text{Nu} \rangle$	$0.664 \text{Re}_L^{1/2} \text{Pr}^{1/3}$	(B)	$(0.037 \text{Re}_L^{4/5} - 871) \text{Pr}^{1/3}$	(E)	$0.037 \text{Re}_L^{4/5} \text{Pr}^{1/3}$	(H)
$\langle \text{Sh} \rangle$	$0.664 \text{Re}_L^{1/2} \text{Sc}^{1/3}$	(C)	$(0.037 \text{Re}_L^{4/5} - 871) \text{Sc}^{1/3}$	(F)	$0.037 \text{Re}_L^{4/5} \text{Sc}^{1/3}$	(I)
	$\text{Re}_L \leq 500,000$		$5 \times 10^5 < \text{Re}_L < 10^8$		$\text{Re}_L > 10^8$	
	$0.6 \leq \text{Pr} \leq 60$		$0.6 \leq \text{Sc} \leq 3000$			

$$\dot{Q} = (WL)\langle h \rangle |T_w - T_\infty| \quad (4.2-11)$$

$$\dot{n}_A = (WL)\langle k_c \rangle |c_{A_w} - c_{A_\infty}| \quad (4.2-12)$$

Engineering problems associated with the flow of a fluid over a flat plate are classified as follows:

- Calculate the transfer rate; given the physical properties, the velocity of the fluid, and the dimensions of the plate.
- Calculate the length of the plate in the direction of flow; given the physical properties, the velocity of the fluid, and the transfer rate.
- Calculate the fluid velocity; given the dimensions of the plate, the transfer rate, and the physical properties of the fluid.

**Example 4.1** *Water at 20°C flows over a 2 m long flat plate with a velocity of 3 m/s. The width of the plate is 1 m. Calculate the drag force on one side of the plate.*

**Solution**

**Physical properties**

$$\text{For water at } 20^\circ\text{C (293 K)} : \begin{cases} \rho = 999 \text{ kg/m}^3 \\ \mu = 1001 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

**Assumption**

1. *Steady-state conditions prevail.*

**Analysis**

*To determine which correlation to use for calculating the average friction factor  $\langle f \rangle$ , we must first determine the Reynolds number:*

$$\text{Re}_L = \frac{L v_\infty \rho}{\mu} = \frac{(2)(3)(999)}{1001 \times 10^{-6}} = 6 \times 10^6$$

*Therefore, both the laminar and the turbulent flow regions exist on the plate. The use of Eq. (D) in Table 4.2 gives the friction factor as*

$$\begin{aligned} \langle f \rangle &= \frac{0.074}{\text{Re}_L^{1/5}} - \frac{1743}{\text{Re}_L} \\ &= \frac{0.074}{(6 \times 10^6)^{1/5}} - \frac{1743}{6 \times 10^6} = 3 \times 10^{-3} \end{aligned}$$

The drag force can then be calculated from Eq. (4.2-10) as

$$\begin{aligned} F_D &= (WL) \left( \frac{1}{2} \rho v_\infty^2 \right) \langle f \rangle \\ &= (1 \times 2) \left[ \frac{1}{2} (999)(3)^2 \right] (3 \times 10^{-3}) = 27 \text{ N} \end{aligned}$$

**Example 4.2** Air at a temperature of 25 °C flows over a 30 cm wide electric resistance flat plate heater with a velocity of 13 m/s. The heater dissipates energy into the air at a constant rate of 2730 W/m<sup>2</sup>. How long must the heater be in the direction of flow for the surface temperature not to exceed 155 °C?

### Solution

#### Physical properties

The film temperature is  $(25 + 155)/2 = 90$  °C.

$$\text{For air at } 90 \text{ °C (363 K) and 1 atm : } \begin{cases} \nu = 21.95 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 30.58 \times 10^{-3} \text{ W/m.K} \\ \text{Pr} = 0.704 \end{cases}$$

#### Assumptions

1. Steady-state conditions prevail.
2. Both the laminar and the turbulent flow regions exist over the plate.

#### Analysis

The average convection heat transfer coefficient can be calculated from Newton's law of cooling as

$$\begin{aligned} \langle h \rangle &= \frac{q_w}{T_w - T_\infty} \\ &= \frac{2730}{155 - 25} = 21 \text{ W/m}^2 \cdot \text{K} \end{aligned} \quad (1)$$

To determine which correlation to use, it is necessary to calculate the Reynolds number. However, the Reynolds number cannot be determined a priori since the length of the heater is unknown. Therefore, a trial-and-error procedure must be used. Since we assumed that both the laminar and the turbulent flow regions exist over the heater, the use of Eq. (E) in Table 4.2 gives

$$\begin{aligned} \langle \text{Nu} \rangle &= \frac{\langle h \rangle L}{k} = \left( 0.037 \text{Re}_L^{4/5} - 871 \right) \text{Pr}^{1/3} \\ \frac{(21)L}{30.58 \times 10^{-3}} &= \left\{ 0.037 \left[ \frac{(13)L}{21.95 \times 10^{-6}} \right]^{4/5} - 871 \right\} (0.704)^{1/3} \end{aligned} \quad (2)$$

Simplification of Eq. (2) yields

$$F(L) = L - 1.99L^{4/5} + 1.13 = 0 \quad (3)$$

The length of the heater can be determined from Eq. (3) by using one of the numerical methods for root finding given in Section A.7.2 in Appendix A. The iteration scheme for the Newton-Raphson method, Eq. (A.7-18), becomes

$$L_{k+1} = L_k - \frac{F(L_k)}{(dF/dL)_{L_k}} \quad (4)$$

in which the derivative of the function  $F(L)$  is

$$\frac{dF}{dL} = 1 - 1.592L^{-1/5} \quad (5)$$

Assuming  $L^{4/5} \simeq L$ , a starting value can be estimated as  $L_1 = 1.14141$ . Therefore,

$$L_2 = 1.14141 + \frac{0.05930}{0.55044} = 1.24914$$

$$L_3 = 1.24914 + \frac{0.00152}{0.52272} = 1.25205$$

$$L_4 = 1.25205 + \frac{0}{0.52201} = 1.25205$$

Since  $L_3 = L_4$ , the length of the plate is approximately 1.25 m. Now, it is necessary to check the validity of the second assumption:

$$\text{Re}_L = \frac{(1.25)(13)}{21.95 \times 10^{-6}} = 7.4 \times 10^5 \quad \Rightarrow \quad \text{Checks!}$$

**Example 4.3** A water storage tank open to the atmosphere is 12 m in length and 6 m in width. The water and the surrounding air are at a temperature of 25 °C, and the relative humidity of the air is 60%. If the wind blows at a velocity of 2 m/s along the long side of the tank, what is the steady rate of water loss due to evaporation from the surface?

**Solution**

**Physical properties**

For air at 25 °C (298 K) :  $\nu = 15.54 \times 10^{-6} \text{ m}^2/\text{s}$

Diffusion coefficient of water (A) in air (B) at 25 °C (298 K) :

$$\begin{aligned} (\mathcal{D}_{AB})_{298} &= (\mathcal{D}_{AB})_{313} \left( \frac{298}{313} \right)^{3/2} \\ &= (2.88 \times 10^{-5}) \left( \frac{298}{313} \right)^{3/2} = 2.79 \times 10^{-5} \text{ m}^2/\text{s} \end{aligned}$$

The Schmidt number is

$$\begin{aligned} \text{Sc} &= \frac{\nu}{D_{AB}} \\ &= \frac{15.54 \times 10^{-6}}{2.79 \times 10^{-5}} = 0.56 \end{aligned}$$

For water at 25 °C (298 K) :  $P^{sat} = 0.03165$  bar

### Assumptions

1. Steady-state conditions prevail.
2. Ideal gas behavior.

### Analysis

To determine which correlation to use, we must first calculate the Reynolds number:

$$\begin{aligned} \text{Re}_L &= \frac{L v_\infty}{\nu} \\ &= \frac{(12)(2)}{15.54 \times 10^{-6}} = 1.54 \times 10^6 \end{aligned}$$

Since both laminar and turbulent conditions exist, the use of Eq. (F) in Table 4.2 gives

$$\begin{aligned} \langle \text{Sh} \rangle &= \left( 0.037 \text{Re}_L^{4/5} - 871 \right) \text{Sc}^{1/3} \\ &= \left[ 0.037 (1.54 \times 10^6)^{4/5} - 871 \right] (0.56)^{1/3} = 2000 \end{aligned}$$

Therefore, the average mass transfer coefficient is

$$\begin{aligned} \langle k_c \rangle &= \frac{\langle \text{Sh} \rangle D_{AB}}{L} \\ &= \frac{(2000)(2.79 \times 10^{-5})}{12} = 4.65 \times 10^{-3} \text{ m/s} \end{aligned}$$

The number of moles of H<sub>2</sub>O (A) evaporated in unit time is

$$\begin{aligned} \dot{n}_A &= A \langle k_c \rangle [c_A^{sat} - c_A(\text{air})] \\ &= A \langle k_c \rangle (c_A^{sat} - 0.6 c_A^{sat}) = 0.4 A \langle k_c \rangle c_A^{sat} \end{aligned}$$

Saturation concentration of water,  $c_A^{sat}$ , is

$$\begin{aligned} c_A^{sat} &= \frac{P_A^{sat}}{R T} \\ &= \frac{0.03165}{(8.314 \times 10^{-2})(25 + 273)} = 1.28 \times 10^{-3} \text{ kmol/m}^3 \end{aligned}$$

Hence, the rate of water loss is

$$\begin{aligned} \dot{m}_A &= \dot{n}_A \mathcal{M}_A = 0.4 A \langle k_c \rangle c_A^{sat} \mathcal{M}_A \\ &= (0.4)(12 \times 6)(4.65 \times 10^{-3})(1.28 \times 10^{-3})(18)(3600) = 11.1 \text{ kg/h} \end{aligned}$$

### 4.3 FLOW PAST A SINGLE SPHERE

Consider a single sphere immersed in an infinite fluid. We may consider two cases which are exactly equivalent: (i) the sphere is stagnant, the fluid flows over the sphere, (ii) the fluid is stagnant, the sphere moves through the fluid.

According to Newton's second law of motion, the balance of forces acting on a single spherical particle of diameter  $D_P$ , falling in a stagnant fluid with a constant terminal velocity  $v_t$ , is expressed in the form

$$\text{Gravitational force} = \text{Buoyancy} + \text{Drag force} \quad (4.3-1)$$

or,

$$\left(\frac{\pi D_P^3}{6}\right) \rho_P g = \left(\frac{\pi D_P^3}{6}\right) \rho g + \left(\frac{\pi D_P^2}{4}\right) \left(\frac{1}{2} \rho v_t^2\right) f \quad (4.3-2)$$

where  $\rho_P$  and  $\rho$  represent the densities of the particle and fluid, respectively. In the literature, the friction factor  $f$  is also called the *drag coefficient* and denoted by  $C_D$ . Simplification of Eq. (4.3-2) gives

$$f v_t^2 = \frac{4}{3} \frac{g D_P (\rho_P - \rho)}{\rho} \quad (4.3-3)$$

Equation (4.3-3) can be rearranged in dimensionless form as

$$\boxed{f \text{Re}_P^2 = \frac{4}{3} \text{Ar}} \quad (4.3-4)$$

where the Reynolds number,  $\text{Re}_P$ , and the Archimedes number,  $\text{Ar}$ , are defined by

$$\text{Re}_P = \frac{D_P v_t \rho}{\mu} \quad (4.3-5)$$

$$\text{Ar} = \frac{D_P^3 g \rho (\rho_P - \rho)}{\mu^2} \quad (4.3-6)$$

Engineering problems associated with the motion of spherical particles in fluids are classified as follows:

- Calculate the terminal velocity,  $v_t$ ; given the viscosity of fluid,  $\mu$ , and the particle diameter,  $D_P$ .
- Calculate the particle diameter,  $D_P$ ; given the viscosity of the fluid,  $\mu$ , and the terminal velocity,  $v_t$ .
- Calculate the fluid viscosity,  $\mu$ ; given the particle diameter,  $D_P$ , and the terminal velocity,  $v_t$ .

The difficulty in these problems arises from the fact that the friction factor  $f$  in Eq. (4.3-4) is a complex function of the Reynolds number and the Archimedes number cannot be determined *a priori*.

### 4.3.1 Friction Factor Correlations

For flow of a sphere through a stagnant fluid, Lapple and Shepherd (1940) presented their experimental data in the form of  $f$  versus  $Re_P$ . Their data can be approximated as

$$f = \frac{24}{Re_P} \quad Re_P < 2 \quad (4.3-7)$$

$$f = \frac{18.5}{Re_P^{0.6}} \quad 2 \leq Re_P < 500 \quad (4.3-8)$$

$$f = 0.44 \quad 500 \leq Re_P < 2 \times 10^5 \quad (4.3-9)$$

Equations (4.3-7) and (4.3-9) are generally referred to as *Stokes' law* and *Newton's law*, respectively.

In recent years, efforts have been directed to obtain a single comprehensive equation for the friction factor that covers the entire range of  $Re_P$ . Turton and Levenspiel (1986) proposed the following five-constant equation which correlates the experimental data for  $Re_P \leq 2 \times 10^5$ :

$$f = \frac{24}{Re_P} (1 + 0.173 Re_P^{0.657}) + \frac{0.413}{1 + 16,300 Re_P^{-1.09}} \quad (4.3-10)$$

#### 4.3.1.1 Solutions to the engineering problems

Solutions to the engineering problems described above can now be summarized as follows:

■ Calculate  $v_t$ ; given  $\mu$  and  $D_P$

Substitution of Eq. (4.3-10) into Eq. (4.3-4) gives

$$Ar = 18 (Re_P + 0.173 Re_P^{1.657}) + \frac{0.31 Re_P^2}{1 + 16,300 Re_P^{-1.09}} \quad (4.3-11)$$

Since Eq. (4.3-11) expresses the Archimedes number as a function of the Reynolds number, calculation of the terminal velocity for a given particle diameter and fluid viscosity requires an iterative solution. To circumvent this problem, it is necessary to express the Reynolds number as a function of the Archimedes number. The following explicit expression relating the Archimedes number to the Reynolds number is proposed by Turton and Clark (1987):

$$Re_P = \frac{Ar}{18} (1 + 0.0579 Ar^{0.412})^{-1.214} \quad (4.3-12)$$

The procedure to calculate the terminal velocity is as follows:

- a) Calculate the Archimedes number from Eq. (4.3-6),  
 b) Substitute the Archimedes number into Eq. (4.3-12) and determine the Reynolds number,  
 c) Once the Reynolds number is determined, the terminal velocity can be calculated from the equation

$$v_t = \frac{\mu \text{Re}_P}{\rho D_P} \quad (4.3-13)$$

**Example 4.4** Calculate the velocities at which a drop of water, 5 mm in diameter, would fall in air at 20°C and the same size air bubble would rise through water at 20°C.

**Solution**

**Physical properties**

$$\text{For water at } 20^\circ\text{C (293 K)} : \begin{cases} \rho = 999 \text{ kg/m}^3 \\ \mu = 1001 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

$$\text{For air at } 20^\circ\text{C (293 K)} : \begin{cases} \rho = 1.2047 \text{ kg/m}^3 \\ \mu = 18.17 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

**Analysis**

*Water droplet falling in air*

To determine the terminal velocity of water, it is necessary to calculate the Archimedes number using Eq. (4.3-6):

$$\begin{aligned} \text{Ar} &= \frac{D_P^3 g \rho (\rho_P - \rho)}{\mu^2} \\ &= \frac{(5 \times 10^{-3})^3 (9.8)(1.2047)(999 - 1.2047)}{(18.17 \times 10^{-6})^2} = 4.46 \times 10^6 \end{aligned}$$

The Reynolds number is calculated from Eq. (4.3-12):

$$\begin{aligned} \text{Re}_P &= \frac{\text{Ar}}{18} (1 + 0.0579 \text{Ar}^{0.412})^{-1.214} \\ &= \frac{4.46 \times 10^6}{18} [1 + 0.0579 (4.46 \times 10^6)^{0.412}]^{-1.214} = 3581 \end{aligned}$$

Hence, the terminal velocity is

$$\begin{aligned} v_t &= \frac{\mu \text{Re}_P}{\rho D_P} \\ &= \frac{(18.17 \times 10^{-6})(3581)}{(1.2047)(5 \times 10^{-3})} = 10.8 \text{ m/s} \end{aligned}$$

*Air bubble rising in water*

*In this case, the Archimedes number is*

$$\begin{aligned} Ar &= \frac{D_P^3 g \rho (\rho_P - \rho)}{\mu^2} \\ &= \frac{(5 \times 10^{-3})^3 (9.8)(999)(1.2047 - 999)}{(1001 \times 10^{-6})^2} = -1.219 \times 10^6 \end{aligned}$$

*The minus sign indicates that the motion of a bubble is in the direction opposite to gravity, i.e., it is rising. The Reynolds number and the terminal velocity are*

$$\begin{aligned} Re_P &= \frac{Ar}{18} (1 + 0.0579 Ar^{0.412})^{-1.214} \\ &= \frac{1.219 \times 10^6}{18} [1 + 0.0579 (1.219 \times 10^6)^{0.412}]^{-1.214} = 1825 \end{aligned}$$

$$\begin{aligned} v_t &= \frac{\mu Re_P}{\rho D_P} \\ &= \frac{(1001 \times 10^{-6})(1825)}{(999)(5 \times 10^{-3})} = 0.37 \text{ m/s} \end{aligned}$$

■ Calculate  $D_P$ ; given  $\mu$  and  $v_t$

In this case Eq. (4.3-4) must be rearranged such that the particle diameter is eliminated. If both sides of Eq. (4.3-4) are divided by  $Re_P^3$ , the result is

$$\frac{f}{Re_P} = Y \quad (4.3-14)$$

where  $Y$ , which is independent of  $D_P$ , is a dimensionless number defined by

$$Y = \frac{4}{3} \frac{g(\rho_P - \rho)\mu}{\rho^2 v_t^3} \quad (4.3-15)$$

Substitution of Eq. (4.3-10) into Eq. (4.3-14) yields

$$Y = \frac{24}{Re_P^2} (1 + 0.173 Re_P^{0.657}) + \frac{0.413}{Re_P + 16,300 Re_P^{-0.09}} \quad (4.3-16)$$

Since Eq. (4.3-16) expresses  $Y$  as a function of the Reynolds number, calculation of the particle diameter for a given terminal velocity and fluid viscosity requires an iterative solution. To circumvent this problem, the following explicit expression relating  $Y$  to the Reynolds number is proposed by Tosun and Akşahin (1992) as

$$Re_P = \frac{\Psi(Y)}{(6Y^{13/20} - Y^{6/11})^{17/20}} \quad (4.3-17)$$

where  $\Psi(Y)$  is given by

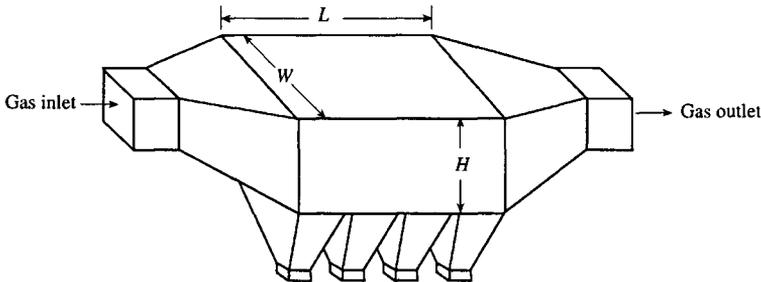
$$\Psi(Y) = \exp\left(3.15 + \frac{0.052}{Y^{1/4}} + \frac{0.007}{Y^{1/2}} - \frac{0.00019}{Y^{3/4}}\right) \quad (4.3-18)$$

The procedure to calculate the particle diameter is as follows:

- a) Calculate  $Y$  from Eq. (4.3-15),
- b) Substitute  $Y$  into Eqs. (4.3-17) and (4.3-18) and determine  $Re_P$ ,
- c) Once the Reynolds number is determined, the particle diameter can be calculated from the equation

$$D_P = \frac{\mu Re_P}{\rho v_t} \quad (4.3-19)$$

**Example 4.5** *A gravity settling chamber is one of the diverse range of equipment used to remove particulate solids from gas streams. In a settling chamber, the entering gas stream encounters an abrupt and large increase in cross-sectional area as shown in the figure below. As a result of the sharp decrease in the gas velocity, the solid particles settle down by gravity. In practice, the gas velocity through the chamber should be kept below 3 m/s to prevent the re-entrainment of the settled particles.*



*Spherical dust particles having a density of 2200 kg/m<sup>3</sup> are to be separated from an air stream at a temperature of 25 °C. Determine the diameter of the smallest particle that can be removed in a settling chamber 7 m long, 2 m wide, and 1 m high.*

**Solution**

**Physical properties**

$$\text{For air at } 25^\circ\text{C (298 K)} : \begin{cases} \rho = 1.1845 \text{ kg/m}^3 \\ \mu = 18.41 \times 10^{-6} \text{ kg/m.s} \end{cases}$$

**Analysis**

For the minimum particle size that can be removed with 100% efficiency, the time required for this particle to fall a distance  $H$  must be equal to the time required to move this particle horizontally a distance  $L$ , i.e.,

$$t = \frac{H}{v_t} = \frac{L}{\langle v \rangle}$$

where  $\langle v \rangle$  represents the average gas velocity in the settling chamber. Taking  $\langle v \rangle = 3 \text{ m/s}$ , the settling velocity of the particles can be calculated as

$$\begin{aligned} v_t &= \langle v \rangle \left( \frac{H}{L} \right) \\ &= (3) \left( \frac{1}{7} \right) = 0.43 \text{ m/s} \end{aligned}$$

The value of  $Y$  is calculated from Eq. (4.3-15) as

$$\begin{aligned} Y &= \frac{4}{3} \frac{g(\rho_P - \rho)\mu}{\rho^2 v_t^3} \\ &= \frac{4}{3} \frac{(9.8)(2200 - 1.1845)(18.41 \times 10^{-6})}{(1.1845)^2 (0.43)^3} = 4.74 \end{aligned}$$

Substitution of the value of  $Y$  into Eq. (4.3-18) gives

$$\begin{aligned} \Psi(Y) &= \exp \left( 3.15 + \frac{0.052}{Y^{1/4}} + \frac{0.007}{Y^{1/2}} - \frac{0.00019}{Y^{3/4}} \right) \\ &= \exp \left[ 3.15 + \frac{0.052}{(4.74)^{1/4}} + \frac{0.007}{(4.74)^{1/2}} - \frac{0.00019}{(4.74)^{3/4}} \right] = 24.3 \end{aligned}$$

Therefore, the Reynolds number and the particle diameter are

$$\begin{aligned} \text{Re}_P &= \frac{\Psi(Y)}{(6Y^{13/20} - Y^{6/11})^{17/20}} \\ &= \frac{24.3}{[6(4.74)^{13/20} - (4.74)^{6/11}]^{17/20}} = 2.55 \end{aligned}$$

$$\begin{aligned} D_P &= \frac{\mu \text{Re}_P}{\rho v_t} \\ &= \frac{(18.41 \times 10^{-6})(2.55)}{(1.1845)(0.43)} = 92 \times 10^{-6} \text{ m} \end{aligned}$$

■ Calculate  $\mu$ ; given  $D_P$  and  $v_t$

In this case Eq. (4.3-4) must be rearranged so that the fluid viscosity can be eliminated. If both sides of Eq. (4.3-4) are divided by  $\text{Re}_P^2$ , the result is

$$f = X \quad (4.3-20)$$

where  $X$ , which is independent of  $\mu$ , is a dimensionless number defined by

$$X = \frac{4}{3} \frac{gD_P(\rho_P - \rho)}{\rho v_t^2} \quad (4.3-21)$$

Substitution of Eq. (4.3-10) into Eq. (4.3-20) gives

$$X = \frac{24}{\text{Re}_P} (1 + 0.173 \text{Re}_P^{0.657}) + \frac{0.413}{1 + 16,300 \text{Re}_P^{-1.09}} \quad (4.3-22)$$

Since Eq. (4.3-22) expresses  $X$  as a function of the Reynolds number, calculation of the fluid viscosity for a given terminal velocity and particle diameter requires an iterative solution. To circumvent this problem, the following explicit expression relating  $X$  to the Reynolds number is proposed by Tosun and Akşahin (1992) as

$$\boxed{\text{Re}_P = \frac{24}{X} (1 + 120 X^{-20/11})^{4/11}} \quad X \geq 0.5 \quad (4.3-23)$$

The procedure to calculate the fluid viscosity is as follows:

- a) Calculate  $X$  from Eq. (4.3-21),
- b) Substitute  $X$  into Eq. (4.3-23) and determine the Reynolds number,
- c) Once the Reynolds number is determined, the fluid viscosity can be calculated from the equation

$$\mu = \frac{D_P v_t \rho}{\text{Re}_P} \quad (4.3-24)$$

**Example 4.6** *One way of measuring fluid viscosity is to use a falling ball viscometer in which a spherical ball of known density is dropped into a fluid-filled graduated cylinder and the time of fall for the ball for a specified distance is recorded.*

*A spherical ball, 5 mm in diameter, has a density of 1000 kg/m<sup>3</sup>. It falls through a liquid of density 910 kg/m<sup>3</sup> at 25 °C and travels a distance of 10 cm in 1.8 min. Determine the viscosity of the liquid.*

**Solution**

*The terminal velocity of the sphere is*

$$\begin{aligned} v_t &= \frac{\text{Distance}}{\text{Time}} \\ &= \frac{10 \times 10^{-2}}{(1.8)(60)} = 9.26 \times 10^{-4} \text{ m/s} \end{aligned}$$

The value of  $X$  is calculated from Eq. (4.3-21) as

$$\begin{aligned} X &= \frac{4}{3} \frac{gD_P(\rho_P - \rho)}{\rho v_t^2} \\ &= \frac{4}{3} \frac{(9.8)(5 \times 10^{-3})(1000 - 910)}{(910)(9.26 \times 10^{-4})^2} = 7536 \end{aligned}$$

Substitution of the value of  $X$  into Eq. (4.3-23) gives the Reynolds number as

$$\begin{aligned} \text{Re}_P &= \frac{24}{X} \left(1 + 120 X^{-20/11}\right)^{4/11} \\ &= \frac{24}{7536} \left[1 + 120 (7536)^{-20/11}\right]^{4/11} = 3.2 \times 10^{-3} \end{aligned}$$

Hence, the viscosity of the fluid is

$$\begin{aligned} \mu &= \frac{D_P v_t \rho}{\text{Re}_P} \\ &= \frac{(5 \times 10^{-3})(9.26 \times 10^{-4})(910)}{3.2 \times 10^{-3}} = 1.32 \text{ kg/m.s} \end{aligned}$$

#### 4.3.1.2 Deviations from ideal behavior

It should be noted that Eqs. (4.3-4) and (4.3-10) are only valid for a single spherical particle falling in an unbounded fluid. The presence of container walls and other particles as well as any deviations from spherical shape affect the terminal velocity of particles. For example, as a result of the upflow of displaced fluid in a suspension of uniform particles, the settling velocity of particles in suspension is slower than the terminal velocity of a single particle of the same size. The most general empirical equation relating the settling velocity to the volume fraction of particles,  $\omega$ , is given by

$$\frac{v_t(\text{suspension})}{v_t(\text{single sphere})} = (1 - \omega)^n \quad (4.3-25)$$

where the exponent  $n$  depends on the Reynolds number based on the terminal velocity of a particle in an unbounded fluid. In the literature, values of  $n$  are reported as

$$n = \begin{cases} 4.65 - 5.00 & \text{Re}_P < 2 \\ 2.30 - 2.65 & 500 \leq \text{Re}_P \leq 2 \times 10^5 \end{cases} \quad (4.3-26)$$

The particle shape is another factor affecting terminal velocity. The terminal velocity of a non-spherical particle is less than that of a spherical one by a factor of *sphericity*,  $\phi$ , i.e.,

$$\frac{v_t(\text{non-spherical})}{v_t(\text{spherical})} = \phi < 1 \quad (4.3-27)$$

Sphericity is defined as the ratio of the surface area of a sphere having the same volume as the non-spherical particle to the actual surface area of the particle.

### 4.3.2 Heat Transfer Correlations

When a sphere is immersed in an infinite stagnant fluid, the analytical solution for the steady-state conduction is possible<sup>1</sup> and the result is expressed in the form

$$\text{Nu} = 2 \quad (4.3-28)$$

In the case of fluid motion, contribution of the convective mechanism must be included in Eq. (4.3-28). Correlations for including convective heat transfer are as follows:

#### Ranz-Marshall correlation

Ranz and Marshall (1952) proposed the following correlation for constant surface temperature:

$$\text{Nu} = 2 + 0.6 \text{Re}_P^{1/2} \text{Pr}^{1/3} \quad (4.3-29)$$

All properties in Eq. (4.3-29) must be evaluated at the film temperature.

#### Whitaker correlation

Whitaker (1972) considered heat transfer from the sphere to be a result of two parallel processes occurring simultaneously. He assumed that the laminar and turbulent contributions are additive and proposed the following equation:

$$\text{Nu} = 2 + \left( 0.4 \text{Re}_P^{1/2} + 0.06 \text{Re}_P^{2/3} \right) \text{Pr}^{0.4} (\mu_\infty / \mu_w)^{1/4} \quad (4.3-30)$$

All properties except  $\mu_w$  should be evaluated at  $T_\infty$ . Equation (4.3-30) is valid for

$$3.5 \leq \text{Re}_P \leq 7.6 \times 10^4$$

$$0.71 \leq \text{Pr} \leq 380$$

$$1.0 \leq \mu_\infty / \mu_w \leq 3.2$$

#### 4.3.2.1 Calculation of the heat transfer rate

Once the average heat transfer coefficient is estimated by using correlations, the rate of heat transferred is calculated as

$$\dot{Q} = (\pi D_P^2) \langle h \rangle |T_w - T_\infty| \quad (4.3-31)$$

**Example 4.7** *An instrument is enclosed in a protective spherical shell, 5 cm in diameter, and submerged in a river to measure the concentrations of pollutants. The temperature and the velocity of the river are 10°C and 1.2 m/s, respectively. To prevent any damage to the instrument as a result of the cold river temperature, the surface temperature is kept constant at 32°C by installing electrical heaters in the protective shell. Calculate the electrical power dissipated under steady conditions.*

<sup>1</sup>See Example 8.9 in Chapter 8.

**Solution****Physical properties**

$$\text{For water at } 10^\circ\text{C (283 K): } \begin{cases} \rho = 1000 \text{ kg/m}^3 \\ \mu = 1304 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ k = 587 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ \text{Pr} = 9.32 \end{cases}$$

$$\text{For water at } 32^\circ\text{C (305 K): } \mu = 769 \times 10^{-6} \text{ kg/m}\cdot\text{s}$$

**Analysis**

*System: Protective shell*

*Under steady conditions, the electrical power dissipated is equal to the rate of heat loss from the shell surface to river. The rate of heat loss is given by*

$$\dot{Q} = (\pi D_P^2) \langle h \rangle (T_w - T_\infty) \quad (1)$$

*To determine  $\langle h \rangle$ , it is necessary to calculate the Reynolds number*

$$\begin{aligned} \text{Re}_P &= \frac{D_P v_\infty \rho}{\mu} \\ &= \frac{(5 \times 10^{-2})(1.2)(1000)}{1304 \times 10^{-6}} = 4.6 \times 10^4 \end{aligned} \quad (2)$$

*The Whitaker correlation, Eq. (4.3-30), gives*

$$\text{Nu} = 2 + \left( 0.4 \text{Re}_P^{1/2} + 0.06 \text{Re}_P^{2/3} \right) \text{Pr}^{0.4} (\mu_\infty / \mu_w)^{1/4}$$

or,

$$\begin{aligned} \text{Nu} &= 2 + \left[ 0.4 (4.6 \times 10^4)^{1/2} + 0.06 (4.6 \times 10^4)^{2/3} \right] (9.32)^{0.4} \\ &\quad \times \left( \frac{1304 \times 10^{-6}}{769 \times 10^{-6}} \right)^{1/4} = 456 \end{aligned} \quad (3)$$

*The average heat transfer coefficient is*

$$\begin{aligned} \langle h \rangle &= \text{Nu} \left( \frac{k}{D_P} \right) \\ &= (456) \left( \frac{587 \times 10^{-3}}{5 \times 10^{-2}} \right) = 5353 \text{ W/m}^2 \cdot \text{K} \end{aligned} \quad (4)$$

*Therefore, the rate of heat loss is calculated from Eq. (1) as*

$$\dot{Q} = [\pi (5 \times 10^{-2})^2] (5353)(32 - 10) = 925 \text{ W} \quad (5)$$

### 4.3.3 Mass Transfer Correlations

When a sphere is immersed in an infinite stagnant fluid, the analytical solution for the steady-state diffusion is possible<sup>2</sup> and the result is expressed in the form

$$\text{Sh} = 2 \quad (4.3-32)$$

In the case of fluid motion, contribution of convection must be taken into consideration. Correlations for convective mass transfer are as follows:

#### Ranz-Marshall correlation

For constant surface composition and low mass transfer rates, Eq. (4.3-29) may be applied to mass transfer problems simply by replacing Nu and Pr with Sh and Sc, respectively, i.e.,

$$\boxed{\text{Sh} = 2 + 0.6 \text{Re}_P^{1/2} \text{Sc}^{1/3}} \quad (4.3-33)$$

Equation (4.3-33) is valid for

$$2 \leq \text{Re}_P \leq 200$$

$$0.6 \leq \text{Sc} \leq 2.7$$

#### Frossling correlation

Frossling (1938) proposed the following correlation:

$$\boxed{\text{Sh} = 2 + 0.552 \text{Re}_P^{1/2} \text{Sc}^{1/3}} \quad (4.3-34)$$

Equation (4.3-34) is valid for

$$2 \leq \text{Re}_P \leq 800$$

$$0.6 \leq \text{Sc} \leq 2.7$$

Steinberger and Treybal (1960) modified Frossling correlation as

$$\boxed{\text{Sh} = 2 + 0.552 \text{Re}_P^{0.53} \text{Sc}^{1/3}} \quad (4.3-35)$$

which is valid for

$$1500 \leq \text{Re}_P \leq 12,000$$

$$0.6 \leq \text{Sc} \leq 1.85$$

---

<sup>2</sup>See Example 8.13 in Chapter 8.

**Steinberger-Treybal correlation**

The correlation originally proposed by Steinberger and Treybal (1960) includes a correction term for natural convection. The lack of experimental data, however, makes this term very difficult to calculate in most cases. The effect of natural convection becomes negligible when the Reynolds number is high and Steinberger-Treybal correlation reduces to

$$\text{Sh} = 0.347 \text{Re}_p^{0.62} \text{Sc}^{1/3} \quad (4.3-36)$$

Equation (4.3-36) is recommended for liquids when

$$2000 \leq \text{Re}_p \leq 16,900$$

**4.3.3.1 Calculation of the mass transfer rate**

Once the average mass transfer coefficient is estimated by using correlations, the rate of mass of species  $A$  transferred is calculated as

$$\dot{m}_A = (\pi D_p^2) \langle k_c \rangle |c_{A_w} - c_{A_\infty}| \mathcal{M}_A \quad (4.3-37)$$

**Example 4.8** *A solid sphere of benzoic acid ( $\rho = 1267 \text{ kg/m}^3$ ) with a diameter of 12 mm is dropped in a long cylindrical tank filled with pure water at 25°C. If the height of the tank is 3 m, determine the amount of benzoic acid dissolved from the sphere when it reaches the bottom of the tank. The saturation solubility of benzoic acid in water is 3.412 kg/m<sup>3</sup>.*

**Solution****Physical properties**

$$\text{For water (B) at } 25^\circ\text{C (298 K)} : \begin{cases} \rho = 1000 \text{ kg/m}^3 \\ \mu = 892 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ \mathcal{D}_{AB} = 1.21 \times 10^{-9} \text{ m}^2/\text{s} \end{cases}$$

The Schmidt number is

$$\begin{aligned} \text{Sc} &= \frac{\mu}{\rho \mathcal{D}_{AB}} \\ &= \frac{892 \times 10^{-6}}{(1000)(1.21 \times 10^{-9})} = 737 \end{aligned}$$

**Assumptions**

1. *Initial acceleration period is negligible and the sphere reaches its terminal velocity instantaneously.*

2. The diameter of the sphere does not change appreciably. Thus, the Reynolds number and the terminal velocity remain constant.
3. Steady-state conditions prevail.
4. Physical properties of water do not change as a result of mass transfer.

### Analysis

To determine the terminal velocity of the benzoic acid sphere, it is necessary to calculate the Archimedes number using Eq. (4.3-6):

$$\begin{aligned} Ar &= \frac{D_P^3 g \rho (\rho_P - \rho)}{\mu^2} \\ &= \frac{(12 \times 10^{-3})^3 (9.8) (1000) (1267 - 1000)}{(892 \times 10^{-6})^2} = 5.68 \times 10^6 \end{aligned}$$

The Reynolds number is calculated from Eq. (4.3-12):

$$\begin{aligned} Re_P &= \frac{Ar}{18} (1 + 0.0579 Ar^{0.412})^{-1.214} \\ &= \frac{5.68 \times 10^6}{18} [1 + 0.0579 (5.68 \times 10^6)^{0.412}]^{-1.214} = 4056 \end{aligned}$$

Hence, the terminal velocity is

$$\begin{aligned} v_t &= \frac{\mu Re_P}{\rho D_P} \\ &= \frac{(892 \times 10^{-6})(4056)}{(1000)(12 \times 10^{-3})} = 0.3 \text{ m/s} \end{aligned}$$

Since the benzoic acid sphere falls the distance of 3 m with a velocity of 0.3 m/s, then the falling time is

$$\begin{aligned} t &= \frac{\text{Distance}}{\text{Time}} \\ &= \frac{3}{0.3} = 10 \text{ s} \end{aligned}$$

The Sherwood number is calculated from the Steinberger-Treybal correlation, Eq. (4.3-36), as

$$\begin{aligned} Sh &= 0.347 Re_P^{0.62} Sc^{1/3} \\ &= 0.347 (4056)^{0.62} (737)^{1/3} = 541 \end{aligned}$$

The average mass transfer coefficient is

$$\begin{aligned} \langle k_c \rangle &= Sh \left( \frac{D_{AB}}{D_P} \right) \\ &= (541) \left( \frac{1.21 \times 10^{-9}}{12 \times 10^{-3}} \right) = 5.46 \times 10^{-5} \text{ m/s} \end{aligned}$$

The rate of transfer of benzoic acid (species  $A$ ) to water is calculated by using Eq. (4.3-37):

$$\begin{aligned}\dot{m}_A &= (\pi D_P^2) \langle k_c \rangle (c_{A_w} - c_{A_\infty}) \mathcal{M}_A = (\pi D_P^2) \langle k_c \rangle (\rho_{A_w} - \rho_{A_\infty}) \\ &= [\pi(12 \times 10^{-3})^2] (5.46 \times 10^{-5})(3.412 - 0) = 8.43 \times 10^{-8} \text{ kg/s}\end{aligned}$$

The amount of benzoic acid dissolved in 10 s is

$$\begin{aligned}M_A &= \dot{m}_A t \\ &= (8.43 \times 10^{-8})(10) = 8.43 \times 10^{-7} \text{ kg}\end{aligned}$$

### Verification of assumption # 2

The initial mass of the benzoic acid sphere,  $M_o$ , is

$$M_o = \left[ \frac{\pi(12 \times 10^{-3})^3}{6} \right] (1267) = 1.146 \times 10^{-3} \text{ kg}$$

The percent decrease in the mass of the sphere is given by

$$\left( \frac{8.43 \times 10^{-7}}{1.146 \times 10^{-3}} \right) \times 100 = 0.074\%$$

Therefore, the assumed constancy of  $D_P$  and  $v_t$  is justified.

## 4.4 FLOW NORMAL TO A SINGLE CYLINDER

### 4.4.1 Friction Factor Correlations

For cross flow over an infinitely long circular cylinder, Lapple and Shepherd (1940) presented their experimental data in the form of  $f$  versus  $\text{Re}_D$ , the Reynolds number based on the diameter of the cylinder. Their data can be approximated as

$$f = \frac{6.18}{\text{Re}_D^{8/9}} \quad \text{Re}_D < 2 \quad (4.4-1)$$

$$f = 1.2 \quad 10^4 \leq \text{Re}_D \leq 1.5 \times 10^5 \quad (4.4-2)$$

The friction factor  $f$  in Eqs. (4.4-1) and (4.4-2) is based on the projected area of a cylinder, i.e., diameter times length, and  $\text{Re}_D$  is defined by

$$\text{Re}_D = \frac{Dv_\infty\rho}{\mu} \quad (4.4-3)$$

Tosun and Akşahin (1992) proposed the following single equation for the friction factor that covers the entire range of the Reynolds number in the form

$$f = \frac{6.18}{\text{Re}_D^{8/9}} \left(1 + 0.36 \text{Re}_D^{5/9}\right)^{8/5} \quad \text{Re}_D \leq 1.5 \times 10^5 \quad (4.4-4)$$

Once the friction factor is determined, the drag force is calculated from

$$F_D = (DL) \left(\frac{1}{2} \rho v_\infty^2\right) f \quad (4.4-5)$$

**Example 4.9** A distillation column has an outside diameter of 80 cm and a height of 10 m. Calculate the drag force exerted by air on the column if the wind speed is 2.5 m/s.

### Solution

#### Physical properties

$$\text{For air at } 25^\circ\text{C (298 K)} : \begin{cases} \rho = 1.1845 \text{ kg/m}^3 \\ \mu = 18.41 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

#### Assumption

1. Air temperature is  $25^\circ\text{C}$ .

#### Analysis

From Eq. (4.4-3) the Reynolds number is

$$\begin{aligned} \text{Re}_D &= \frac{Dv_\infty\rho}{\mu} \\ &= \frac{(0.8)(2.5)(1.1845)}{18.41 \times 10^{-6}} = 1.29 \times 10^5 \end{aligned}$$

The use of Eq. (4.4-4) gives the friction factor as

$$\begin{aligned} f &= \frac{6.18}{\text{Re}_D^{8/9}} \left(1 + 0.36 \text{Re}_D^{5/9}\right)^{8/5} \\ &= \frac{6.18}{(1.29 \times 10^5)^{8/9}} \left[1 + 0.36 (1.29 \times 10^5)^{5/9}\right]^{8/5} = 1.2 \end{aligned}$$

Therefore, the drag force is calculated from Eq. (4.4-5) as

$$\begin{aligned} F_D &= (DL) \left(\frac{1}{2} \rho v_\infty^2\right) f \\ &= (0.8 \times 10) \left[\frac{1}{2} (1.1845)(2.5)^2\right] (1.2) = 35.5 \text{ N} \end{aligned}$$

### 4.4.2 Heat Transfer Correlations

As stated in Section 4.3.2, the analytical solution for steady-state conduction from a sphere to a stagnant medium gives  $Nu = 2$ . Therefore, the correlations for heat transfer in spherical geometry require that  $Nu \rightarrow 2$  as  $Re \rightarrow 0$ . In the case of a single cylinder, however, no solution for the case of steady-state conduction exists. Hence, it is required that  $Nu \rightarrow 0$  as  $Re \rightarrow 0$ . The following heat transfer correlations are available in this case:

#### Whitaker correlation

Whitaker (1972) proposed a correlation in the form

$$Nu = \left( 0.4 Re_D^{1/2} + 0.06 Re_D^{2/3} \right) Pr^{0.4} (\mu_\infty / \mu_w)^{1/4} \quad (4.4-6)$$

in which all properties except  $\mu_w$  are evaluated at  $T_\infty$ . Equation (4.4-6) is valid for

$$\begin{aligned} 1.0 &\leq Re_D \leq 1.0 \times 10^5 \\ 0.67 &\leq Pr \leq 300 \\ 0.25 &\leq \mu_\infty / \mu_w \leq 5.2 \end{aligned}$$

#### Zhukauskas correlation

The correlation proposed by Zhukauskas (1972) is given by

$$Nu = C Re_D^m Pr^n (Pr_\infty / Pr_w)^{1/4} \quad (4.4-7)$$

where

$$n = \begin{cases} 0.37 & \text{if } Pr \leq 10 \\ 0.36 & \text{if } Pr > 10 \end{cases}$$

and the values of  $C$  and  $m$  are given in Table 4.3. All properties except  $Pr_w$  should be evaluated at  $T_\infty$  in Eq. (4.4-7).

**Table 4.3** Constants of Eq. (4.4-7) for the circular cylinder in cross flow.

$Re_D$	$C$	$m$
1 – 40	0.75	0.4
40 – 1000	0.51	0.5
$1 \times 10^3 - 2 \times 10^5$	0.26	0.6
$2 \times 10^5 - 1 \times 10^6$	0.076	0.7

### Churchill-Bernstein correlation

Churchill and Bernstein (1977) proposed a single comprehensive equation that covers the entire range of  $Re_D$  for which data are available, as well as for a wide range of  $Pr$ , which is in the form

$$\boxed{Nu = 0.3 + \frac{0.62 Re_D^{1/2} Pr^{1/3}}{\left[1 + (0.4/Pr)^{2/3}\right]^{1/4}} \left[1 + \left(\frac{Re_D}{28,200}\right)^{5/8}\right]^{4/5}} \quad (4.4-8)$$

where all properties are evaluated at the film temperature. Equation (4.4-8) is recommended when

$$Re_D Pr > 0.2$$

#### 4.4.2.1 Calculation of the heat transfer rate

Once the average heat transfer coefficient is estimated by using correlations, the rate of heat transferred is calculated as

$$\boxed{\dot{Q} = (\pi DL)\langle h \rangle |T_w - T_\infty|} \quad (4.4-9)$$

**Example 4.10** Assume that a person can be approximated as a cylinder of 0.3 m diameter and 1.8 m height with a surface temperature of 30°C. Calculate the rate of heat loss from the body while this person is subjected to a 4 m/s wind with a temperature of -10°C.

#### Solution

##### Physical properties

The film temperature is  $(30 - 10)/2 = 10^\circ\text{C}$

$$\text{For air at } -10^\circ\text{C (263 K)} : \begin{cases} \mu = 16.7 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ \nu = 12.44 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 23.28 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ Pr = 0.72 \end{cases}$$

$$\text{For air at } 10^\circ\text{C (280 K)} : \begin{cases} \nu = 14.18 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 24.86 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ Pr = 0.714 \end{cases}$$

$$\text{For air at } 30^\circ\text{C (303 K)} : \begin{cases} \mu = 18.64 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ Pr = 0.71 \end{cases}$$

#### Assumption

1. Steady-state conditions prevail.

**Analysis**

The rate of heat loss from the body can be calculated from Eq. (4.4-9):

$$\dot{Q} = (\pi DL)\langle h \rangle (T_w - T_\infty) \quad (1)$$

Determination of  $\langle h \rangle$  in Eq. (1) requires the Reynolds number to be known. The Reynolds numbers at  $T_\infty$  and  $T_f$  are

$$\text{at } T_\infty = -10^\circ\text{C} \quad \text{Re}_D = \frac{D v_\infty}{\nu} = \frac{(0.3)(4)}{12.44 \times 10^{-6}} = 9.65 \times 10^4$$

$$\text{at } T_f = 10^\circ\text{C} \quad \text{Re}_D = \frac{D v_\infty}{\nu} = \frac{(0.3)(4)}{14.18 \times 10^{-6}} = 8.46 \times 10^4$$

**Whitaker correlation**

The use of Eq. (4.4-6) gives the Nusselt number as

$$\begin{aligned} \text{Nu} &= \left( 0.4 \text{Re}_D^{1/2} + 0.06 \text{Re}_D^{2/3} \right) \text{Pr}^{0.4} (\mu_\infty / \mu_w)^{1/4} \\ &= \left[ 0.4 (9.65 \times 10^4)^{1/2} + 0.06 (9.65 \times 10^4)^{2/3} \right] (0.72)^{0.4} \left( \frac{16.7 \times 10^{-6}}{18.64 \times 10^{-6}} \right)^{1/4} \\ &= 214 \end{aligned}$$

Hence, the average heat transfer coefficient is

$$\begin{aligned} \langle h \rangle &= \text{Nu} \left( \frac{k}{D} \right) \\ &= (214) \left( \frac{23.28 \times 10^{-3}}{0.3} \right) = 16.6 \text{ W/m}^2 \cdot \text{K} \end{aligned}$$

Substitution of this result into Eq. (1) gives the rate of heat loss as

$$\dot{Q} = (\pi \times 0.3 \times 1.8) (16.6) [30 - (-10)] = 1126 \text{ W}$$

**Zhukauskas correlation**

Since  $\text{Re}_D = 9.65 \times 10^4$  and  $\text{Pr} < 10$ , from Table 4.3 the constants are:  $C = 0.26$ ,  $m = 0.6$  and  $n = 0.37$ . Hence, the use of Eq. (4.4-7) gives

$$\begin{aligned} \text{Nu} &= 0.26 \text{Re}_D^{0.6} \text{Pr}^{0.37} (\text{Pr}_\infty / \text{Pr}_w)^{1/4} \\ &= 0.26 (9.65 \times 10^4)^{0.6} (0.72)^{0.37} \left( \frac{0.72}{0.71} \right)^{1/4} = 226 \end{aligned}$$

Therefore, the average heat transfer coefficient and the rate of heat loss from the body are

$$\begin{aligned}\langle h \rangle &= \text{Nu} \left( \frac{k}{D} \right) \\ &= (226) \left( \frac{23.28 \times 10^{-3}}{0.3} \right) = 17.5 \text{ W/m}^2 \cdot \text{K}\end{aligned}$$

$$\dot{Q} = (\pi \times 0.3 \times 1.8) (17.5) [30 - (-10)] = 1188 \text{ W}$$

### Churchill-Bernstein correlation

The use of Eq. (4.4-8) gives

$$\begin{aligned}\text{Nu} &= 0.3 + \frac{0.62 \text{Re}_D^{1/2} \text{Pr}^{1/3}}{\left[ 1 + (0.4/\text{Pr})^{2/3} \right]^{1/4}} \left[ 1 + \left( \frac{\text{Re}_D}{28,200} \right)^{5/8} \right]^{4/5} \\ &= 0.3 + \frac{0.62 (8.46 \times 10^4)^{1/2} (0.714)^{1/3}}{\left[ 1 + (0.4/0.714)^{2/3} \right]^{1/4}} \left[ 1 + \left( \frac{8.46 \times 10^4}{28,200} \right)^{5/8} \right]^{4/5} = 340\end{aligned}$$

The average heat transfer coefficient and the rate of heat loss from the body are

$$\begin{aligned}\langle h \rangle &= \text{Nu} \left( \frac{k}{D} \right) \\ &= (340) \left( \frac{24.86 \times 10^{-3}}{0.3} \right) = 28.2 \text{ W/m}^2 \cdot \text{K}\end{aligned}$$

$$\dot{Q} = (\pi \times 0.3 \times 1.8) (28.2) [30 - (-10)] = 1914 \text{ W}$$

**Comment:** The heat transfer coefficient predicted by the Churchill-Bernstein correlation is 70% greater than the one calculated using the Whitaker correlation. It is important to note that no two correlations will exactly give the same result.

### 4.4.3 Mass Transfer Correlations

Bedingfield and Drew (1950) proposed the following correlation for cross- and parallel-flow of gases to the cylinder in which mass transfer to or from the ends of the cylinder is not considered:

$$\boxed{\text{Sh} = 0.281 \text{Re}_D^{1/2} \text{Sc}^{0.44}} \quad (4.4-10)$$

Equation (4.4-10) is valid for

$$400 \leq \text{Re}_D \leq 25,000$$

$$0.6 < \text{Sc} < 2.6$$

For liquids the correlation obtained by Linton and Sherwood (1950) may be used:

$$\boxed{\text{Sh} = 0.281 \text{Re}_D^{0.6} \text{Sc}^{1/3}} \quad (4.4-11)$$

Equation (4.4-11) is valid for

$$400 \leq \text{Re}_D \leq 25,000$$

$$\text{Sc} \leq 3,000$$

#### 4.4.3.1 Calculation of the mass transfer rate

Once the average mass transfer coefficient is estimated by using correlations, the rate of mass of species  $A$  transferred is calculated as

$$\boxed{\dot{m}_A = (\pi DL) \langle k_c \rangle |c_{A_w} - c_{A_\infty}| \mathcal{M}_A} \quad (4.4-12)$$

where  $\mathcal{M}_A$  is the molecular weight of species  $A$ .

**Example 4.11** *A cylindrical pipe of 5 cm outside diameter is covered with a thin layer of ethanol. Air at 30°C flows normal to the pipe with a velocity of 3 m/s. Determine the average mass transfer coefficient.*

#### Solution

##### Physical properties

*Diffusion coefficient of ethanol (A) in air (B) at 30°C (303 K) :*

$$(\mathcal{D}_{AB})_{303} = (\mathcal{D}_{AB})_{313} \left( \frac{303}{313} \right)^{3/2}$$

$$= (1.45 \times 10^{-5}) \left( \frac{303}{313} \right)^{3/2} = 1.38 \times 10^{-5} \text{ m}^2/\text{s}$$

*For air at 30°C (303 K) :  $\nu = 16 \times 10^{-6} \text{ m}^2/\text{s}$*

*The Schmidt number is*

$$\text{Sc} = \frac{\nu}{\mathcal{D}_{AB}}$$

$$= \frac{16 \times 10^{-6}}{1.38 \times 10^{-5}} = 1.16$$

##### Assumptions

1. *Steady-state conditions prevail.*
2. *Isothermal system.*

**Analysis**

The Reynolds number is

$$\begin{aligned} \text{Re}_D &= \frac{D v_\infty}{\nu} \\ &= \frac{(5 \times 10^{-2})(3)}{16 \times 10^{-6}} = 9375 \end{aligned}$$

The use of the correlation proposed by Bedingfield and Drew, Eq. (4.4-10), gives

$$\begin{aligned} \text{Sh} &= 0.281 \text{Re}_D^{1/2} \text{Sc}^{0.44} \\ &= 0.281 (9375)^{1/2} (1.16)^{0.44} = 29 \end{aligned}$$

Therefore, the average mass transfer coefficient is

$$\begin{aligned} \langle k_c \rangle &= \text{Sh} \left( \frac{\mathcal{D}_{AB}}{D} \right) \\ &= (29) \left( \frac{1.38 \times 10^{-5}}{5 \times 10^{-2}} \right) = 8 \times 10^{-3} \text{ m/s} \end{aligned}$$

**4.5 FLOW IN CIRCULAR PIPES**

The rate of work done,  $\dot{W}$ , to pump a fluid can be determined from the expression

$$\dot{W} = \dot{m} \hat{W} = \dot{m} \left( \int \hat{V} dP \right) \quad (4.5-1)$$

where  $\dot{m}$  and  $\hat{V}$  are the mass flow rate and the specific volume of the fluid, respectively. Note that the term in parenthesis on the right-hand side of Eq. (4.5-1) is known as the *shaft work* in thermodynamics<sup>3</sup>. For an incompressible fluid, i.e.,  $\hat{V} = 1/\rho = \text{constant}$ , Eq. (4.5-1) simplifies to

$$\dot{W} = Q |\Delta P| \quad (4.5-2)$$

where  $Q$  is the volumetric flow rate of the fluid. Combination of Eq. (4.5-2) with Eq. (3.1-11) gives

$$F_D \langle v \rangle = Q |\Delta P| \quad (4.5-3)$$

or,

$$\left[ (\pi DL) \left( \frac{1}{2} \rho \langle v \rangle^2 \right) f \right] \langle v \rangle = Q |\Delta P| \quad (4.5-4)$$

Expressing the average velocity in terms of the volumetric flow rate

$$\langle v \rangle = \frac{Q}{\pi D^2/4} \quad (4.5-5)$$

---

<sup>3</sup>Work done on the system is considered positive.

reduces Eq. (4.5-4) to

$$\boxed{|\Delta P| = \frac{32 \rho L f Q^2}{\pi^2 D^5}} \quad (4.5-6)$$

Engineering problems associated with pipe flow are classified as follows:

- Determine the pressure drop,  $|\Delta P|$ , or the pump size,  $\dot{W}$ ; given the volumetric flow rate,  $Q$ , the pipe diameter,  $D$ , and the physical properties of the fluid,  $\rho$  and  $\mu$ .
- Determine the volumetric flow rate,  $Q$ ; given the pressure drop,  $|\Delta P|$ , the pipe diameter,  $D$ , and the physical properties of the fluid,  $\rho$  and  $\mu$ .
- Determine the pipe diameter,  $D$ ; given the volumetric flow rate,  $Q$ , the pressure drop,  $|\Delta P|$ , and the physical properties of the fluid,  $\rho$  and  $\mu$ .

## 4.5.1 Friction Factor Correlations

### 4.5.1.1 Laminar flow correlation

For laminar flow in a circular pipe, i.e.,  $Re = D(v)\rho/\mu < 2100$ , the solution of the equations of change gives<sup>4</sup>

$$\boxed{f = \frac{16}{Re}} \quad (4.5-7)$$

The friction factor  $f$  appearing in Eqs. (4.5-6) and (4.5-7) is also called the *Fanning friction factor*. However, this is not the only definition for  $f$  available in the literature. Another commonly used definition for  $f$  is the *Darcy friction factor*,  $f_D$ , which is four times larger than the Fanning friction factor, i.e.,  $f_D = 4f$ . Therefore, for laminar flow

$$f_D = \frac{64}{Re} \quad (4.5-8)$$

### 4.5.1.2 Turbulent flow correlation

Since no theoretical solution exists for turbulent flow, the friction factor is usually determined from the *Moody chart* (1944) in which it is expressed as a function of the Reynolds number,  $Re$ , and the relative pipe wall roughness,  $\varepsilon/D$ . Moody prepared this chart by using the equation proposed by Colebrook (1938)

$$\boxed{\frac{1}{\sqrt{f}} = -4 \log \left( \frac{\varepsilon/D}{3.7065} + \frac{1.2613}{Re \sqrt{f}} \right)} \quad (4.5-9)$$

where  $\varepsilon$  is the surface roughness of the pipe wall in meters.

<sup>4</sup>See Section 9.1.3.1 in Chapter 9.

## 4.5.1.3 Solutions to the engineering problems

## I. Laminar flow

For flow in a pipe, the Reynolds number is defined by

$$\text{Re} = \frac{D\langle v \rangle \rho}{\mu} = \frac{4\rho Q}{\pi\mu D} \quad (4.5-10)$$

Substitution of Eq. (4.5-10) into Eq. (4.5-7) yields

$$f = \frac{4\pi\mu D}{\rho Q} \quad (4.5-11)$$

■ Calculate  $|\Delta P|$  or  $\dot{W}$ ; given  $Q$  and  $D$

Substitution of Eq. (4.5-11) into Eq. (4.5-6) gives

$$|\Delta P| = \frac{128\mu L Q}{\pi D^4} \quad (4.5-12)$$

The pump size can be calculated from Eq. (4.5-2) as

$$\dot{W} = \frac{128\mu L Q^2}{\pi D^4} \quad (4.5-13)$$

■ Calculate  $Q$ ; given  $|\Delta P|$  and  $D$

Rearrangement of Eq. (4.5-12) gives

$$Q = \frac{\pi D^4 |\Delta P|}{128\mu L} \quad (4.5-14)$$

■ Calculate  $D$ ; given  $Q$  and  $|\Delta P|$

Rearrangement of Eq. (4.5-12) gives

$$D = \left( \frac{128\mu L Q}{\pi |\Delta P|} \right)^{1/4} \quad (4.5-15)$$

## II. Turbulent flow

### ■ Calculate $|\Delta P|$ or $\dot{W}$ ; given $Q$ and $D$

For the given values of  $Q$  and  $D$ , the Reynolds number can be determined using Eq. (4.5-10). However, when the values of  $Re$  and  $\varepsilon/D$  are known, determination of  $f$  from Eq. (4.5-9) requires an iterative procedure since  $f$  appears on both sides of the equation. To avoid the iterative solutions, efforts have been directed to express the friction factor,  $f$ , as an explicit function of the Reynolds number,  $Re$ , and the relative pipe wall roughness,  $\varepsilon/D$ .

Gregory and Fogarasi (1985) compared the predictions of the twelve explicit relations with Eq. (4.5-9) and recommended the use of the correlation proposed by Chen (1979):

$$\frac{1}{\sqrt{f}} = -4 \log \left( \frac{\varepsilon/D}{3.7065} - \frac{5.0452}{Re} \log A \right) \quad (4.5-16)$$

where

$$A = \left( \frac{\varepsilon/D}{2.5497} \right)^{1.1098} + \left( \frac{7.1490}{Re} \right)^{0.8981} \quad (4.5-17)$$

Thus, in order to calculate the pressure drop using Eq. (4.5-16), the following procedure should be followed through which an iterative solution is avoided:

- Calculate the Reynolds number from Eq. (4.5-10),
- Substitute  $Re$  into Eq. (4.5-16) and determine  $f$ ,
- Use Eq. (4.5-6) to find the pressure drop. Finally, the pump size can be determined by using Eq. (4.5-2).

**Example 4.12** *What is the required pressure drop per unit length in order to pump water at a volumetric flow rate of  $0.03 \text{ m}^3/\text{s}$  at  $20^\circ\text{C}$  through a commercial steel pipe ( $\varepsilon = 4.6 \times 10^{-5} \text{ m}$ ) 20 cm in diameter?*

### Solution

#### Physical properties

$$\text{For water at } 20^\circ\text{C (293 K)} : \begin{cases} \rho = 999 \text{ kg/m}^3 \\ \mu = 1001 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

#### Analysis

The Reynolds number is determined from Eq. (4.5-10) as

$$\begin{aligned} Re &= \frac{4\rho Q}{\pi\mu D} \\ &= \frac{(4)(999)(0.03)}{\pi(1001 \times 10^{-6})(0.2)} = 191 \times 10^3 \end{aligned}$$

Substitution of this value into Eqs. (4.5-17) and (4.5-16) gives

$$A = \left( \frac{\varepsilon/D}{2.5497} \right)^{1.1098} + \left( \frac{7.1490}{\text{Re}} \right)^{0.8981}$$

$$= \left[ \frac{(4.6 \times 10^{-5}/0.2)}{2.5497} \right]^{1.1098} + \left( \frac{7.1490}{191 \times 10^3} \right)^{0.8981} = 1.38 \times 10^{-4}$$

$$\frac{1}{\sqrt{f}} = -4 \log \left( \frac{\varepsilon/D}{3.7065} - \frac{5.0452}{\text{Re}} \log A \right)$$

$$= -4 \log \left[ \frac{(4.6 \times 10^{-5}/0.2)}{3.7065} - \frac{5.0452}{191 \times 10^3} \log(1.38 \times 10^{-4}) \right] = 15.14$$

Hence, the friction factor is

$$f = 4.36 \times 10^{-3}$$

Thus, Eq. (4.5-6) gives the pressure drop per unit pipe length as

$$\frac{|\Delta P|}{L} = \frac{32 \rho f Q^2}{\pi^2 D^5}$$

$$= \frac{(32)(999)(4.36 \times 10^{-3})(0.03)^2}{\pi^2 (0.2)^5} = 40 \text{ Pa/m}$$

■ Calculate  $Q$ ; given  $|\Delta P|$  and  $D$

In this case rearrangement of Eq. (4.5-6) gives

$$f = \left( \frac{Y}{Q} \right)^2 \quad (4.5-18)$$

where  $Y$  is defined by

$$Y = \sqrt{\frac{\pi^2 D^5 |\Delta P|}{32 \rho L}} \quad (4.5-19)$$

Substitution of Eqs. (4.5-10) and (4.5-18) into Eq. (4.5-9) yields

$$\boxed{Q = -4Y \log \left( \frac{\varepsilon/D}{3.7065} + \frac{\mu D}{\rho Y} \right)} \quad (4.5-20)$$

Thus, the procedure to calculate the volumetric flow rate becomes:

- a) Calculate  $Y$  from Eq. (4.5-19),
- b) Substitute  $Y$  into Eq. (4.5-20) and determine the volumetric flow rate.

**Example 4.13** What is the volumetric flow rate of water in  $\text{m}^3/\text{s}$  at  $20^\circ\text{C}$  that can be delivered through a commercial steel pipe ( $\varepsilon = 4.6 \times 10^{-5} \text{ m}$ ) 20 cm in diameter when the pressure drop per unit length of the pipe is  $40 \text{ Pa/m}$ ?

**Solution****Physical properties**

$$\text{For water at } 20^\circ\text{C (293 K)} : \begin{cases} \rho = 999 \text{ kg/m}^3 \\ \mu = 1001 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

**Analysis**

Substitution of the given values into Eq. (4.5-19) yields

$$\begin{aligned} Y &= \sqrt{\frac{\pi^2 D^5 |\Delta P|}{32 \rho L}} \\ &= \sqrt{\frac{\pi^2 (0.2)^5 (40)}{(32)(999)}} = 1.99 \times 10^{-3} \end{aligned}$$

Hence, Eq. (4.5-20) gives the volumetric flow rate as

$$\begin{aligned} Q &= -4Y \log \left( \frac{\varepsilon/D}{3.7065} + \frac{\mu D}{\rho Y} \right) \\ &= -(4)(1.99 \times 10^{-3}) \log \left[ \frac{(4.6 \times 10^{-5}/0.2)}{3.7065} + \frac{(1001 \times 10^{-6})(0.2)}{(999)(1.99 \times 10^{-3})} \right] \\ &= 0.03 \text{ m}^3/\text{s} \end{aligned}$$

**■ Calculate  $D$ ; given  $Q$  and  $|\Delta P|$** 

Swamee and Jain (1976) and Cheng and Turton (1990) presented explicit equations to solve problems of this type. These equations, however, are unnecessarily complex. A simpler equation can be obtained by using the procedure suggested by Tosun and Akşahin (1993) as follows. Equation (4.5-6) can be rearranged in the form

$$f = (DN)^5 \quad (4.5-21)$$

where  $N$  is defined by

$$N = \left( \frac{\pi^2 |\Delta P|}{32 \rho L Q^2} \right)^{1/5} \quad (4.5-22)$$

For turbulent flow, the value of  $f$  changes between 0.00025 and 0.01925. Using an average value of 0.01 for  $f$  gives a relationship between  $D$  and  $N$  as

$$D = \frac{0.4}{N} \quad (4.5-23)$$

Substitution of Eq. (4.5-21) to the left-hand side of Eq. (4.5-9), and substitution of Eqs. (4.5-10) and (4.5-23) to the right-hand side of Eq. (4.5-9) gives

$$D = \frac{0.575}{N} \left( \left\{ \left[ \log(\varepsilon N) + 5.806 \left( \frac{\mu}{\rho Q N} \right) \right] - 0.171 \right\}^2 \right)^{-1/5} \quad (4.5-24)$$

The procedure to calculate the pipe diameter becomes:

- a) Calculate  $N$  from Eq. (4.5-22),
- b) Substitute  $N$  into Eq. (4.5-24) and determine the pipe diameter.

**Example 4.14** *Water at 20 °C is to be pumped through a commercial steel pipe ( $\varepsilon = 4.6 \times 10^{-5}$  m) at a volumetric flow rate of 0.03 m<sup>3</sup>/s. Determine the diameter of the pipe if the allowable pressure drop per unit length of pipe is 40 Pa/m.*

### Solution

#### Physical properties

$$\text{For water at } 20^\circ\text{C (293 K)} : \begin{cases} \rho = 999 \text{ kg/m}^3 \\ \mu = 1001 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

#### Analysis

Equation (4.5-22) gives

$$\begin{aligned} N &= \left( \frac{\pi^2 |\Delta P|}{32 \rho L Q^2} \right)^{1/5} \\ &= \left[ \frac{\pi^2 (40)}{(32)(999)(0.03)^2} \right]^{1/5} = 1.69 \end{aligned}$$

Hence, Eq. (4.5-24) gives the pipe diameter as

$$\begin{aligned} D &= \frac{0.575}{N} \left( \left\{ \left[ \log(\varepsilon N) + 5.806 \left( \frac{\mu}{\rho Q N} \right) \right] - 0.171 \right\}^2 \right)^{-1/5} \\ &= \frac{0.575}{1.69} \left( \left\{ \left[ \log [(4.6 \times 10^{-5})(1.69)] + 5.806 \left( \frac{1001 \times 10^{-6}}{(999)(0.03)(1.69)} \right) \right] - 0.171 \right\}^2 \right)^{-1/5} = 0.2 \text{ m} \end{aligned}$$

## 4.5.2 Heat Transfer Correlations

For heat transfer in circular pipes, various correlations have been suggested depending on the flow conditions, i.e., laminar or turbulent.

### 4.5.2.1 Laminar flow correlation

For laminar flow heat transfer in a circular tube with constant wall temperature, Sieder and Tate (1936) proposed the following correlation:

$$\boxed{\text{Nu} = 1.86 [\text{Re Pr} (D/L)]^{1/3} (\mu/\mu_w)^{0.14}} \quad (4.5-25)$$

in which all properties except  $\mu_w$  are evaluated at the mean bulk temperature. Equation (4.5-25) is valid for

$$13 \leq \text{Re} \leq 2030$$

$$0.48 \leq \text{Pr} \leq 16,700$$

$$0.0044 \leq \mu/\mu_w \leq 9.75$$

The analytical solution<sup>5</sup> to this problem is only possible for very long tubes, i.e.,  $L/D \rightarrow \infty$ . In this case the Nusselt number remains constant at the value of 3.66.

#### 4.5.2.2 Turbulent flow correlations

The following correlations approximate the physical situation quite well for the cases of constant wall temperature and constant wall heat flux:

##### Dittus-Boelter correlation

Dittus and Boelter (1930) proposed the following correlation in which all physical properties are evaluated at the mean bulk temperature:

$$\text{Nu} = 0.023 \text{Re}_P^{4/5} \text{Pr}^n \quad (4.5-26)$$

where

$$n = \begin{cases} 0.4 & \text{for heating} \\ 0.3 & \text{for cooling} \end{cases}$$

The Dittus-Boelter correlation is valid when

$$0.7 \leq \text{Pr} \leq 160$$

$$\text{Re} \geq 10,000$$

$$L/D \geq 10$$

##### Sieder-Tate correlation

Sieder and Tate (1936) correlation is

$$\text{Nu} = 0.027 \text{Re}_P^{4/5} \text{Pr}^{1/3} (\mu/\mu_w)^{0.14} \quad (4.5-27)$$

in which all properties except  $\mu_w$  are evaluated at the mean bulk temperature. Equation (4.5-27) is valid for

$$0.7 \leq \text{Pr} \leq 16,700$$

$$\text{Re} \geq 10,000$$

$$L/D \geq 10$$

---

<sup>5</sup>See Section 9.3.1.2 in Chapter 9.

**Whitaker correlation**

The equation proposed by Whitaker (1972) is

$$\boxed{\text{Nu} = 0.015 \text{Re}_P^{0.83} \text{Pr}^{0.42} (\mu/\mu_w)^{0.14}} \quad (4.5-28)$$

in which the Prandtl number dependence is based on the work of Friend and Metzner (1958), and the functional dependence of  $\mu/\mu_w$  is from the work of Sieder and Tate (1936). All physical properties except  $\mu_w$  are evaluated at the mean bulk temperature. The Whitaker correlation is valid for

$$2,300 \leq \text{Re} \leq 1 \times 10^5$$

$$0.48 \leq \text{Pr} \leq 592$$

$$0.44 \leq \mu/\mu_w \leq 2.5$$

**4.5.2.3 Calculation of the heat transfer rate**

Once the average heat transfer coefficient is calculated from correlations by using Eqs. (4.5-25)-(4.5-28), then the rate of energy transferred is calculated as

$$\boxed{\dot{Q} = (\pi DL)\langle h \rangle \Delta T_{LM}} \quad (4.5-29)$$

where  $\Delta T_{LM}$ , *logarithmic mean temperature difference*, is defined by

$$\Delta T_{LM} = \frac{(T_w - T_b)_{in} - (T_w - T_b)_{out}}{\ln \left[ \frac{(T_w - T_b)_{in}}{(T_w - T_b)_{out}} \right]} \quad (4.5-30)$$

The derivation of Eq. (4.5-29) is given in Section 9.3 in Chapter 9.

**Example 4.15** *Steam condensing on the outer surface of a thin-walled circular tube of 65 mm diameter maintains a uniform surface temperature of 100 °C. Oil flows through the tube at an average velocity of 1 m/s. Determine the length of the tube in order to increase oil temperature from 40 °C to 60 °C. Physical properties of the oil are as follows:*

$$\text{At } 50^\circ\text{C} : \begin{cases} \mu = 12.4 \times 10^{-3} \text{ kg/m}\cdot\text{s} \\ \nu = 4.28 \times 10^{-5} \text{ m}^2/\text{s} \\ \text{Pr} = 143 \end{cases}$$

$$\text{At } 100^\circ\text{C} : \mu = 9.3 \times 10^{-3} \text{ kg/m}\cdot\text{s}$$

**Solution****Assumptions**

1. *Steady-state conditions prevail.*
2. *Physical properties remain constant.*
3. *Changes in kinetic and potential energies are negligible.*

**Analysis**

*System: Oil in the pipe*

*The inventory rate equation for mass becomes*

$$\text{Rate of mass in} = \text{Rate of mass out} = \dot{m} = \rho \langle v \rangle (\pi D^2 / 4) \quad (1)$$

*On the other hand, the inventory rate equation for energy reduces to*

$$\text{Rate of energy in} = \text{Rate of energy out} \quad (2)$$

*The terms in Eq. (2) are expressed by*

$$\text{Rate of energy in} = \dot{m} \hat{C}_P (T_{b_{in}} - T_{ref}) + \pi DL \langle h \rangle \Delta T_{LM} \quad (3)$$

$$\text{Rate of energy out} = \dot{m} \hat{C}_P (T_{b_{out}} - T_{ref}) \quad (4)$$

*Since the wall temperature is constant, the expression for  $\Delta T_{LM}$ , Eq. (4.5-30), becomes*

$$\Delta T_{LM} = \frac{T_{b_{out}} - T_{b_{in}}}{\ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right)} \quad (5)$$

*Substitution of Eqs. (1), (3), (4) and (5) into Eq. (2) gives*

$$\frac{L}{D} = \frac{1}{4} \frac{\langle v \rangle \rho \hat{C}_P}{\langle h \rangle} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \quad (6)$$

*Noting that  $St_H = \langle h \rangle / (\langle v \rangle \rho \hat{C}_P) = Nu / (Re Pr)$ , Eq. (6) becomes*

$$\frac{L}{D} = \frac{1}{4} \frac{1}{St_H} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) = \frac{1}{4} \frac{Re Pr}{Nu} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \quad (7)$$

*To determine Nu (or,  $\langle h \rangle$ ), first the Reynolds number must be calculated. The mean bulk temperature is  $(40 + 60)/2 = 50^\circ\text{C}$  and the Reynolds number is*

$$\begin{aligned} Re &= \frac{D \langle v \rangle}{\nu} \\ &= \frac{(65 \times 10^{-3})(1)}{4.28 \times 10^{-5}} = 1519 \quad \Rightarrow \quad \text{Laminar flow} \end{aligned}$$

Since the flow is laminar, Eq. (4.5-25) must be used, i.e.,

$$\text{Nu} = 1.86 [\text{Re Pr} (D/L)]^{1/3} (\mu/\mu_w)^{0.14} \quad (8)$$

Substitution of Eq. (8) into Eq. (7) yields

$$\begin{aligned} \frac{L}{D} &= \text{Re Pr} \left[ \frac{(\mu/\mu_w)^{-0.14}}{(4)(1.86)} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \right]^{3/2} \\ &= (1519)(143) \left[ \frac{(12.4 \times 10^{-3}/9.3 \times 10^{-3})^{-0.14}}{(4)(1.86)} \ln \left( \frac{100 - 40}{100 - 60} \right) \right]^{3/2} \\ &= 2602 \end{aligned}$$

The tube length is then

$$L = (2602)(65 \times 10^{-3}) = 169 \text{ m}$$

**Example 4.16** Air at 20 °C enters a circular pipe of 1.5 cm internal diameter with a velocity of 50 m/s. Steam condenses on the outside of the pipe so as to keep the surface temperature of the pipe at 150 °C.

- Calculate the length of the pipe required to increase air temperature to 90 °C.
- Discuss the effect of surface roughness on the length of the pipe.

### Solution

#### Physical properties

The mean bulk temperature is  $(20 + 90)/2 = 55^\circ\text{C}$

For air at 20 °C (293 K) :  $\rho = 1.2047 \text{ kg/m}^3$

For air at 55 °C (328 K) :  $\begin{cases} \mu = 19.8 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ \nu = 18.39 \times 10^{-6} \text{ m}^2/\text{s} \\ \text{Pr} = 0.707 \end{cases}$

For air at 150 °C (423 K) :  $\mu = 23.86 \times 10^{-6} \text{ kg/m}\cdot\text{s}$

#### Analysis

- System: Air in the pipe

The inventory rate equation for mass reduces to

$$\text{Rate of mass of air in} = \text{Rate of mass of air out} = \dot{m} \quad (1)$$

Note that for compressible fluids like air, both density and average velocity depend on temperature and pressure. Therefore, using the inlet conditions

$$\begin{aligned} \dot{m} &= (\pi D^2/4) (\rho v)_{inlet} \\ &= \left[ \frac{\pi(0.015)^2}{4} \right] (1.2047)(50) = 1.06 \times 10^{-2} \text{ kg/s} \end{aligned}$$

In problems dealing with the flow of compressible fluids, it is customary to define mass velocity,  $G$ , as

$$G = \frac{\dot{m}}{A} = \rho(v) \quad (2)$$

The advantage of using  $G$  is the fact that it remains constant for steady flow of compressible fluids through ducts of uniform cross-section. In this case

$$G = (1.2047)(50) = 60.24 \text{ kg/m}^2 \cdot \text{s}$$

The inventory rate equation for energy is written as

$$\text{Rate of energy in} = \text{Rate of energy out} \quad (3)$$

Equations (3)-(5) of Example 4.15 are also applicable to this problem. Therefore, we get

$$\frac{L}{D} = \frac{1}{4} \frac{\text{Re Pr}}{\text{Nu}} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \quad (4)$$

The Nusselt number in Eq. (4) can be determined only if the Reynolds number is known. The Reynolds number is calculated as

$$\begin{aligned} \text{Re} &= \frac{DG}{\mu} \\ &= \frac{(0.015)(60.24)}{19.80 \times 10^{-6}} = 45,636 \quad \Rightarrow \quad \text{Turbulent flow} \end{aligned}$$

The value of  $L$  depends on the correlations as follows:

#### Dittus-Boelter correlation

Substitution of Eq. (4.5-26) into Eq. (4) gives

$$\begin{aligned} \frac{L}{D} &= \frac{\text{Re}^{0.2} \text{Pr}^{0.6}}{0.092} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \\ &= \frac{(45,636)^{0.2} (0.707)^{0.6}}{0.092} \ln \left( \frac{150 - 20}{150 - 90} \right) = 58.3 \end{aligned}$$

Therefore, the required length is

$$L = (58.3)(1.5) = 87 \text{ cm}$$

#### Sieder-Tate correlation

Substitution of Eq. (4.5-27) into Eq. (4) gives

$$\begin{aligned} \frac{L}{D} &= \frac{\text{Re}^{0.2} \text{Pr}^{2/3} \left( \mu/\mu_w \right)^{-0.14}}{0.108} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \\ &= \frac{(45,636)^{0.2} (0.707)^{2/3}}{0.108} \left( \frac{19.80 \times 10^{-6}}{23.86 \times 10^{-6}} \right)^{-0.14} \ln \left( \frac{150 - 20}{150 - 90} \right) = 49.9 \end{aligned}$$

Therefore, the required length is

$$L = (49.9)(1.5) = 75 \text{ cm}$$

### Whitaker correlation

Substitution of Eq. (4.5-28) into Eq. (4) gives

$$\begin{aligned} \frac{L}{D} &= \frac{\text{Re}^{0.17} \text{Pr}^{0.58} \left(\mu/\mu_w\right)^{-0.14}}{0.06} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \\ &= \frac{(45,636)^{0.17} (0.707)^{0.58} \left(\frac{19.80 \times 10^{-6}}{23.86 \times 10^{-6}}\right)^{-0.14}}{0.06} \ln \left( \frac{150 - 20}{150 - 90} \right) = 67 \end{aligned}$$

Therefore, the required length is

$$L = (67)(1.5) = 101 \text{ cm}$$

b) Note that Eq. (4) is also expressed in the form

$$\frac{L}{D} = \frac{1}{4} \frac{1}{\text{St}_H} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \quad (5)$$

The use of the Chilton-Colburn analogy, i.e.,  $f/2 = \text{St}_H \text{Pr}^{2/3}$ , reduces Eq. (5) to

$$\begin{aligned} \frac{L}{D} &= \frac{1}{2} \frac{\text{Pr}^{2/3}}{f} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \\ &= \frac{1}{2} \frac{(0.707)^{2/3}}{f} \ln \left( \frac{150 - 20}{150 - 90} \right) = \frac{0.3068}{f} \end{aligned} \quad (6)$$

The friction factor can be calculated from the Chen correlation, Eq. (4.5-16)

$$\frac{1}{\sqrt{f}} = -4 \log \left( \frac{\varepsilon/D}{3.7065} - \frac{5.0452}{\text{Re}} \log A \right)$$

where

$$A = \left( \frac{\varepsilon/D}{2.5497} \right)^{1.1098} + \left( \frac{7.1490}{\text{Re}} \right)^{0.8981}$$

For various values of  $\varepsilon/D$ , the calculated values of  $f$ ,  $L/D$  and  $L$  are given as follows:

$\varepsilon/D$	$f$	$L/D$	$L$ (cm)
0	0.0053	57.9	86.9
0.001	0.0061	50.3	75.5
0.002	0.0067	45.8	68.7
0.003	0.0072	42.6	63.9
0.004	0.0077	39.8	59.7

**Comment:** *The increase in surface roughness increases the friction factor and hence power consumption. On the other hand, the increase in surface roughness causes an increase in the heat transfer coefficient with a concomitant decrease in pipe length.*

### 4.5.3 Mass Transfer Correlations

Mass transfer in cylindrical tubes is encountered in a variety of operations such as wetted wall columns, reverse osmosis, and cross-flow ultrafiltration. As in the case of heat transfer, mass transfer correlations depend on whether the flow is laminar or turbulent.

#### 4.5.3.1 Laminar flow correlation

For laminar flow mass transfer in a circular tube with a constant wall concentration, an analogous expression to Eq. (4.5-25) is given by

$$\boxed{\text{Sh} = 1.86 [\text{Re Sc} (D/L)]^{1/3}} \quad (4.5-31)$$

Equation (4.5-31) is valid for

$$[\text{Re Sc} (D/L)]^{1/3} \geq 2$$

#### 4.5.3.2 Turbulent flow correlations

##### Gilliland-Sherwood correlation

Gilliland and Sherwood (1934) correlated the experimental results obtained from wetted wall columns in the form

$$\boxed{\text{Sh} = 0.023 \text{Re}^{0.83} \text{Sc}^{0.44}} \quad (4.5-32)$$

which is valid for

$$2,000 \leq \text{Re} \leq 35,000$$

$$0.6 \leq \text{Sc} \leq 2.5$$

##### Linton-Sherwood correlation

The correlation proposed by Linton and Sherwood (1950) is given by

$$\boxed{\text{Sh} = 0.023 \text{Re}^{0.83} \text{Sc}^{1/3}} \quad (4.5-33)$$

Equation (4.5-33) is valid for

$$2,000 \leq \text{Re} \leq 70,000$$

$$0.6 \leq \text{Sc} \leq 2,500$$

### 4.5.3.3 Calculation of the mass transfer rate

Once the average mass transfer coefficient is calculated from correlations given by Eqs. (4.5-31)-(4.5-33), then the rate of mass of species  $\mathcal{A}$  transferred is calculated as

$$\dot{m}_A = (\pi DL)\langle k_c \rangle (\Delta c_A)_{LM} \mathcal{M}_A \quad (4.5-34)$$

where  $\mathcal{M}_A$  is the molecular weight of species  $\mathcal{A}$ , and  $(\Delta c_A)_{LM}$ , *logarithmic mean concentration difference*, is defined by

$$(\Delta c_A)_{LM} = \frac{(c_{A_w} - c_{A_b})_{in} - (c_{A_w} - c_{A_b})_{out}}{\ln \left[ \frac{(c_{A_w} - c_{A_b})_{in}}{(c_{A_w} - c_{A_b})_{out}} \right]} \quad (4.5-35)$$

The derivation of Eq. (4.5-34) is given in Section 9.5 in Chapter 9.

**Example 4.17** *A smooth tube with an internal diameter of 2.5 cm is cast from solid naphthalene. Pure air enters the tube at an average velocity of 9 m/s. If the average air pressure is 1 atm and the temperature is 40°C, estimate the tube length required for the average concentration of naphthalene vapor in the air to reach 25% of the saturation value.*

**Solution**

**Physical properties**

*Diffusion coefficient of naphthalene (A) in air (B) at 40°C (313 K) :*

$$\begin{aligned} (\mathcal{D}_{AB})_{313} &= (\mathcal{D}_{AB})_{300} \left( \frac{313}{300} \right)^{3/2} \\ &= (0.62 \times 10^{-5}) \left( \frac{313}{300} \right)^{3/2} = 6.61 \times 10^{-6} \text{ m}^2/\text{s} \end{aligned}$$

*For air at 40°C (313 K) :  $\nu = 16.95 \times 10^{-6} \text{ m}^2/\text{s}$*

*The Schmidt number is*

$$\begin{aligned} \text{Sc} &= \frac{\nu}{\mathcal{D}_{AB}} \\ &= \frac{16.95 \times 10^{-6}}{6.61 \times 10^{-6}} = 2.56 \end{aligned}$$

**Assumptions**

1. *Steady-state conditions prevail.*
2. *The system is isothermal.*

**Analysis**

*System: Air in the naphthalene tube*

*If naphthalene is designated as species A, then the rate equation for the conservation of species A becomes*

$$\text{Rate of moles of A in} = \text{Rate of moles of A out} \quad (1)$$

*The terms in Eq. (1) are expressed by*

$$\text{Rate of moles of A in} = \pi DL \langle k_c \rangle (\Delta c_A)_{LM} \quad (2)$$

$$\text{Rate of moles of A out} = Q(c_{A_b})_{out} = (\pi D^2/4) \langle v \rangle (c_{A_b})_{out} \quad (3)$$

*Since the concentration at the wall is constant, the expression for  $(\Delta c_A)_{LM}$ , Eq. (4.5-35), becomes*

$$(\Delta c_A)_{LM} = \frac{(c_{A_b})_{out}}{\ln \left[ \frac{c_{A_w}}{c_{A_w} - (c_{A_b})_{out}} \right]} \quad (4)$$

*Substitution of Eqs. (2)-(4) into Eq. (1) gives*

$$\begin{aligned} \frac{L}{D} &= -\frac{1}{4} \frac{\langle v \rangle}{\langle k_c \rangle} \ln \left[ 1 - \frac{(c_{A_b})_{out}}{c_{A_w}} \right] \\ &= -\frac{1}{4} \frac{\langle v \rangle}{\langle k_c \rangle} \ln(1 - 0.25) = 0.072 \left( \frac{\langle v \rangle}{\langle k_c \rangle} \right) \end{aligned} \quad (5)$$

*Note that Eq. (5) can also be expressed in the form*

$$\frac{L}{D} = 0.072 \left( \frac{1}{St_M} \right) = 0.072 \left( \frac{Re Sc}{Sh} \right) \quad (6)$$

*The value of L depends on the correlations as follows:*

**Chilton-Colburn analogy**

*Substitution of Eq. (3.5-13) into Eq. (6) gives*

$$\frac{L}{D} = 0.072 \frac{2}{f} Sc^{2/3} \quad (7)$$

*The Reynolds number is*

$$\begin{aligned} Re &= \frac{D \langle v \rangle}{\nu} \\ &= \frac{(2.5 \times 10^{-2})(9)}{16.95 \times 10^{-6}} = 13,274 \quad \Rightarrow \quad \text{Turbulent flow} \end{aligned}$$

The friction factor can be calculated from the Chen correlation, Eq. (4.5-16). Taking  $\varepsilon/D \approx 0$ ,

$$\begin{aligned} A &= \left( \frac{\varepsilon/D}{2.5497} \right)^{1.1098} + \left( \frac{7.1490}{\text{Re}} \right)^{0.8981} \\ &= \left( \frac{7.1490}{13,274} \right)^{0.8981} = 1.16 \times 10^{-3} \end{aligned}$$

$$\begin{aligned} \frac{1}{\sqrt{f}} &= -4 \log \left( \frac{\varepsilon/D}{3.7065} - \frac{5.0452}{\text{Re}} \log A \right) \\ &= -4 \log \left[ -\frac{5.0452}{13,274} \log(1.16 \times 10^{-3}) \right] \Rightarrow f = 0.0072 \end{aligned}$$

Hence Eq. (7) becomes

$$\frac{L}{D} = \frac{(0.072)(2)(2.56)^{2/3}}{0.0072} = 37.4$$

The required length is then

$$L = (37.4)(2.5) = 93.5 \text{ cm}$$

#### Linton-Sherwood correlation

Substitution of Eq. (4.5-33) into Eq. (6) gives

$$\begin{aligned} \frac{L}{D} &= 3.13 \text{Re}^{0.17} \text{Sc}^{2/3} \\ &= 3.13 (13,274)^{0.17} (2.56)^{2/3} = 29.4 \end{aligned}$$

The tube length is

$$L = (29.4)(2.5) = 73.5 \text{ cm}$$

### 4.5.4 Flow in Non-Circular Ducts

The correlations given for friction factor, heat transfer coefficient, and mass transfer coefficient are only valid for ducts of circular cross-section. These correlations can be used for flow in non-circular ducts by introducing the concept of *hydraulic equivalent diameter*,  $D_h$ , defined by

$$D_h = 4 \left( \frac{\text{Flow area}}{\text{Wetted perimeter}} \right) \quad (4.5-36)$$

The Reynolds number based on the hydraulic equivalent diameter is

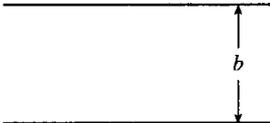
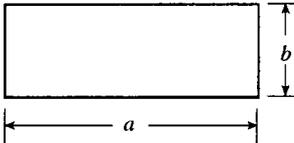
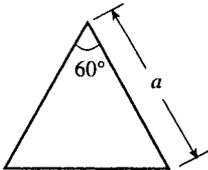
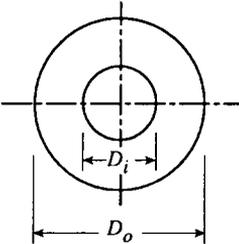
$$\text{Re}_h = \frac{D_h \langle v \rangle \rho}{\mu} \quad (4.5-37)$$

so that the friction factor, based on the hydraulic equivalent diameter, is related to  $Re_h$  in the form

$$f_h = \Omega \left( \frac{16}{Re_h} \right) \tag{4.5-38}$$

where  $\Omega$  depends on the geometry of the system. Since  $\Omega = 1$  only for a circular pipe, the use of the hydraulic equivalent diameter has not been recommended for laminar flow (Bird *et al.*, 1960; Fahien, 1983). The hydraulic equivalent diameter for various geometries is shown in Table 4.4.

**Table 4.4** The hydraulic equivalent diameter for various geometries.

Geometry	$D_h$
	$2b$
	$\frac{2ab}{a + b}$
	$\frac{a}{\sqrt{3}}$
	$D_o - D_i$

**Example 4.18** Water flows at an average velocity of 5 m/s through a duct of equilateral triangular cross-section with one side,  $a$ , being equal to 2 cm. Electric wires are wrapped around the outer surface of the duct to provide a constant wall heat flux of  $100 \text{ W/cm}^2$ . If the inlet water temperature is  $25^\circ\text{C}$  and the duct length is 1.5 m, calculate:

- The power required to pump water through the duct,
- The exit water temperature,
- The average heat transfer coefficient.

### Solution

#### Physical properties

$$\text{For water at } 25^\circ\text{C (298 K)} : \begin{cases} \rho = 997 \text{ kg/m}^3 \\ \mu = 892 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ \hat{C}_P = 4180 \text{ J/kg}\cdot\text{K} \end{cases}$$

#### Assumptions

- Steady-state conditions prevail.
- Changes in kinetic and potential energies are negligible.
- Variations in  $\rho$  and  $\hat{C}_P$  with temperature are negligible.

#### Analysis

System: Water in the duct

- The power required is calculated from Eq. (3.1-11)

$$\dot{W} = F_D \langle v \rangle = \left[ (3aL) \left( \frac{1}{2} \rho \langle v \rangle^2 \right) f \right] \langle v \rangle \quad (1)$$

The friction factor in Eq. (1) can be calculated from the modified form of the Chen correlation, Eq. (4.5-16)

$$\frac{1}{\sqrt{f}} = -4 \log \left( \frac{\varepsilon/D}{3.7065} - \frac{5.0452}{\text{Re}_h} \log A \right) \quad (2)$$

where

$$A = \left( \frac{\varepsilon/D}{2.5497} \right)^{1.1098} + \left( \frac{7.1490}{\text{Re}_h} \right)^{0.8981} \quad (3)$$

The hydraulic equivalent diameter and the Reynolds number are

$$\begin{aligned} D_h &= \frac{a}{\sqrt{3}} \\ &= \frac{2}{\sqrt{3}} = 1.155 \text{ cm} \end{aligned}$$

$$\begin{aligned} \text{Re}_h &= \frac{D_h \langle v \rangle \rho}{\mu} \\ &= \frac{(1.155 \times 10^{-2})(5)(997)}{892 \times 10^{-6}} = 64,548 \quad \Rightarrow \quad \text{Turbulent flow} \end{aligned}$$

Substitution of these values into Eqs. (3) and (2) and taking  $\varepsilon/D \approx 0$  gives

$$\begin{aligned} A &= \left( \frac{7.1490}{\text{Re}_h} \right)^{0.8981} \\ &= \left( \frac{7.1490}{64,548} \right)^{0.8981} = 2.8 \times 10^{-4} \end{aligned}$$

$$\begin{aligned} \frac{1}{\sqrt{f}} &= -4 \log \left( -\frac{5.0452}{\text{Re}_h} \log A \right) \\ &= -4 \log \left[ -\frac{5.0452}{64,548} \log(2.8 \times 10^{-4}) \right] \quad \Rightarrow \quad f = 0.0049 \end{aligned}$$

Hence, the power required is calculated from Eq. (1) as

$$\dot{W} = \left\{ (3)(2 \times 10^{-2})(1.5) \left[ \frac{1}{2} (997)(5)^2 \right] (0.0049) \right\} (5) = 27.5 \text{ W}$$

b) The inventory rate equation for mass is

$$\text{Rate of mass in} = \text{Rate of mass out} = \dot{m} = \rho \langle v \rangle \left( \frac{\sqrt{3} a^2}{4} \right) \quad (4)$$

$$\dot{m} = (997)(5) \left[ \frac{\sqrt{3} (2 \times 10^{-2})^2}{4} \right] = 0.863 \text{ kg/s}$$

The inventory rate equation for energy reduces to

$$\text{Rate of energy in} = \text{Rate of energy out} \quad (5)$$

The terms in Eq. (5) are expressed by

$$\text{Rate of energy in} = \dot{m} \hat{C}_P (T_{b_{in}} - T_{ref}) + \dot{Q}_w \quad (6)$$

$$\text{Rate of energy out} = \dot{m} \hat{C}_P (T_{b_{out}} - T_{ref}) \quad (7)$$

where  $\dot{Q}_w$  is the rate of heat transfer to water from the lateral surfaces of the duct. Substitution of Eqs. (6) and (7) into Eq. (5) gives

$$\begin{aligned} T_{b_{out}} &= T_{b_{in}} + \frac{\dot{Q}_w}{\dot{m} \hat{C}_P} \\ &= 25 + \frac{(3)(2)(150)(100)}{(0.863)(4180)} = 50^\circ \text{C} \end{aligned}$$

c) The mean bulk temperature is  $(25 + 50)/2 = 37.5^\circ\text{C}$ . At this temperature

$$k = 628 \times 10^{-3} \text{ W/m}\cdot\text{K} \quad \text{and} \quad \text{Pr} = 4.62$$

The use of the Dittus-Boelter correlation, Eq. (4.5-26), gives

$$\begin{aligned} \text{Nu} &= 0.023 \text{Re}_P^{4/5} \text{Pr}^{0.4} \\ &= 0.023 (64,548)^{4/5} (4.62)^{0.4} = 299 \end{aligned}$$

Therefore, the average heat transfer coefficient is

$$\begin{aligned} \langle h \rangle &= \text{Nu} \left( \frac{k}{D_h} \right) \\ &= (299) \left( \frac{628 \times 10^{-3}}{1.155 \times 10^{-2}} \right) = 16,257 \text{ W/m}^2\cdot\text{K} \end{aligned}$$

## 4.6 FLOW IN PACKED BEDS

The chemical and energy industries deal predominantly with multiphase and multicomponent systems in which considerable attention is devoted to increasing the interfacial contact between the phases to enhance property transfers and chemical reactions at these extended surface interfaces. As a result, packed beds are extensively used in the chemical process industries. Some examples are gas absorption, catalytic reactors, and deep bed filtration.

### 4.6.1 Friction Factor Correlations

The friction factor for packed beds,  $f_{pb}$ , is defined by

$$f_{pb} = \frac{\epsilon^3}{1 - \epsilon} \frac{D_P |\Delta P|}{\rho v_o^2 L} \quad (4.6-1)$$

where  $\epsilon$  is the *porosity* (or, *void volume fraction*),  $D_P$  is the particle diameter, and  $v_o$  is the *superficial velocity*. The superficial velocity is obtained by dividing the volumetric flow rate to the total cross-sectional area of the bed. Note that the actual flow area is a fraction of the total cross-sectional area.

**Example 4.19** *Water flows through an annulus at a volumetric flow rate of  $5 \text{ m}^3/\text{min}$ . The diameters of the inner and the outer pipes are 30 cm and 50 cm, respectively. Calculate the superficial velocity.*

**Solution**

If the inside and outside pipe diameters are designated by  $D_i$  and  $D_o$ , respectively, the superficial velocity,  $v_o$ , is defined by

$$v_o = \frac{Q}{\pi D_o^2/4} = \frac{5}{\pi(0.5)^2/4} = 25.5 \text{ m/min}$$

The actual average velocity,  $\langle v \rangle_{act}$ , in the annulus is

$$\langle v \rangle_{act} = \frac{Q}{\pi(D_o^2 - D_i^2)/4} = \frac{5}{\pi[(0.5)^2 - (0.3)^2]/4} = 40 \text{ m/min}$$

**Comment:** The superficial velocity is always less than the actual average velocity by a factor of porosity, which is equal to  $[1 - (D_i/D_o)^2]$  in this example.

For packed beds, the Reynolds number is defined by

$$\text{Re}_{pb} = \frac{D_P v_o \rho}{\mu} \frac{1}{1 - \epsilon} \quad (4.6-2)$$

For laminar flow, the relationship between the friction factor and the Reynolds number is given by

$$\boxed{f_{pb} = \frac{150}{\text{Re}_{pb}}} \quad \text{Re}_{pb} < 10 \quad (4.6-3)$$

which is known as the *Kozeny-Carman equation*.

In the case of turbulent flow, i.e.,  $\text{Re}_{pb} > 1000$ , the relationship between  $\text{Re}_{pb}$  and  $f_{pb}$  is given by the *Burke-Plummer equation* in the form

$$\boxed{f_{pb} = 1.75} \quad \text{Re}_{pb} > 1000 \quad (4.6-4)$$

The so-called *Ergun equation* (1952) is simply the summation of the Kozeny-Carman and the Burke-Plummer equations

$$\boxed{f_{pb} = \frac{150}{\text{Re}_{pb}} + 1.75} \quad (4.6-5)$$

**Example 4.20** A column of  $0.8 \text{ m}^2$  cross-section and 30 m height is packed with spherical particles of diameter 6 mm. A fluid with  $\rho = 1.2 \text{ kg/m}^3$  and  $\mu = 1.8 \times 10^{-5} \text{ kg/m} \cdot \text{s}$  flows through the bed at a mass flow rate of  $0.65 \text{ kg/s}$ . If the pressure drop is measured as  $3200 \text{ Pa}$ , calculate the porosity of the bed:

- Analytically,
- By using Newton-Raphson method.

**Solution****Assumption**

1. The system is isothermal.

**Analysis**

The superficial velocity through the packed bed is

$$v_o = \frac{0.65}{(1.2)(0.8)} = 0.677 \text{ m/s}$$

Substitution of the values into Eqs. (4.6-1) and (4.6-2) gives the friction factor and the Reynolds number as a function of porosity in the form

$$\begin{aligned} f_{pb} &= \frac{\epsilon^3}{1-\epsilon} \frac{D_P |\Delta P|}{\rho v_o^2 L} \\ &= \frac{\epsilon^3}{1-\epsilon} \left[ \frac{(6 \times 10^{-3})(3200)}{(1.2)(0.677)^2(30)} \right] = 1.164 \left( \frac{\epsilon^3}{1-\epsilon} \right) \end{aligned} \quad (1)$$

$$\begin{aligned} \text{Re}_{pb} &= \frac{D_P v_o \rho}{\mu} \frac{1}{1-\epsilon} \\ &= \left[ \frac{(6 \times 10^{-3})(0.677)(1.2)}{1.8 \times 10^{-5}} \right] \frac{1}{1-\epsilon} = 270.8 \left( \frac{1}{1-\epsilon} \right) \end{aligned} \quad (2)$$

Substitution of Eqs. (1) and (2) into Eq. (4.6-5) gives

$$\epsilon^3 - 0.476 \epsilon^2 + 2.455 \epsilon - 1.979 = 0 \quad (3)$$

a) Equation (3) can be solved analytically by using the procedure described in Section A.7.1.2 in Appendix A. In order to calculate the discriminant, the terms  $M$  and  $N$  must be calculated from Eqs. (A.7-5) and (A.7-6), respectively:

$$\begin{aligned} M &= \frac{(3)(2.455) - (0.476)^2}{9} = 0.793 \\ N &= \frac{-(9)(0.476)(2.455) + (27)(1.979) + (2)(0.476)^3}{54} = 0.799 \end{aligned}$$

Therefore, the discriminant is

$$\begin{aligned} \Delta &= M^3 + N^2 \\ &= (0.793)^3 + (0.799)^2 = 1.137 \end{aligned}$$

Since  $\Delta > 0$ , Eq. (3) has only one real root as given by Eq. (A.7-7). The terms  $S$  and  $T$  in this equation are calculated as

$$\begin{aligned} S &= \left( N + \sqrt{\Delta} \right)^{1/3} \\ &= \left( 0.799 + \sqrt{1.137} \right)^{1/3} = 1.231 \end{aligned}$$

$$\begin{aligned}
 T &= (N - \sqrt{\Delta})^{1/3} \\
 &= (0.799 - \sqrt{1.137})^{1/3} = -0.644
 \end{aligned}$$

Hence the average porosity of the bed is

$$\epsilon = 1.231 - 0.644 + \frac{0.476}{3} = 0.746$$

b) Equation (3) is rearranged as

$$F(\epsilon) = \epsilon^3 - 0.476\epsilon^2 + 2.455\epsilon - 1.979 = 0 \quad (4)$$

From Eq. (A.7-18) the iteration scheme is

$$\epsilon_{k+1} = \epsilon_k - \frac{F(\epsilon_k)}{\left. \frac{dF}{d\epsilon} \right|_{\epsilon_k}} \quad (5)$$

The derivative of the function  $F$  is given by

$$\frac{dF}{d\epsilon} = 3\epsilon^2 - 0.952\epsilon + 2.455$$

Assuming a starting value of 0.7, the calculation scheme is

$$\begin{aligned}
 \epsilon_2 &= 0.7 + \frac{0.151}{3.259} = 0.746 \\
 \epsilon_3 &= 0.746 - \frac{0.003}{3.414} = 0.745
 \end{aligned}$$

Since  $\epsilon_2 \approx \epsilon_3$ , the value of porosity is 0.746.

## 4.6.2 Heat Transfer Correlation

Whitaker (1972) proposed the following correlation for heat transfer in packed beds:

$$\boxed{\text{Nu}_{pb} = (0.4 \text{Re}_{pb}^{1/2} + 0.2 \text{Re}_{pb}^{2/3}) \text{Pr}^{0.4}} \quad (4.6-6)$$

The Nusselt number in Eq. (4.6-6) is defined by

$$\text{Nu}_{pb} = \frac{\langle h \rangle D_P}{k} \frac{\epsilon}{1 - \epsilon} \quad (4.6-7)$$

Equation (4.6-6) is valid when

$$3.7 \leq \text{Re}_{pb} \leq 8000$$

$$0.34 \leq \epsilon \leq 0.74$$

$$\text{Pr} \approx 0.7$$

All properties in Eq. (4.6-6) are evaluated at the average fluid temperature in the bed.

#### 4.6.2.1 Calculation of the heat transfer rate

Once the average heat transfer coefficient is determined, the rate of heat transfer is calculated from

$$\dot{Q} = a_v V \langle h \rangle \Delta T_{LM} \quad (4.6-8)$$

where  $V$  is the total volume of the packed bed and  $a_v$  is the packing surface area per unit volume defined by

$$a_v = \frac{6(1-\epsilon)}{D_P} \quad (4.6-9)$$

### 4.6.3 Mass Transfer Correlation

Dwivedi and Upadhyay (1977) proposed a single correlation for both gases and liquids in packed and fluidized beds in terms of the  $j$ -factor as

$$\epsilon j_{M_{pb}} = \frac{0.765}{(\text{Re}_{pb}^*)^{0.82}} + \frac{0.365}{(\text{Re}_{pb}^*)^{0.386}} \quad (4.6-10)$$

which is valid for  $0.01 \leq \text{Re}_{pb}^* \leq 15,000$ . The terms  $j_{M_{pb}}$  and  $\text{Re}_{pb}^*$  in Eq. (4.6-10) are defined by

$$j_{M_{pb}} = \left( \frac{\langle k_c \rangle}{v_o} \right) \text{Sc}^{2/3} \quad (4.6-11)$$

and

$$\text{Re}_{pb}^* = \frac{D_P v_o \rho}{\mu} \quad (4.6-12)$$

#### 4.6.3.1 Calculation of the mass transfer rate

Once the average mass transfer coefficient is determined, the rate of mass transfer of species  $A$ ,  $\dot{m}_A$ , is given by

$$\dot{m}_A = a_v V \langle k_c \rangle (\Delta c_A)_{LM} \mathcal{M}_A \quad (4.6-13)$$

**Example 4.21** *Instead of using a naphthalene pipe as in Example 4.17, it is suggested to form a packed bed of porosity 0.45 in a pipe, 2.5 cm in internal diameter, by using naphthalene spheres of 5 mm in diameter. Pure air at 40°C flows at a superficial velocity of 9 m/s through the bed. Determine the length of the packed bed required for the average concentration of naphthalene vapor in the air to reach 25% of the saturation value.*

**Solution****Physical properties**

*Diffusion coefficient of naphthalene (A) in air (B) at 40°C (313 K) :*

$$\begin{aligned} (\mathcal{D}_{AB})_{313} &= (\mathcal{D}_{AB})_{300} \left( \frac{313}{300} \right)^{3/2} \\ &= (0.62 \times 10^{-5}) \left( \frac{313}{300} \right)^{3/2} = 6.61 \times 10^{-6} \text{ m}^2/\text{s} \end{aligned}$$

*For air at 40°C (313 K) :  $\nu = 16.95 \times 10^{-6} \text{ m}^2/\text{s}$*

*The Schmidt number is*

$$\begin{aligned} \text{Sc} &= \frac{\nu}{\mathcal{D}_{AB}} \\ &= \frac{16.95 \times 10^{-6}}{6.61 \times 10^{-6}} = 2.56 \end{aligned}$$

**Assumptions**

1. *Steady-state conditions prevail.*
2. *The system is isothermal.*
3. *The diameter of the naphthalene spheres does not change appreciably.*

**Analysis**

*System: Air in the packed bed*

*Under steady conditions, the conservation statement for naphthalene, species A, becomes*

$$\text{Rate of moles of A in} = \text{Rate of moles of A out} \quad (1)$$

*The terms in Eq. (1) are expressed by*

$$\text{Rate of moles of A in} = a_v V \langle k_c \rangle (\Delta c_A)_{LM} \quad (2)$$

$$\text{Rate of moles of A out} = \mathcal{Q} (c_{A_b})_{out} = (\pi D^2/4) v_o (c_{A_b})_{out} \quad (3)$$

*Since the concentration at the surface of the naphthalene spheres is constant, the expression for  $(\Delta c_A)_{LM}$ , Eq. (4.5-35), becomes*

$$(\Delta c_A)_{LM} = \frac{(c_{A_b})_{out}}{\ln \left[ \frac{c_{A_w}}{c_{A_w} - (c_{A_b})_{out}} \right]} \quad (4)$$

Substitution of Eqs. (2)-(4) into Eq. (1) and noting that  $V = (\pi D^2/4)L$  gives

$$L = -\frac{v_o}{\langle k_c \rangle a_v} \ln \left[ 1 - \frac{(c_{A_b})_{out}}{c_{A_w}} \right] \quad (5)$$

Note that for a circular pipe, i.e.,  $a_v = 4/D$ , the above equation reduces to Eq. (5) in Example 4.17.

The interfacial area per unit volume,  $a_v$ , is calculated from Eq. (4.6-9) as

$$\begin{aligned} a_v &= \frac{6(1-\epsilon)}{D_P} \\ &= \frac{6(1-0.45)}{0.005} = 660 \text{ m}^{-1} \end{aligned}$$

To determine the average mass transfer coefficient from Eq. (4.6-10), first it is necessary to calculate the Reynolds number

$$\begin{aligned} \text{Re}_{pb}^* &= \frac{D_P v_o}{\nu} \\ &= \frac{(0.005)(9)}{16.95 \times 10^{-6}} = 2655 \end{aligned}$$

Substitution of this value into Eq. (4.6-10) gives

$$\begin{aligned} \epsilon j_{M_{pb}} &= \frac{0.765}{(\text{Re}_{pb}^*)^{0.82}} + \frac{0.365}{(\text{Re}_{pb}^*)^{0.386}} \\ &= \frac{0.765}{(2655)^{0.82}} + \frac{0.365}{(2655)^{0.386}} = 0.0186 \end{aligned}$$

in which  $\epsilon j_{M_{pb}}$  is given by Eq. (4.6-11). Therefore, the average mass transfer coefficient is

$$\begin{aligned} \langle k_c \rangle &= 0.0186 \frac{v_o}{\epsilon \text{Sc}^{2/3}} \\ &= \frac{(0.0186)(9)}{(0.45)(2.56)^{2/3}} = 0.2 \text{ m/s} \end{aligned}$$

The length of the bed is calculated from Eq. (5) as

$$L = -\frac{9}{(0.2)(660)} \ln(1-0.25) = 0.02 \text{ m}$$

**Comment:** The use of a packed bed increases the mass transfer area between air and solid naphthalene. This in turn causes a drastic decrease in the length of the equipment.

## NOTATION

$A$	area, $\text{m}^2$
$a_v$	packing surface area per unit volume, $1/\text{m}$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ}/\text{kg}\cdot\text{K}$
$c_i$	concentration of species $i$ , $\text{kmol}/\text{m}^3$
$D$	diameter, $\text{m}$
$D_h$	hydraulic equivalent diameter, $\text{m}$
$D_P$	particle diameter, $\text{m}$
$D_{AB}$	diffusion coefficient for system $A$ - $B$ , $\text{m}^2/\text{s}$
$F_D$	drag force, $\text{N}$
$f$	friction factor
$G$	mass velocity, $\text{kg}/\text{m}^2\cdot\text{s}$
$g$	acceleration of gravity, $\text{m}/\text{s}^2$
$j_H$	Chilton-Colburn $j$ – factor for heat transfer
$j_M$	Chilton-Colburn $j$ – factor for mass transfer
$k$	thermal conductivity, $\text{W}/\text{m}\cdot\text{K}$
$k_c$	mass transfer coefficient, $\text{m}/\text{s}$
$L$	length, $\text{m}$
$M$	mass, $\text{kg}$
$\dot{m}$	mass flow rate, $\text{kg}/\text{s}$
$\mathcal{M}$	molecular weight, $\text{kg}/\text{kmol}$
$\dot{n}$	molar flow rate, $\text{kmol}/\text{s}$
$P$	pressure, $\text{Pa}$
$\dot{Q}$	heat transfer rate, $\text{W}$
$Q$	volumetric flow rate, $\text{m}^3/\text{s}$
$q$	heat flux, $\text{W}/\text{m}^2$
$\mathcal{R}$	gas constant, $\text{J}/\text{mol}\cdot\text{K}$
$T$	temperature, $^\circ\text{C}$ or $\text{K}$
$t$	time, $\text{s}$
$V$	volume, $\text{m}^3$
$v$	velocity, $\text{m}/\text{s}$
$v_o$	superficial velocity, $\text{m}/\text{s}$
$v_t$	terminal velocity, $\text{m}/\text{s}$
$W$	work, $\text{J}$ ; width, $\text{m}$
$\dot{W}$	rate of work, $\text{W}$
$x$	rectangular coordinate, $\text{m}$
$\Delta$	difference
$\epsilon$	porosity
$\varepsilon$	surface roughness of the pipe, $\text{m}$
$\mu$	viscosity, $\text{kg}/\text{m}\cdot\text{s}$
$\nu$	kinematic viscosity, $\text{m}^2/\text{s}$
$\rho$	density, $\text{kg}/\text{m}^3$

**Overlines**

$\sim$	per mole
$\hat{\phantom{a}}$	per unit mass

**Bracket**

$\langle a \rangle$	average value of $a$
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**Superscript**

$sat$	saturation
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**Subscripts**

$A, B$	species in binary systems
$b$	bulk
$c$	transition from laminar to turbulent
$ch$	characteristic
$f$	film
$i$	species in multicomponent systems
$in$	inlet
$LM$	log-mean
$out$	out
$pb$	packed bed
$w$	wall or surface
$\infty$	free-stream

**Dimensionless Numbers**

$Ar$	Archimedes number
$Pr$	Prandtl number
$Nu$	Nusselt number
$Re$	Reynolds number
$Re_D$	Reynolds number based on the diameter
$Re_h$	Reynolds number based on the hydraulic equivalent diameter
$Re_L$	Reynolds number based on the length
$Re_x$	Reynolds number based on the distance $x$
$Sc$	Schmidt number
$Sh$	Sherwood number
$St_H$	Stanton number for heat transfer
$St_M$	Stanton number for mass transfer

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## PROBLEMS

4.1 Air at atmospheric pressure and 200 °C flows at 8 m/s over a flat plate 150 cm long in the direction of flow and 70 cm wide.

a) Estimate the rate of cooling of the plate so as to keep the surface temperature at 30 °C.

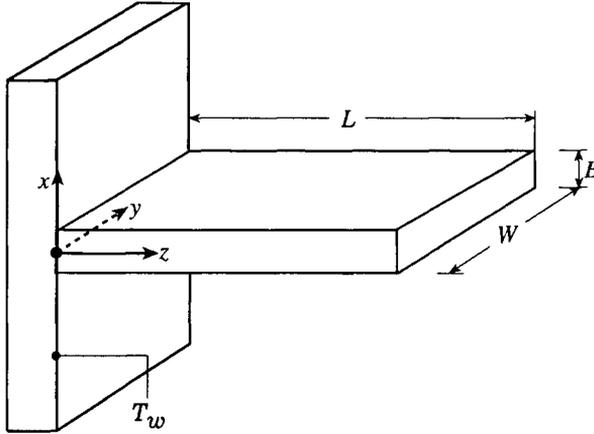
b) Calculate the drag force exerted on the plate.

(Answer: a) 1589 W b) 0.058 N)

4.2 Water at 15 °C flows at 0.15 m/s over a flat plate 1 m long in the direction of flow and 0.3 m wide. If energy is transferred from the top and bottom surfaces of the plate to the flowing stream at a steady rate of 3500 W, determine the temperature of the plate surface.

(Answer: 35 °C)

4.3 Fins are used to increase the area available for heat transfer between metal walls and poorly conducting fluids such as gases. A simple rectangular fin is shown below.



If one assumes,

- $T = T(z)$  only,
- No heat is lost from the end or from the edges,
- The average heat transfer coefficient,  $\langle h \rangle$ , is constant and uniform over the entire surface of the fin,
- The thermal conductivity of the fin,  $k$ , is constant,
- The temperature of the medium surrounding the fin,  $T_\infty$ , is uniform,
- The wall temperature,  $T_w$ , is constant,

the resulting steady-state temperature distribution is given by

$$\frac{T - T_\infty}{T_w - T_\infty} = \frac{\cosh \left[ \Lambda \left( 1 - \frac{z}{L} \right) \right]}{\cosh \Lambda}$$

where

$$\Lambda = \sqrt{\frac{2\langle h \rangle L^2}{kB}}$$

If the rate of heat loss from the fin is 478 W, determine the average heat transfer coefficient for the following conditions:  $T_\infty = 175^\circ\text{C}$ ;  $T_w = 260^\circ\text{C}$ ;  $k = 105 \text{ W/m}\cdot\text{K}$ ;  $L = 4 \text{ cm}$ ;  $W = 30 \text{ cm}$ ;  $B = 5 \text{ mm}$ .

(Answer:  $400 \text{ W/m}^2\cdot\text{K}$ )

4.4 Consider the rectangular fin given in Problem 4.3. One of the problems of practical interest is the determination of the optimum values of  $B$  and  $L$  to maximize the heat transfer rate from the fin for a fixed volume,  $V$ , and  $W$ . Show that the optimum dimensions are given as

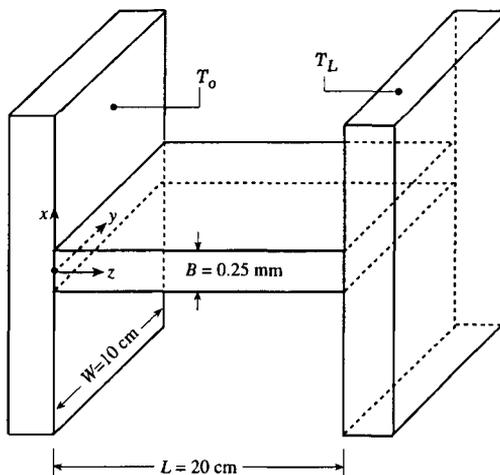
$$B_{opt} \simeq \left( \frac{\langle h \rangle V^2}{k W^2} \right)^{1/3} \quad \text{and} \quad L_{opt} \simeq \left( \frac{k V}{\langle h \rangle W} \right)^{1/3}$$

4.5 Consider the rectangular fin given in Problem 4.3. If a laminar flow region exists over the plate, show that the optimum value of  $W$  for the maximum heat transfer rate from the fin for a fixed volume,  $V$ , and thickness,  $B$ , is given by

$$W_{opt} = 1.2 V^{4/5} B^{-6/5} \left[ \left( \frac{k_f}{k} \right) \text{Pr}^{1/3} \sqrt{\frac{v_\infty}{\nu}} \right]^{2/5}$$

where  $k_f$  is the thermal conductivity of the fluid.

4.6 A thin aluminum fin ( $k = 205 \text{ W/m.K}$ ) of length  $L = 20 \text{ cm}$  has two ends attached to two parallel walls which have temperatures  $T_o = 100^\circ\text{C}$  and  $T_L = 90^\circ\text{C}$  as shown in the figure below. The fin loses heat by convection to the ambient air at  $T_\infty = 30^\circ\text{C}$  with an average heat transfer coefficient of  $\langle h \rangle = 120 \text{ W/m}^2.\text{K}$  through the top and bottom surfaces (heat loss from the edges may be considered negligible).



One of your friends assumes that there is no internal generation of energy within the fin and determines the steady-state temperature distribution within the fin as

$$\frac{T - T_\infty}{T_o - T_\infty} = e^{Nz} - 2\Omega \sinh Nz$$

in which  $N$  and  $\Omega$  are defined as

$$N = \sqrt{\frac{2\langle h \rangle}{kB}}$$

$$\Omega = \frac{e^{NL} - \left( \frac{T_L - T_\infty}{T_o - T_\infty} \right)}{2 \sinh NL}$$

- a) Show that there is indeed no internal generation of energy within the fin.  
 b) Determine the location and the value of the minimum temperature within the fin.

(Answer:  $z = 0.1$  cm,  $T = 30.14^\circ\text{C}$ )

4.7 Rework Example 4.8 by using the Ranz-Marshall correlation, Eq. (4.3-33), the Frossling correlation, Eq. (4.3-34), and the modified Frossling correlation, Eq. (4.3-35). Why are the resulting Sherwood numbers differ significantly from the value of 541?

4.8 In an experiment carried out at  $20^\circ\text{C}$ , a glass sphere of density  $2620 \text{ kg/m}^3$  falls through carbon tetrachloride ( $\rho = 1590 \text{ kg/m}^3$  and  $\mu = 9.58 \times 10^{-4} \text{ kg/m}\cdot\text{s}$ ) with a terminal velocity of  $65 \text{ cm/s}$ . Determine the diameter of the sphere.

(Answer: 21 mm)

4.9 A  $\text{CO}_2$  bubble is rising in a glass of beer 20 cm tall. Estimate the time required for a bubble of 5 mm in diameter to reach the top if the properties of  $\text{CO}_2$  and beer can be taken as equal to that of air and water, respectively.

(Answer: 0.54 s)

4.10 Show that the use of the Dittus-Boelter correlation, Eq. (4.5-26), together with the Chilton-Colburn analogy, Eq. (3.5-12), yields

$$f \simeq 0.046 \text{Re}^{-0.2}$$

which is a good power-law approximation for the friction factor in smooth circular pipes. Calculate  $f$  for  $Re = 10^5$ ,  $10^6$  and  $10^7$  using this approximate equation and compare the values with the ones obtained by using the Chen correlation, Eq. (4.5-16).

4.11 For laminar flow of an incompressible Newtonian fluid in a circular pipe, Eq. (4.5-12) indicates that the pressure drop is proportional to the volumetric flow rate. For fully turbulent flow show that the pressure drop in a pipe is proportional to the square of the volumetric flow rate.

4.12 The purpose of the blood pressure in a human body is to push blood to the tissues of the organism so that they can perform their function. Each time

the heart beats, it pumps out blood into the arteries. The blood pressure reaches its maximum value, i.e., systolic pressure, when the heart contracts to pump the blood. In between beats, the heart is at rest and the blood pressure falls down to a minimum value, diastolic pressure. An average healthy person has systolic and diastolic pressures of 120 and 80 mmHg, respectively. Human body has about 5.6 L of blood. If it takes 20 s for blood to circulate throughout the body, estimate the power output of the heart.

(Answer: 3.73 W)

**4.13** Water is in isothermal turbulent flow at 20°C through a horizontal pipe of circular cross-section with 10 cm inside diameter. The following experimental values of velocity are measured as a function of radial distance  $r$ :

$r$ (cm)	$v_z$ (m/s)
0.5	0.394
1.5	0.380
2.5	0.362
3.5	0.337
4.5	0.288

The velocity distribution is proposed in the form

$$v_z = v_{\max} \left(1 - \frac{r}{R}\right)^n$$

where  $v_{\max}$  is the maximum velocity and  $R$  is the radius of the pipe. Calculate the pressure drop per unit length of the pipe.

(Answer: 12.3 Pa/m)

**4.14** In Example 4.15, the length to diameter ratio is expressed as

$$\frac{L}{D} = \frac{1}{4} \frac{1}{\text{St}_H} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right)$$

Use the Chilton-Colburn analogy, i.e.,

$$\frac{f}{2} = \text{St}_H \text{Pr}^{2/3}$$

and evaluate the value of  $L/D$ . Is it a realistic value? Why?

**4.15** Water at 10°C enters a circular pipe of internal diameter 2.5 cm with a velocity of 1.2 m/s. Steam condenses on the outside of the pipe so as to keep the

surface temperature of the pipe at 82°C. If the length of the pipe is 5 m, determine the outlet temperature of water.

(Answer: 51°C)

**4.16** Dry air at 1 atm pressure and 50°C enters a circular pipe of 12 cm internal diameter with an average velocity of 10 cm/s. The inner surface of the pipe is coated with a thin absorbent material which is soaked with water at 20°C. If the length of the pipe is 6 m, calculate the amount of water vapor carried out of the pipe per hour.

(Answer: 0.067 kg/h)

**4.17** A column with an internal diameter of 50 cm and a height of 2 m is packed with spherical particles of 3 mm in diameter so as to form a packed bed with  $\epsilon = 0.45$ . Estimate the power required to pump a Newtonian liquid ( $\mu = 70 \times 10^{-3}$  kg/m.s;  $\rho = 1200$  kg/m<sup>3</sup>) through the packed bed at a mass flow rate of 1.2 kg/s.

(Answer: 39.6 W)

**4.18** The drag force,  $F_D$ , is defined as the interfacial transfer of momentum from the fluid to the solid. In Chapter 3, power,  $\dot{W}$ , is given by Eq. (3.1-11) as

$$\dot{W} = F_D v_{ch} \quad (1)$$

For flow in conduits, power is also expressed by Eq. (4.5-2) in the form

$$\dot{W} = Q |\Delta P| \quad (2)$$

a) For flow in a circular pipe, the characteristic velocity is taken as the average velocity. For this case, use Eqs. (1) and (2) to show that

$$F_D = A |\Delta P| \quad (3)$$

where  $A$  is the cross-sectional area of the pipe.

b) For flow through packed beds, the characteristic velocity is taken as the actual average velocity or, interstitial velocity, i.e.,

$$v_{ch} = \frac{v_o}{\epsilon} \quad (4)$$

in which  $v_o$  is the superficial velocity and  $\epsilon$  is the porosity of the bed. Show that

$$F_D = \epsilon A |\Delta P| \quad (5)$$

where  $A$  is the cross-sectional area of the packed bed.

c) In fluidization, the drag force on each particle should support its effective weight, i.e., weight minus buoyancy. Show that the drag force is given by

$$F_D = AL(1 - \epsilon)(\rho_P - \rho)g\epsilon \quad (6)$$

where  $L$  is the length of the bed,  $\rho$  and  $\rho_P$  are the densities of the fluid and solid particle, respectively. Note that in the calculation of the buoyancy force, the volume occupied by solid particles should be multiplied by the density of suspension, i.e.,  $\epsilon\rho + (1 - \epsilon)\rho_P$ , instead of  $\rho$ .

Combine Eqs. (5) and (6) to get

$$\frac{|\Delta P|}{L} = g(1 - \epsilon)(\rho_P - \rho) \quad (7)$$

which is a well-known equation in fluidization.

**4.19** A  $15 \times 90$  m lawn is covered by a layer of ice of 0.15 mm thick at  $-4^\circ\text{C}$ . The wind at a temperature of  $0^\circ\text{C}$  with 15% relative humidity blows in the direction of the short side of the lawn. If the wind velocity is 10 m/s, estimate the time required for the ice layer to disappear by sublimation under steady conditions. The vapor pressure and the density of ice at  $-4^\circ\text{C}$  are 3.28 mmHg and  $917 \text{ kg/m}^3$ , respectively.

(Answer: 33 min)

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# Chapter 5

## Rate of Generation in Momentum, Energy and Mass Transfer

In Chapter 1, the generation rate per unit volume is designated by  $\mathfrak{R}$ . Integration of this quantity over the volume of the system gives the generation rate in the conservation statement. In this chapter, explicit expressions for  $\mathfrak{R}$  will be developed for the cases of momentum, energy, and mass transport.

### 5.1 RATE OF GENERATION IN MOMENTUM TRANSPORT

In general, forces acting on a particle can be classified as surface forces and body forces. *Surface forces*, such as, normal stresses (pressure) and tangential stresses, act by direct contact on a surface. *Body forces*, however, act at a distance on a volume. Gravitational, electrical and electromagnetic forces are examples of body forces.

For solid bodies Newton's second law of motion states that

$$\left( \begin{array}{c} \text{Summation of forces} \\ \text{acting on a system} \end{array} \right) = \left( \begin{array}{c} \text{Time rate of change of} \\ \text{momentum of a system} \end{array} \right) \quad (5.1-1)$$

in which forces acting on a system include both surface and body forces. Equation (5.1-1) can be extended to fluid particles by considering the rate of flow of

momentum into and out of the volume element, i.e.,

$$\begin{aligned} \left( \begin{array}{c} \text{Rate of} \\ \text{momentum in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{momentum out} \end{array} \right) + \left( \begin{array}{c} \text{Summation of forces} \\ \text{acting on a system} \end{array} \right) \\ = \left( \begin{array}{c} \text{Time rate of change of} \\ \text{momentum of a system} \end{array} \right) \end{aligned} \quad (5.1-2)$$

On the other hand, for a given system, the inventory rate equation for momentum can be expressed as

$$\begin{aligned} \left( \begin{array}{c} \text{Rate of} \\ \text{momentum in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{momentum out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of momentum} \\ \text{generation} \end{array} \right) \\ = \left( \begin{array}{c} \text{Rate of momentum} \\ \text{accumulation} \end{array} \right) \end{aligned} \quad (5.1-3)$$

Comparison of Eqs. (5.1-2) and (5.1-3) indicates that

$$\left( \begin{array}{c} \text{Rate of momentum} \\ \text{generation} \end{array} \right) = \left( \begin{array}{c} \text{Summation of forces} \\ \text{acting on a system} \end{array} \right) \quad (5.1-4)$$

in which the forces acting on a system are the pressure force (surface force) and the gravitational force (body force).

### 5.1.1 Momentum Generation As a Result of Gravitational Force

Consider a basketball player holding a ball in his hands. When he drops the ball, it starts to accelerate as a result of gravitational force. According to Eq.(5.1-4), the rate of momentum generation is given by

$$\text{Rate of momentum generation} = Mg \quad (5.1-5)$$

where  $M$  is the mass of the ball and  $g$  is the gravitational acceleration. Therefore, the rate of momentum generation per unit volume,  $\mathfrak{R}$ , is given by

$$\boxed{\mathfrak{R} = \rho g} \quad (5.1-6)$$

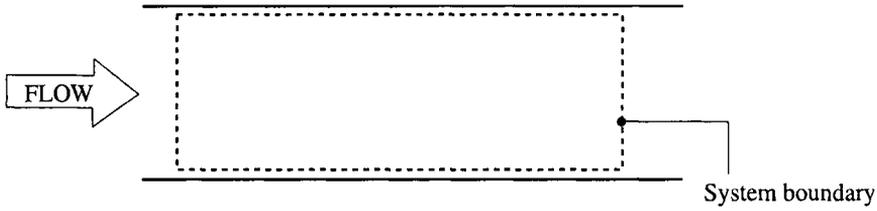
### 5.1.2 Momentum Generation As a Result of Pressure Force

Consider the steady flow of an incompressible fluid in a pipe as shown in Figure 5.1. The rate of mechanical energy required to pump the fluid is given by Eq. (4.5-3) as

$$\dot{W} = F_D \langle v \rangle = Q |\Delta P| \quad (5.1-7)$$

Since the volumetric flow rate,  $Q$ , is the product of average velocity,  $\langle v \rangle$ , with the cross-sectional area,  $A$ , Eq. (5.1-7) reduces to

$$A |\Delta P| - F_D = 0 \quad (5.1-8)$$



**Figure 5.1** Flow through a pipe.

For the system whose boundaries are indicated by a dotted line in Figure 5.1, the conservation of mass states that

$$\dot{m}_{in} = \dot{m}_{out} \quad (5.1-9)$$

or,

$$(\rho\langle v \rangle A)_{in} = (\rho\langle v \rangle A)_{out} \quad \Rightarrow \quad \langle v \rangle_{in} = \langle v \rangle_{out} \quad (5.1-10)$$

On the other hand, the conservation statement for momentum, Eq. (5.1-3), takes the form

$$\left( \begin{array}{c} \text{Rate of} \\ \text{momentum in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{momentum out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of momentum} \\ \text{generation} \end{array} \right) = 0 \quad (5.1-11)$$

and can be expressed as

$$(\dot{m}\langle v \rangle)_{in} - [(\dot{m}\langle v \rangle)_{out} + F_D] + \mathfrak{R}(AL) = 0 \quad (5.1-12)$$

where  $\mathfrak{R}$  is the rate of momentum generation per unit volume. Note that the rate of momentum transfer from the fluid to the pipe wall manifests itself as a drag force. The use of Eqs. (5.1-9) and (5.1-10) simplifies Eq. (5.1-12) to

$$\mathfrak{R}(AL) - F_D = 0 \quad (5.1-13)$$

Comparison of Eqs. (5.1-8) and (5.1-13) indicates that the rate of momentum generation per unit volume is equal to the pressure gradient, i.e.,

$$\boxed{\mathfrak{R} = \frac{|\Delta P|}{L}} \quad (5.1-14)$$

### 5.1.3 Modified Pressure

Equations (5.1-6) and (5.1-14) indicate that the presence of pressure and/or gravity forces can be interpreted as a source of momentum. In fluid mechanics, it is

customary to combine these two forces in a single term and express the rate of momentum generation per unit volume as

$$\mathfrak{R} = \frac{|\Delta \mathcal{P}|}{L} \quad (5.1-15)$$

where  $\mathcal{P}$  is the *modified pressure*<sup>1</sup> defined by

$$\mathcal{P} = P + \rho gh \quad (5.1-16)$$

in which  $h$  is the distance measured in the direction opposite to gravity from any chosen reference plane.

### 5.1.3.1 Physical interpretation of the modified pressure

Consider a stagnant liquid in a storage tank open to the atmosphere. Let  $z$  be the distance measured from the surface of the liquid in the direction of gravity. The hydrostatic pressure distribution within the fluid is given by

$$P = P_{atm} + \rho gz \quad (5.1-17)$$

For this case the modified pressure is defined as

$$\mathcal{P} = P - \rho gz \quad (5.1-18)$$

Substitution of Eq. (5.1-18) into Eq. (5.1-17) gives

$$\mathcal{P} = P_{atm} = \text{constant} \quad (5.1-19)$$

The simplicity of defining the modified pressure comes from the fact that it is always constant under static conditions whereas the hydrostatic pressure varies as a function of position. Suppose that you measure a pressure difference over a length  $L$  of a pipe. It is difficult to estimate whether this pressure difference comes from a flow situation or hydrostatic distribution. However, any variation in  $\mathcal{P}$  implies a flow. Another distinct advantage of defining modified pressure is that the difference in  $\mathcal{P}$  is independent of the orientation of the pipe as shown in Table 5.1.

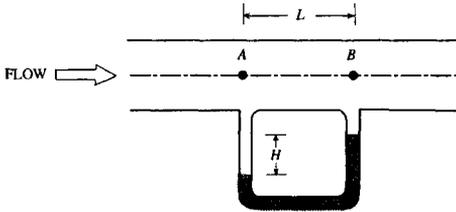
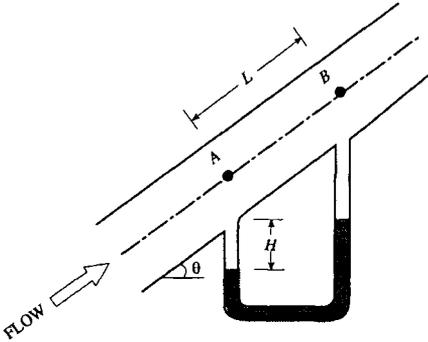
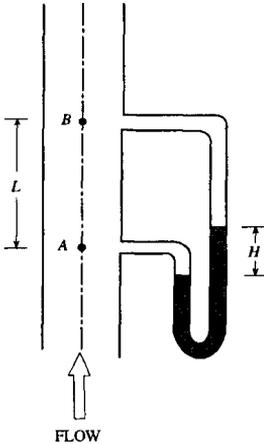
## 5.2 RATE OF GENERATION IN ENERGY TRANSPORT

Let us consider the following paradox: “*One of the most important problems that the world faces today is energy shortage. According to the first law of thermodynamics, energy is converted from one form to another and transferred from one system to another but its total is conserved. If energy is conserved, then there should be no energy shortage.*”

---

<sup>1</sup>The term  $\mathcal{P}$  is also called equivalent pressure, dynamic pressure and piezometric pressure.

**Table 5.1** Pressure difference in flow through a pipe with different orientation.

Geometry	$\mathcal{P}_A - \mathcal{P}_B$	$P_A - P_B$
	$(\rho_m - \rho)gH$	$(\rho_m - \rho)gH$
	$(\rho_m - \rho)gH$	$(\rho_m - \rho)gH + \rho g L \sin \theta$
	$(\rho_m - \rho)gH$	$(\rho_m - \rho)gH + \rho g L$

The answer to this dilemma lies in the fact that although energy is conserved, its ability to produce useful work decreases steadily as a result of the irreversibilities associated with the transformation of energy from one form into another<sup>2</sup>. These irreversibilities give rise to energy generation within the system. Typical examples

<sup>2</sup>Note that 1,000 J at 100 °C is much more valuable than 1,000 J at 20 °C.

are the degradation of mechanical energy into thermal energy during viscous flow and degradation of electrical energy into thermal energy during transmission of an electric current.

Generation of energy can also be attributed to various other factors such as chemical and nuclear reactions, absorption radiation, and presence of magnetic fields. Energy generation as a result of chemical reaction will be explained in detail in Chapter 6.

The rate of energy generation per unit volume may be considered constant in most cases. If it is dependent on temperature, it may be expressed in various forms such as

$$\mathfrak{R} = \begin{cases} a + bT \\ \mathfrak{R}_o e^{\alpha T} \end{cases} \quad (5.2-1)$$

where  $a$  and  $b$  are constants.

## 5.3 RATE OF GENERATION IN MASS TRANSPORT

### 5.3.1 Stoichiometry of a Chemical Reaction

Balancing of a chemical equation is based on the conservation of mass for a closed thermodynamic system. If a chemical reaction takes place in a closed container, the mass does not change even if there is an exchange of energy with the surroundings.

Consider a reaction between nitrogen and hydrogen to form ammonia, i.e.,



If  $A_1 = \text{N}_2$ ,  $A_2 = \text{H}_2$  and  $A_3 = \text{NH}_3$ , Eq. (5.3-1) is expressed as

$$A_1 + 3A_2 = 2A_3 \quad (5.3-2)$$

It is convenient to write all the chemical species on one side of the equation and give a positive sign to the species which are regarded as the products of the reaction. Thus,

$$2A_3 - A_1 - 3A_2 = 0 \quad (5.3-3)$$

or,

$$\sum_{i=1}^s \alpha_i A_i = 0 \quad (5.3-4)$$

where  $\alpha_i$  is the stoichiometric coefficient of  $i^{\text{th}}$  chemical species (positive if species is a product, negative if species is a reactant),  $s$  is the total number of species in the reaction, and  $A_i$  is the chemical symbol for the  $i^{\text{th}}$  chemical species, representing the molecular weight of species.

Each chemical species,  $A_i$ , is the sum of the chemical elements,  $E_j$ , such that

$$A_i = \sum_{j=1}^t \beta_{ji} E_j \quad (5.3-5)$$

where  $\beta_{ji}$  represents the number of chemical elements  $E_j$  in the chemical species  $A_i$ , and  $t$  is the total number of chemical elements. Substitution of Eq. (5.3-5) into Eq. (5.3-4) gives

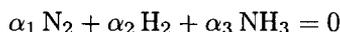
$$\sum_{i=1}^s \alpha_i \left( \sum_{j=1}^t \beta_{ji} E_j \right) = \sum_{j=1}^t \left( \sum_{i=1}^s \alpha_i \beta_{ji} \right) E_j = 0 \quad (5.3-6)$$

Since all the  $E_j$  are linearly independent<sup>3</sup>, then

$$\boxed{\sum_{i=1}^s \alpha_i \beta_{ji} = 0} \quad j = 1, 2, \dots, t \quad (5.3-7)$$

Equation (5.3-7) is used to balance chemical equations.

**Example 5.1** Consider the reaction between  $N_2$  and  $H_2$  to form  $NH_3$



Show how one can apply Eq. (5.3-7) to balance this equation.

**Solution**

If  $A_1 = N_2$ ,  $A_2 = H_2$  and  $A_3 = NH_3$ , the above equation can be expressed as

$$\alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 A_3 = 0 \quad (1)$$

If we let  $E_1 = N$  ( $j = 1$ ) and  $E_2 = H$  ( $j = 2$ ), then Eq. (5.3-7) becomes

$$\alpha_1 E_{11} + \alpha_2 E_{12} + \alpha_3 E_{13} = 0 \quad \text{for } j = 1 \quad (2)$$

$$\alpha_1 E_{21} + \alpha_2 E_{22} + \alpha_3 E_{23} = 0 \quad \text{for } j = 2 \quad (3)$$

---

<sup>3</sup>The expression

$$\sum_{i=1}^n \alpha_i x_i = \alpha_1 x_1 + \alpha_2 x_2 + \dots + \alpha_n x_n$$

where  $\{\alpha_1, \alpha_2, \dots, \alpha_n\}$  is a set of scalars, is called a *linear combination* of the elements of the set  $S = \{x_1, x_2, \dots, x_n\}$ . The elements of the set  $S$  is said to be *linearly dependent* if there exists a set of scalars  $\{\alpha_1, \alpha_2, \dots, \alpha_n\}$  with elements  $\alpha_i$  **not** all equal to zero, such that the linear combination  $\sum_{i=1}^n \alpha_i x_i = 0$  holds. If  $\sum_{i=1}^n \alpha_i x_i = 0$  holds for all  $\alpha_i = 0$ , then the set  $S$  is *linearly independent*.

or,

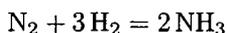
$$\alpha_1(2) + \alpha_2(0) + \alpha_3(1) = 0 \quad (4)$$

$$\alpha_1(0) + \alpha_2(2) + \alpha_3(3) = 0 \quad (5)$$

Solutions of Eqs. (4) and (5) give

$$\alpha_1 = -\frac{1}{2}\alpha_3 \quad \alpha_2 = -\frac{3}{2}\alpha_3 \quad (6)$$

If we take  $\alpha_3 = 2$ , then  $\alpha_1 = -1$  and  $\alpha_2 = -3$ . Hence, the reaction becomes



**Comment:** Stoichiometric coefficients have units. For example, in the above equation the stoichiometric coefficient of  $\text{H}_2$  indicates that there are 3 moles of  $\text{H}_2$  per mole of  $\text{N}_2$ .

### 5.3.2 The Law of Combining Proportions

Stoichiometric coefficients have the units of moles of  $i$  per mole of basis species, where basis species is arbitrarily chosen. The law of combining proportions states that

$$\frac{\text{moles of } i \text{ reacted}}{(\text{moles of } i / \text{mole of basis species})} = \text{moles of basis species} \quad (5.3-8)$$

or,

$$\frac{n_i - n_{i_o}}{\alpha_i} = \varepsilon \quad (5.3-9)$$

where  $\varepsilon$  is called the *molar extent* of the reaction<sup>4</sup>. Rearrangement of Eq. (5.3-9) gives

$$\boxed{n_i = n_{i_o} + \alpha_i \varepsilon} \quad (5.3-10)$$

Note that once  $\varepsilon$  has been determined, the number of moles of any chemical species participating in the reaction can be determined by using Eq. (5.3-10).

The molar extent of the reaction should not be confused with the *fractional conversion variable*,  $X$ , which can only take values between 0 and 1. The molar extent of the reaction is an extensive property measured in moles and its value can be greater than unity.

It is also important to note that the fractional conversion may be different for each of the reacting species, i.e.,

$$\boxed{X_i = \frac{n_{i_o} - n_i}{n_{i_o}}} \quad (5.3-11)$$

<sup>4</sup>The term  $\varepsilon$  has been given various names in the literature, such as, degree of advancement, reaction of coordinate, degree of reaction and progress variable.

On the other hand, molar extent is unique for a given reaction. Comparison of Eqs. (5.3-10) and (5.3-11) indicates that

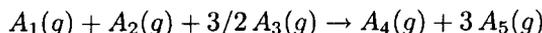
$$\varepsilon = \frac{n_{i_o}}{(-\alpha_i)} X \quad (5.3-12)$$

The total number of moles,  $n_T$ , of a reacting mixture at any instant can be calculated by the summation of Eq. (5.3-10) over all species, i.e.,

$$n_T = n_{T_o} + \bar{\alpha} \varepsilon \quad (5.3-13)$$

where  $n_{T_o}$  is the initial total number of moles and  $\bar{\alpha} = \sum_i \alpha_i$ .

**Example 5.2** A system containing 1 mol  $A_1$ , 2 mol  $A_2$  and 7 mol  $A_3$  undergoes the following reaction



Determine the limiting reactant and fractional conversion with respect to each reactant if the reaction goes to completion.

### Solution

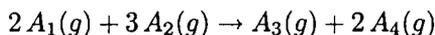
Since  $n_i \geq 0$ , it is possible to conclude from Eq. (5.3-10) that the limiting reactant has the least positive value of  $n_{i_o}/(-\alpha_i)$ . The values given in the following table indicate that the limiting reactant is  $A_1$ .

Species	$n_{i_o}/(-\alpha_i)$
$A_1$	1
$A_2$	2
$A_3$	4.67

Note that the least positive value of  $n_{i_o}/(-\alpha_i)$  is also the greatest possible value of  $\varepsilon$ . Since the reaction goes to completion, species  $A_1$  will be completely depleted and  $\varepsilon = 1$ . Using Eq. (5.3-12), fractional conversion values are given as follows:

Species	$X$
$A_1$	1
$A_2$	0.50
$A_3$	0.21

**Example 5.3** A system containing 3 mol  $A_1$  and 4 mol  $A_2$  undergoes the following reaction



Calculate the mole fractions of each species if  $\varepsilon = 1.1$ . What is the fractional conversion based on the limiting reactant?

**Solution**

Using Eq. (5.3-10), the number of moles of each species is expressed as

$$n_1 = 3 - 2\varepsilon = 3 - (2)(1.1) = 0.8 \text{ mol}$$

$$n_2 = 4 - 3\varepsilon = 4 - (3)(1.1) = 0.7 \text{ mol}$$

$$n_3 = \varepsilon = 1.1 \text{ mol}$$

$$n_4 = 2\varepsilon = (2)(1.1) = 2.2 \text{ mol}$$

Therefore, the total number of moles is 4.8 moles and the mole fraction of each species is

$$x_1 = \frac{0.8}{4.8} = 0.167$$

$$x_2 = \frac{0.7}{4.8} = 0.146$$

$$x_3 = \frac{1.1}{4.8} = 0.229$$

$$x_4 = \frac{2.2}{4.8} = 0.458$$

The fractional conversion,  $X$ , based on the limiting reactant  $A_2$  is

$$X = \frac{4 - 0.7}{4} = 0.825$$

Molar concentration of the  $i^{\text{th}}$  species,  $c_i$ , is defined by

$$c_i = \frac{n_i}{V} \quad (5.3-14)$$

Therefore, division of Eq. (5.3-10) by the volume  $V$  gives

$$\frac{n_i}{V} = \frac{n_{i_o}}{V} + \alpha_i \frac{\varepsilon}{V} \quad (5.3-15)$$

or,

$$\boxed{c_i = c_{i_o} + \alpha_i \xi} \quad (5.3-16)$$

where  $c_{i_o}$  is the initial molar concentration of the  $i^{\text{th}}$  species and  $\xi$  is the *intensive extent* of the reaction in moles per unit volume. Note that  $\xi$  is related to conversion,  $X$ , by

$$\boxed{\xi = \frac{c_{i_o}}{(-\alpha_i)} X_i} \quad (5.3-17)$$

The total molar concentration,  $c$ , of a reacting mixture at any instant can be calculated by the summation of Eq. (5.3-16) over all species, i.e.,

$$\boxed{c = c_o + \bar{\alpha} \xi} \quad (5.3-18)$$

where  $c_o$  is the initial total molar concentration.

When more than one reaction takes place in a reactor, Eq. (5.3-10) takes the form

$$\boxed{n_{ij} = n_{ij_o} + \alpha_{ij} \varepsilon_j} \quad (5.3-19)$$

where

- $n_{ij}$  = number of moles of  $i^{th}$  species in the  $j^{th}$  reaction
- $n_{ij_o}$  = initial number of moles of  $i^{th}$  species in the  $j^{th}$  reaction
- $\alpha_{ij}$  = stoichiometric coefficient of  $i^{th}$  species in the  $j^{th}$  reaction
- $\varepsilon_j$  = extent of the  $j^{th}$  reaction

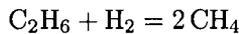
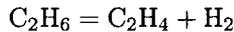
Summation of Eq. (5.3-19) over all reactions taking place in a reactor gives

$$\sum_j n_{ij} = \sum_j n_{ij_o} + \sum_j \alpha_{ij} \varepsilon_j \quad (5.3-20)$$

or,

$$\boxed{n_i = n_{i_o} + \sum_j \alpha_{ij} \varepsilon_j} \quad (5.3-21)$$

**Example 5.4** *The following two reactions occur simultaneously in a batch reactor:*



*A mixture of 85 mol % C<sub>2</sub>H<sub>6</sub> and 15% inerts is fed into a reactor and the reactions proceed until 25% C<sub>2</sub>H<sub>4</sub> and 5% CH<sub>4</sub> are formed. Determine the percentage of each species in a reacting mixture.*

### Solution

*Basis: 1 mole of a reacting mixture*

*Let  $\varepsilon_1$  and  $\varepsilon_2$  be the extents of the first and second reactions, respectively. Then, the number of moles of each species can be expressed as*

$$n_{\text{C}_2\text{H}_6} = 0.85 - \varepsilon_1 - \varepsilon_2$$

$$n_{\text{C}_2\text{H}_4} = \varepsilon_1$$

$$n_{\text{H}_2} = \varepsilon_1 - \varepsilon_2$$

$$n_{\text{CH}_4} = 2\varepsilon_2$$

$$n_{\text{inert}} = 0.15$$

*The total number of moles,  $n_T$ , is*

$$n_T = 1 + \varepsilon_1$$

The mole fractions of  $C_2H_4$  and  $CH_4$  are given in the problem statement. These values are used to determine the extent of the reactions as

$$x_{C_2H_4} = \frac{\varepsilon_1}{1 + \varepsilon_1} = 0.25 \quad \Rightarrow \quad \varepsilon_1 = 0.333$$

$$x_{CH_4} = \frac{2\varepsilon_2}{1 + \varepsilon_1} = 0.05 \quad \Rightarrow \quad \varepsilon_2 = 0.033$$

Therefore, the mole fractions of  $C_2H_6$ ,  $H_2$  and the inerts are

$$x_{C_2H_6} = \frac{0.85 - \varepsilon_1 - \varepsilon_2}{1 + \varepsilon_1} = \frac{0.85 - 0.333 - 0.033}{1 + 0.333} = 0.363$$

$$x_{H_2} = \frac{\varepsilon_1 - \varepsilon_2}{1 + \varepsilon_1} = \frac{0.333 - 0.033}{1 + 0.333} = 0.225$$

$$x_{inert} = \frac{0.15}{1 + 0.333} = 0.112$$

### 5.3.3 Rate of Reaction

The rate of a chemical reaction,  $r$ , is defined by

$$r = \frac{1}{V} \frac{d\varepsilon}{dt} \quad (5.3-22)$$

where  $V$  is the volume physically occupied by the reacting fluid. Since both  $V$  and  $d\varepsilon/dt$  are positive, the reaction rate is intrinsically positive. Note that the reaction rate has the units of moles reacted per unit time per unit volume of the reaction mixture. The reaction rate expression,  $r$ , has the following characteristics:

- It is an intensive property,
- It is independent of the reactor type,
- It is independent of a process.

Changes in the molar extent of the reaction can be related to the changes in the number of moles of species  $i$  by differentiating Eq. (5.3-10). The result is

$$d\varepsilon = \frac{1}{\alpha_i} dn_i \quad (5.3-23)$$

Substitution of Eq. (5.3-23) into Eq. (5.3-22) gives

$$r = \frac{1}{\alpha_i} \frac{1}{V} \frac{dn_i}{dt} \quad (5.3-24)$$

If the rate of generation of species  $i$  per unit volume,  $\mathfrak{R}_i$ , is defined by

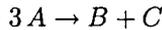
$$\mathfrak{R}_i = \frac{1}{V} \frac{dn_i}{dt} \quad (5.3-25)$$

then

$$\mathfrak{R}_i = \alpha_i r \quad (5.3-26)$$

Therefore,  $\mathfrak{R}_i$  is negative if  $i$  appears as a reactant;  $\mathfrak{R}_i$  is positive if  $i$  is a product.

**Example 5.5** For the reaction



express the reaction rate in terms of the time rate of change of species  $A$ ,  $B$ , and  $C$ .

**Solution**

Application of Eq. (5.3-24) gives the rate as

$$r = -\frac{1}{3} \frac{1}{V} \frac{dn_A}{dt} = \frac{1}{V} \frac{dn_B}{dt} = \frac{1}{V} \frac{dn_C}{dt} \quad (1)$$

If  $V$  is constant, then Eq. (1) reduces to

$$r = -\frac{1}{3} \frac{dc_A}{dt} = \frac{dc_B}{dt} = \frac{dc_C}{dt} \quad (2)$$

**Comment:** The rate of reaction is equal to the time derivative of a concentration only when the volume of the reacting mixture is constant.

In the case of several reactions,  $\mathfrak{R}_i$  is defined by

$$\mathfrak{R}_i = \sum_j \alpha_{ij} r_j \quad (5.3-27)$$

where  $r_j$  is the rate of  $j^{\text{th}}$  reaction.

The reaction rate is a function of temperature and concentration and is assumed to be the product of two functions, one is dependent only on the temperature and the other is dependent only on the concentration, i.e.,

$$r(T, c_i) = k(T)f(c_i) \quad (5.3-28)$$

The function  $k(T)$  is called the *rate constant* and its dependence on the temperature is given by

$$k(T) = AT^m e^{-\mathcal{E}/\mathcal{R}T} \quad (5.3-29)$$

where  $A$  is a constant,  $\mathcal{E}$  is the activation energy,  $\mathcal{R}$  is the gas constant and  $T$  is the absolute temperature. The power of temperature,  $m$ , is given by

$$m = \begin{cases} 0 & \text{from the Arrhenius relation} \\ 1/2 & \text{from the kinetic theory of gases} \\ 1 & \text{from statistical mechanics} \end{cases} \quad (5.3-30)$$

In engineering practice the *Arrhenius relation*, i.e.,

$$k(T) = A e^{-\mathcal{E}/\mathcal{R}T} \quad (5.3-31)$$

is generally considered valid<sup>5</sup> and the rate constant can be determined by running the same reaction at different temperatures. The data from these experiments are found to be linear on a semi-log plot of  $k$  versus  $1/T$ .

The function  $f(c_i)$  depends on the concentration of all the species in the chemical reaction. Since the reaction rate is usually largest at the start of the reaction and eventually decreases to reach a zero-rate at equilibrium, the function  $f(c_i)$  is taken to be a power function of the concentration of the reactants.

If  $f(c_i)$  were a power function of the products of the reaction, the reaction rate would increase, rather than decrease with time. These reactions are called *autocatalytic*.

For normal decreasing rate reactions

$$f(c_i) = \prod_i c_i^{\gamma_i} \quad (5.3-32)$$

where  $c_i$  is the concentration of a reactant. Thus, the constitutive equation for the reaction rate is

$$r = k \prod_i c_i^{\gamma_i} \quad (5.3-33)$$

The *order of a reaction*,  $n$ , refers to the powers to which the concentrations are raised, i.e.,

$$n = \sum_i \gamma_i \quad (5.3-34)$$

It should be pointed out that there is no necessary connection between the order and the stoichiometry of the reaction.

## NOTATION

$A$	area, $\text{m}^2$
$c$	concentration, $\text{kmol}/\text{m}^3$
$\mathcal{E}$	activation energy, $\text{kJ}/\text{kmol}$
$F_D$	drag force, $\text{N}$
$g$	acceleration of gravity, $\text{m}/\text{s}^2$
$h$	elevation, $\text{m}$
$k$	reaction rate constant
$L$	length, $\text{m}$

<sup>5</sup>Deviations from the Arrhenius relationship are discussed by Maheswari and Akella (1988).

$M$	mass, kg
$\dot{m}$	mass flow rate, kg/s
$n$	number of moles, kmol
$n_{ij}$	number of moles of $i^{\text{th}}$ species in the $j^{\text{th}}$ reaction
$P$	pressure, Pa
$\mathcal{P}$	modified pressure, Pa
$Q$	volumetric flow rate, $\text{m}^3/\text{s}$
$r$	rate of a chemical reaction, $\text{kmol}/\text{m}^3 \cdot \text{s}$
$\mathfrak{R}$	rate of generation (momentum, energy, mass) per unit volume
$T$	temperature, $^{\circ}\text{C}$ or $\text{K}$
$t$	time, s
$V$	volume, $\text{m}^3$
$v$	velocity, $\text{m}/\text{s}$
$\dot{W}$	rate of work, $\text{W}$
$X$	fractional conversion
$x_i$	mole fraction of species $i$
$z$	rectangular coordinate, m
$\alpha_i$	stoichiometric coefficient of species $i$
$\alpha_{ij}$	stoichiometric coefficient of $i^{\text{th}}$ species in the $j^{\text{th}}$ reaction
$\bar{\alpha}$	$\sum_i \alpha_i$
$\Delta$	difference
$\varepsilon$	molar extent of a reaction, kmol
$\xi$	intensive extent of a reaction, $\text{kmol}/\text{m}^3$
$\rho$	density, $\text{kg}/\text{m}^3$
$\rho_m$	density of manometer fluid, $\text{kg}/\text{m}^3$

**Bracket**

$\langle a \rangle$  average value of  $a$

**Subscripts**

$atm$	atmospheric
$in$	inlet
$o$	initial
$out$	out
$T$	total

**REFERENCE**

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## Chapter 6

# Steady-State Macroscopic Balances

The use of correlations in the determination of momentum, energy and mass transfer from one phase to another under steady-state conditions was covered in Chapter 4. Although some examples of Chapter 4 make use of steady-state macroscopic balances, systematic treatment of these balances for the conservation of chemical species, mass and energy was not presented. The basic steps in the development of steady-state macroscopic balances are as follows:

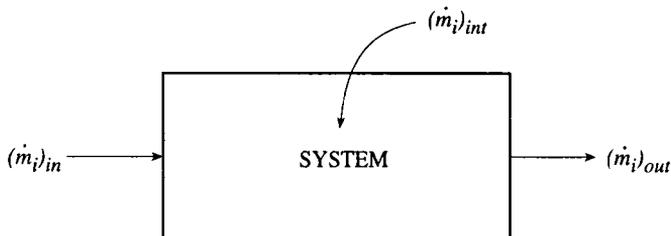
- *Define your system:* A system is any region which occupies a volume and has a boundary.
- *If possible, draw a simple sketch:* A simple sketch helps in the understanding of the physical picture.
- *List the assumptions:* Simplify the complicated problem to a mathematically tractable form by making reasonable assumptions.
- *Write down the inventory rate equation for each of the basic concepts relevant to the problem at hand:* Since the accumulation term vanishes for steady-state cases, macroscopic inventory rate equations reduce to algebraic equations. Note that in order to have a mathematically determinate system, the number of independent inventory rate equations must be equal to the number of dependent variables.
- *Use engineering correlations to evaluate the transfer coefficients:* In macroscopic modeling, empirical equations that represent transfer phenomena from one phase to another contain transfer coefficients, such as the heat transfer coefficient in Newton's law of cooling. These coefficients can be evaluated by using engineering correlations given in Chapter 4.
- *Solve the algebraic equations.*

## 6.1 CONSERVATION OF CHEMICAL SPECIES

The inventory rate equation given by Eq. (1.1-1) holds for every conserved quantity  $\varphi$ . Therefore, the conservation statement for the mass of the  $i^{\text{th}}$  chemical species under steady conditions is given by

$$\left( \begin{array}{c} \text{Rate of mass} \\ \text{of } i \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of mass} \\ \text{of } i \text{ out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of generation} \\ \text{of mass } i \end{array} \right) = 0 \quad (6.1-1)$$

The mass of  $i$  may enter or leave the system by two means: (i) by inlet or outlet streams, (ii) by exchange of mass between the system and its surroundings through the boundaries of the system, i.e., interphase mass transfer.



**Figure 6.1** Steady-state flow system with fixed boundaries.

For a system with a single inlet and a single outlet stream as shown in Figure 6.1, Eq. (6.1-1) can be expressed as

$$\boxed{(\dot{m}_i)_{in} - (\dot{m}_i)_{out} \pm (\dot{m}_i)_{int} + \left( \sum_j \alpha_{ij} r_j \right) \mathcal{M}_i V_{sys} = 0} \quad (6.1-2)$$

in which the molar rate of generation of species  $i$  per unit volume,  $\mathfrak{R}_i$ , is expressed by Eq. (5.3-27). The terms  $(\dot{m}_i)_{in}$  and  $(\dot{m}_i)_{out}$  represent the inlet and outlet mass flow rates of species  $i$ , respectively, and  $\mathcal{M}_i$  is the molecular weight of species  $i$ . The interphase mass transfer rate,  $(\dot{m}_i)_{int}$ , is expressed as

$$(\dot{m}_i)_{int} = A_M \langle k_c \rangle (\Delta c_i)_{ch} \mathcal{M}_i \quad (6.1-3)$$

where  $(\Delta c_i)_{ch}$  is the characteristic concentration difference. Note that  $(\dot{m}_i)_{int}$  is considered *positive* when mass is added to the system.

As stated in Section 2.4.1, the mass flow rate of species  $i$ ,  $\dot{m}_i$ , is given by

$$\dot{m}_i = \rho_i \langle v \rangle A = \rho_i \mathcal{Q} \quad (6.1-4)$$

Therefore, Eq. (6.1-2) takes the form

$$\boxed{(\mathcal{Q}\rho_i)_{in} - (\mathcal{Q}\rho_i)_{out} \pm A_M \langle k_c \rangle (\Delta c_i)_{ch} \mathcal{M}_i + \left( \sum_j \alpha_{ij} r_j \right) \mathcal{M}_i V_{sys} = 0} \quad (6.1-5)$$

Sometimes it is more convenient to work on molar basis. Division of Eqs. (6.1-2) and (6.1-5) by the molecular weight of species  $i$ ,  $\mathcal{M}_i$ , gives

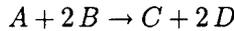
$$\boxed{(\dot{n}_i)_{in} - (\dot{n}_i)_{out} \pm (\dot{n}_i)_{int} + \left( \sum_j \alpha_{ij} r_j \right) V_{sys} = 0} \quad (6.1-6)$$

and

$$\boxed{(\mathcal{Q}c_i)_{in} - (\mathcal{Q}c_i)_{out} \pm A_M \langle k_c \rangle (\Delta c_i)_{ch} + \left( \sum_j \alpha_{ij} r_j \right) V_{sys} = 0} \quad (6.1-7)$$

where  $\dot{n}_i$  and  $c_i$  are the molar flow rate and molar concentration of species  $i$ , respectively.

### Example 6.1 *The liquid phase reaction*



takes place in an isothermal, constant-volume stirred tank reactor. The rate of reaction is expressed by

$$r = k c_A c_B \quad \text{with} \quad k = 0.025 \text{ L/mol}\cdot\text{min}$$

The feed stream consists of equal concentrations of species  $A$  and  $B$  at a value of 1 mol/L. Determine the residence time required to achieve 60% conversion of species  $B$  under steady conditions.

### Solution

#### Assumption

1. As a result of perfect mixing, concentrations of species within the reactor are uniform, i.e.,  $(c_i)_{out} = (c_i)_{sys}$ .

**Analysis**

*System: Contents of the reactor*

Since the reactor volume is constant, the inlet and outlet volumetric flow rates are the same and equal to  $Q$ . Therefore, the inventory rate equation for conservation of species B, Eq. (6.1-7), becomes

$$Q(c_B)_{in} - Q c_{B_{sys}} - (2k c_{A_{sys}} c_{B_{sys}}) V_{sys} = 0 \quad (1)$$

where  $c_{A_{sys}}$  and  $c_{B_{sys}}$  represent the molar concentration of species A and B in the reactor, respectively. Dropping the subscript "sys" and defining the residence time,  $\tau$ , as  $\tau = V/Q$  reduces Eq. (1) to

$$(c_B)_{in} - c_B - (2k c_A c_B) \tau = 0 \quad (2)$$

or,

$$\tau = \frac{(c_B)_{in} - c_B}{2k c_A c_B} \quad (3)$$

Using Eq. (5.3-17), the extent of the reaction can be calculated as

$$\begin{aligned} \xi &= \frac{(c_B)_{in}}{(-\alpha_B)} X_B \\ &= \frac{(1)(0.6)}{2} = 0.3 \text{ mol/L} \end{aligned} \quad (4)$$

Therefore, the concentrations of species A and B in the reactor are

$$c_A = (c_A)_{in} + \alpha_A \xi = 1 - 0.3 = 0.7 \text{ mol/L} \quad (5)$$

$$c_B = (c_B)_{in} + \alpha_B \xi = 1 - (2)(0.3) = 0.4 \text{ mol/L} \quad (6)$$

Substitution of the numerical values into Eq. (3) gives

$$\tau = \frac{1 - 0.4}{(2)(0.025)(0.7)(0.4)} = 42.9 \text{ min}$$

**6.2 CONSERVATION OF MASS**

Summation of Eq. (6.1-2) over all species gives the total mass balance in the form

$$\boxed{\dot{m}_{in} - \dot{m}_{out} \pm \dot{m}_{int} = 0} \quad (6.2-1)$$

Note that the term

$$\sum_i \left( \sum_j \alpha_{ij} r_j \right) \mathcal{M}_i = 0 \quad (6.2-2)$$

since mass is conserved. Equation (6.2-2) implies that the rate of production of mass for the entire system is zero. However, if chemical reactions take place within the system, an individual species may be produced.

On the other hand, summation of Eq. (6.1-6) over all species gives the total mole balance as

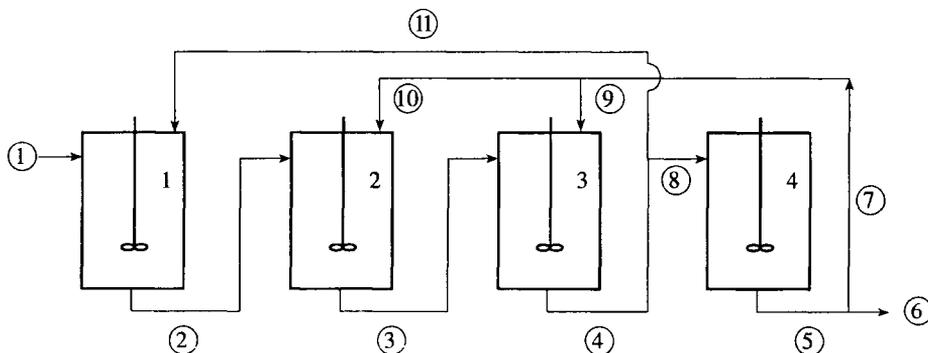
$$\dot{n}_{in} - \dot{n}_{out} \pm \dot{n}_{int} + \left[ \sum_i \left( \sum_j \alpha_{ij} r_j \right) \right] V_{sys} = 0 \quad (6.2-3)$$

In this case the generation term is not zero because moles are not conserved.

**Example 6.2** *A liquid phase irreversible reaction*



takes place in a series of 4 continuous stirred tank reactors as shown in the figure below.



The rate of reaction is given by

$$r = kc_A \quad \text{with} \quad k = 3 \times 10^5 \exp\left(-\frac{4200}{T}\right)$$

in which  $k$  is in  $\text{h}^{-1}$  and  $T$  is in degrees Kelvin. The temperature and the volume of each reactor are given as follows:

Reactor No	Temperature ( $^{\circ}\text{C}$ )	Volume (L)
1	35	800
2	45	1000
3	70	1200
4	60	900

Determine the concentration of species  $A$  in each reactor if the feed to the first reactor contains 1.5 mol/L of  $A$  and the volumetric flow rates of the streams are given as follows:

Stream No	Volumetric Flow Rate (L/h)
1	500
7	200
9	50
11	100

### Solution

#### Assumptions

1. Steady-state conditions prevail.
2. Concentrations of species within the reactor are uniform as a result of perfect mixing.
3. Liquid density remains constant.

#### Analysis

Conservation of total mass, Eq. (6.2-1), reduces to

$$\dot{m}_{in} = \dot{m}_{out} \quad (1)$$

Since the liquid density is constant, Eq. (1) simplifies to

$$Q_{in} = Q_{out} \quad (2)$$

Only four out of eleven streams are given in the problem statement. Therefore, it is necessary to write the following mass balances to calculate the remaining seven streams:

$$\begin{aligned} Q_1 &= Q_6 = 500 \\ 500 + 100 &= Q_2 \\ Q_2 + Q_{10} &= Q_3 \\ Q_3 + 50 &= Q_4 \\ Q_8 &= Q_5 \\ Q_5 &= Q_6 + 200 \\ 200 &= 50 + Q_{10} \end{aligned}$$

Simultaneous solution of the above equations gives the volumetric flow rate of each stream as:

Stream No	Volumetric Flow Rate (L/h)
1	500
2	600
3	750
4	800
5	700
6	500
7	200
8	700
9	50
10	150
11	100

For each reactor, the reaction rate constant is

$$k = 3 \times 10^5 \exp \left[ -\frac{4200}{(35 + 273)} \right] = 0.359 \text{ h}^{-1} \quad \text{for reactor \# 1}$$

$$k = 3 \times 10^5 \exp \left[ -\frac{4200}{(45 + 273)} \right] = 0.551 \text{ h}^{-1} \quad \text{for reactor \# 2}$$

$$k = 3 \times 10^5 \exp \left[ -\frac{4200}{(70 + 273)} \right] = 1.443 \text{ h}^{-1} \quad \text{for reactor \# 3}$$

$$k = 3 \times 10^5 \exp \left[ -\frac{4200}{(60 + 273)} \right] = 0.999 \text{ h}^{-1} \quad \text{for reactor \# 4}$$

For each reactor, the conservation statement for species  $A$ , Eq. (6.1-7), can be written in the form

$$(500)(1.5) + 100 c_{A_3} - 600 c_{A_1} - (0.359 c_{A_1})(800) = 0$$

$$600 c_{A_1} + 150 c_{A_4} - 750 c_{A_2} - (0.551 c_{A_2})(1000) = 0$$

$$750 c_{A_2} + 50 c_{A_4} - 800 c_{A_3} - (1.443 c_{A_3})(1200) = 0$$

$$700 c_{A_3} - 700 c_{A_4} - (0.999 c_{A_4})(900) = 0$$

Simplification gives

$$8.872 c_{A_1} - c_{A_3} = 7.5$$

$$4 c_{A_1} - 8.673 c_{A_2} + c_{A_4} = 0$$

$$15 c_{A_2} - 50.632 c_{A_3} + c_{A_4} = 0$$

$$c_{A_3} - 2.284 c_{A_4} = 0$$

The above equations are written in matrix notation<sup>1</sup> as

$$\begin{bmatrix} 8.872 & 0 & -1 & 0 \\ 4 & -8.673 & 0 & 1 \\ 0 & 15 & -50.632 & 1 \\ 0 & 0 & 1 & -2.284 \end{bmatrix} \begin{bmatrix} c_{A_1} \\ c_{A_2} \\ c_{A_3} \\ c_{A_4} \end{bmatrix} = \begin{bmatrix} 7.5 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Therefore, the solution is

$$\begin{aligned} \begin{bmatrix} c_{A_1} \\ c_{A_2} \\ c_{A_3} \\ c_{A_4} \end{bmatrix} &= \begin{bmatrix} 8.872 & 0 & -1 & 0 \\ 4 & -8.673 & 0 & 1 \\ 0 & 15 & -50.632 & 1 \\ 0 & 0 & 1 & -2.284 \end{bmatrix}^{-1} \begin{bmatrix} 7.5 \\ 0 \\ 0 \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} 0.115 & -0.004 & -0.002 & -0.003 \\ 0.054 & -0.119 & -0.002 & -0.053 \\ 0.016 & -0.036 & -0.021 & -0.025 \\ 0.007 & -0.016 & -0.009 & -0.449 \end{bmatrix} \begin{bmatrix} 7.5 \\ 0 \\ 0 \\ 0 \end{bmatrix} \end{aligned}$$

The multiplication gives the concentrations in each reactor as

$$\begin{bmatrix} c_{A_1} \\ c_{A_2} \\ c_{A_3} \\ c_{A_4} \end{bmatrix} = \begin{bmatrix} 0.859 \\ 0.402 \\ 0.120 \\ 0.053 \end{bmatrix}$$

### 6.3 CONSERVATION OF ENERGY

The conservation statement for *total* energy under steady conditions takes the form

$$\left( \begin{array}{c} \text{Rate of} \\ \text{energy in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{energy out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of energy} \\ \text{generation} \end{array} \right) = 0 \quad (6.3-1)$$

The first law of thermodynamics states that total energy can neither be created nor destroyed. Therefore, rate of generation term in Eq. (6.3-1) equals zero.

Energy may enter or leave the system by two means: (i) by inlet and/or outlet streams, (ii) by exchange of energy between the system and its surroundings through the boundaries of the system in the form of heat and work.

For a system with a single inlet and a single outlet stream as shown in Figure 6.2, Eq. (6.3-1) can be expressed as

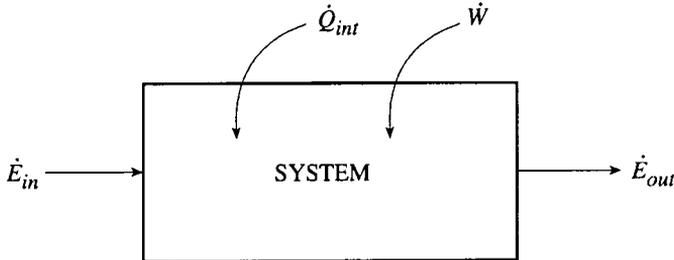
$$(\dot{E}_{in} + \dot{Q}_{int} + \dot{W}) - \dot{E}_{out} = 0 \quad (6.3-2)$$

where the interphase heat transfer rate,  $\dot{Q}_{int}$ , is expressed as

$$\dot{Q}_{int} = A_H (h) (\Delta T)_{ch} \quad (6.3-3)$$

<sup>1</sup>Matrix operations are given in Section A.9 in Appendix A.

in which  $(\Delta T)_{ch}$  is the characteristic temperature difference. Note that  $\dot{Q}_{int}$  is considered positive when energy is added to the system. In a similar way,  $\dot{W}$  is also considered positive when work is done on the system.



**Figure 6.2** Steady-state flow system with fixed boundaries interchanging energy in the form of heat and work with the surroundings.

As stated in Section 2.4.2, the rate of energy entering or leaving the system,  $\dot{E}$ , is expressed as

$$\dot{E} = \hat{E} \dot{m} \quad (6.3-4)$$

Therefore, Eq. (6.3-2) becomes

$$(\hat{E} \dot{m})_{in} - (\hat{E} \dot{m})_{out} + \dot{Q}_{int} + \dot{W} = 0 \quad (6.3-5)$$

To determine the total energy per unit mass,  $\hat{E}$ , consider an astronaut on the space shuttle *Atlantis*. When the astronaut looks at the earth, (s)he sees that the earth has an external kinetic energy due to its rotation and its motion around the sun. The earth also has an internal kinetic energy as a result of all the objects, i.e., people, cars, planes, etc., moving on its surface which the astronaut cannot see. A physical object is usually composed of smaller objects, each of which can have a variety of internal and external energies. The sum of the internal and external energies of the smaller objects is usually apparent as internal energy of the larger objects.

The above discussion indicates that the total energy of any system is expressed as the sum of its internal and external energies. Kinetic and potential energies constitute the external energy, while the energy associated with the translational, rotational, and vibrational motion of molecules and atoms is considered as the internal energy. Therefore, total energy per unit mass can be expressed as

$$\hat{E} = \hat{U} + \hat{E}_K + \hat{E}_P \quad (6.3-6)$$

where  $\hat{U}$ ,  $\hat{E}_K$  and  $\hat{E}_P$  represent internal, kinetic and potential energies per unit mass, respectively. Substitution of Eq. (6.3-6) into Eq. (6.3-5) gives

$$\left[ (\hat{U} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{in} - \left[ (\hat{U} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{out} + \dot{Q}_{int} + \dot{W} = 0 \quad (6.3-7)$$

The rate of work done on the system by the surroundings is given by

$$\dot{W} = \underbrace{\dot{W}_s}_{\text{Shaft work}} + \underbrace{(P\hat{V}\dot{m})_{in} - (P\hat{V}\dot{m})_{out}}_{\text{Flow work}} \quad (6.3-8)$$

In Figure 6.2, when the stream enters the system, work is done on the system by the surroundings. When the stream leaves the system, however, work is done by the system on the surroundings. Note that the boundaries of the system are fixed in the case of a steady-state flow system. Therefore, work associated with volume change is not included in Eq. (6.3-8).

Substitution of Eq. (6.3-8) into Eq. (6.3-7) and the use of the definition of enthalpy, i.e.,  $\hat{H} = \hat{U} + P\hat{V}$ , gives

$$\boxed{\left[ (\hat{H} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{in} - \left[ (\hat{H} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \quad (6.3-9)$$

which is known as the *steady-state energy equation*.

Kinetic and potential energy terms in Eq. (6.3-9) are expressed in the form

$$\hat{E}_K = \frac{1}{2} v^2 \quad (6.3-10)$$

and

$$\hat{E}_P = g h \quad (6.3-11)$$

where  $g$  is the acceleration of gravity and  $h$  is the elevation with respect to a reference plane.

Enthalpy, on the other hand, depends on temperature and pressure. Change in enthalpy is expressed by

$$d\hat{H} = \hat{C}_P dT + \hat{V}(1 - \beta T) dP \quad (6.3-12)$$

where  $\beta$  is the *coefficient of volume expansion* and is defined by

$$\beta = \frac{1}{\hat{V}} \left( \frac{\partial \hat{V}}{\partial T} \right)_P = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_P \quad (6.3-13)$$

Note that

$$\beta = \begin{cases} 0 & \text{for an incompressible fluid} \\ 1/T & \text{for an ideal gas} \end{cases} \quad (6.3-14)$$

When the changes in the kinetic and potential energies between the inlet and outlet of the system are negligible, Eq. (6.3-9) reduces to

$$\boxed{(\hat{H} \dot{m})_{in} - (\hat{H} \dot{m})_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \quad (6.3-15)$$

In terms of molar quantities, Eqs. (6.3-9) and (6.3-15) are written as

$$\boxed{\left[ (\tilde{H} + \tilde{E}_K + \tilde{E}_P) \dot{n} \right]_{in} - \left[ (\tilde{H} + \tilde{E}_K + \tilde{E}_P) \dot{n} \right]_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \quad (6.3-16)$$

and

$$\boxed{(\tilde{H} \dot{n})_{in} - (\tilde{H} \dot{n})_{out} + \dot{Q}_{int} + \dot{W}_s = 0} \quad (6.3-17)$$

### 6.3.1 Energy Equation Without Chemical Reaction

In the case of no chemical reaction, Eqs. (6.3-9) and (6.3-16) are used to determine energy interactions. If kinetic and potential energy changes are negligible, then these equations reduce to Eqs. (6.3-15) and (6.3-17), respectively. The use of the energy equation requires the enthalpy change to be known or calculated. For some substances, such as steam and ammonia, enthalpy values are either tabulated or given in the form of a graph as a function of temperature and pressure. In that case enthalpy changes can be determined easily. If enthalpy values are not tabulated, then the determination of enthalpy depending on the values of temperature and pressure in a given process are given below.

#### 6.3.1.1 Constant pressure and no phase change

Since  $dP = 0$ , integration of Eq. (6.3-12) gives

$$\hat{H} = \int_{T_{ref}}^T \hat{C}_P dT \quad (6.3-18)$$

in which  $\hat{H}$  is taken as zero at  $T_{ref}$ . Substitution of Eq. (6.3-18) into Eq. (6.3-15) gives

$$\dot{m}_{in} \left( \int_{T_{ref}}^{T_{in}} \hat{C}_P dT \right) - \dot{m}_{out} \left( \int_{T_{ref}}^{T_{out}} \hat{C}_P dT \right) + \dot{Q}_{int} + \dot{W}_s = 0 \quad (6.3-19)$$

If  $\hat{C}_P$  is independent of temperature, Eq. (6.3-19) reduces to

$$\dot{m}_{in} \hat{C}_P (T_{in} - T_{ref}) - \dot{m}_{out} \hat{C}_P (T_{out} - T_{ref}) + \dot{Q}_{int} + \dot{W}_s = 0 \quad (6.3-20)$$

**Example 6.3** *It is required to cool a gas composed of 75 mole % N<sub>2</sub>, 15% CO<sub>2</sub> and 10% O<sub>2</sub> from 800 °C to 350 °C. Determine the cooling duty of the heat exchanger if the heat capacity expressions are in the form*

$$\tilde{C}_P (\text{J/mol} \cdot \text{K}) = a + bT + cT^2 + dT^3 \quad T [=] \text{K}$$

where the coefficients  $a$ ,  $b$ ,  $c$  and  $d$  are given by

Species	$a$	$b \times 10^2$	$c \times 10^5$	$d \times 10^5$
N <sub>2</sub>	28.882	-0.1570	0.8075	-2.8706
O <sub>2</sub>	25.460	1.5192	-0.7150	1.3108
CO <sub>2</sub>	21.489	5.9768	-3.4987	7.4643

**Solution****Assumptions**

1. *Ideal gas behavior.*
2. *Changes in kinetic and potential energies are negligible.*
3. *Pressure drop in the heat exchanger is negligible.*

**Analysis**

*System: Gas stream in the heat exchanger*

Since  $\dot{n}_{int} = 0$  and there is no chemical reaction, Eq. (6.2-3) reduces to

$$\dot{n}_{in} = \dot{n}_{out} = \dot{n} \quad (1)$$

Therefore, Eq. (6.3-19) becomes

$$\begin{aligned} \dot{Q}_{int} &= \dot{n} \left( \int_{T_{ref}}^{T_{out}} \tilde{C}_P dT - \int_{T_{ref}}^{T_{in}} \tilde{C}_P dT \right) \\ &= \dot{n} \left( \int_{T_{in}}^{T_{out}} \tilde{C}_P dT \right) \end{aligned} \quad (2)$$

or,

$$\tilde{Q}_{int} = \int_{T_{in}}^{T_{out}} \tilde{C}_P dT \quad (3)$$

where  $\tilde{Q}_{int} = \dot{Q}_{int}/\dot{n}$ ,  $T_{in} = 1073 \text{ K}$ , and  $T_{out} = 623 \text{ K}$ .

The molar heat capacity of the gas stream,  $\tilde{C}_P$ , can be calculated by multiplying the mole fraction of each component by the respective heat capacity and adding them together, i.e.,

$$\begin{aligned} \tilde{C}_P &= \sum_{i=1}^3 x_i (a_i + b_i T + c_i T^2 + d_i T^3) \\ &= 27.431 + 0.931 \times 10^{-2} T + 0.009 \times 10^{-5} T^2 - 0.902 \times 10^{-9} T^3 \end{aligned} \quad (4)$$

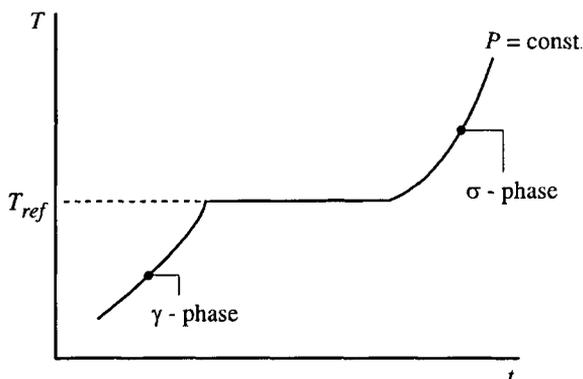
Substitution of Eq. (4) into Eq. (3) and integration gives

$$\tilde{Q}_{int} = -15,662 \text{ J/mol}$$

The minus sign indicates that heat must be removed from the gas stream.

## 6.3.1.2 Constant pressure with phase change

When we start heating a substance at constant pressure, a typical variation in temperature as a function of time is given in Figure 6.3.



**Figure 6.3** Temperature-time relationship as the substance transforms from the  $\gamma$ -phase to  $\sigma$ -phase.

Let  $T_{ref}$  be the temperature at which phase change from the  $\gamma$ -phase to the  $\sigma$ -phase, or vice versa, takes place. If we choose the  $\gamma$ -phase enthalpy as zero at the reference temperature, then enthalpies of the  $\sigma$ - and  $\gamma$ -phases at any given temperature  $T$  are given as

$$\hat{H} = \begin{cases} \int_{T_{ref}}^T (\hat{C}_P)_\sigma dT & \sigma - \text{phase} \\ -\hat{\lambda} - \int_T^{T_{ref}} (\hat{C}_P)_\gamma dT & \gamma - \text{phase} \end{cases} \quad (6.3-21)$$

where  $\hat{\lambda} = \hat{H}_\sigma - \hat{H}_\gamma$  at the reference temperature.

**Example 6.4** One way of cooling a can of coke on a hot summer day is to wrap a piece of wet cloth around the can and expose it to a gentle breeze. Calculate the steady-state temperature of the can if the air temperature is  $35^\circ\text{C}$ .

**Solution****Assumptions**

1. Steady-state conditions prevail.
2. Ideal gas behavior.

**Analysis**

*System: Wet cloth and the coke can*

*The inventory rate equation for energy becomes*

$$\text{Rate of energy in} = \text{Rate of energy out} \quad (1)$$

*Let the steady-state temperature of the cloth and that of coke be  $T_w$ . The rate of energy entering the system is given by*

$$\text{Rate of energy in} = A_H \langle h \rangle (T_\infty - T_w) \quad (2)$$

*in which  $A_H$  and  $T_\infty$  represent the heat transfer area and air temperature, respectively. On the other hand, the rate of energy leaving the system is expressed in the form*

$$\text{Rate of energy out} = \dot{n}_A \left[ \tilde{\lambda}_A + (\tilde{C}_P)_A (T_\infty - T_w) \right] \quad (3)$$

*where  $\dot{n}_A$  represents the rate of moles of water, i.e., species  $A$ , evaporated and is given by*

$$\dot{n}_A = A_M \langle k_c \rangle (c_{A_w} - c_{A_\infty}) \quad (4)$$

*in which  $A_M$  represents the mass transfer area. Substitution of Eqs. (2), (3) and (4) into Eq. (1) and using*

$$A_H = A_M$$

$$c_{A_\infty} \simeq 0$$

$$\tilde{\lambda}_A \gg (\tilde{C}_P)_A (T_\infty - T_w)$$

*gives*

$$T_\infty - T_w = c_{A_w} \tilde{\lambda}_A \left( \frac{\langle k_c \rangle}{\langle h \rangle} \right) \quad (5)$$

*The ratio  $\langle k_c \rangle / \langle h \rangle$  can be estimated by the use of the Chilton-Colburn analogy, i.e.,  $j_H = j_M$ , as*

$$\frac{\text{St}_H}{\text{St}_M} = \left( \frac{\text{Sc}}{\text{Pr}} \right)^{2/3} \Rightarrow \frac{\langle k_c \rangle}{\langle h \rangle} = \frac{1}{\rho \hat{C}_P} \left( \frac{\text{Pr}}{\text{Sc}} \right)^{2/3} \quad (6)$$

*The use of Eq. (6) in Eq. (5) yields*

$$T_\infty - T_w = \frac{c_{A_w} \tilde{\lambda}_A}{(\rho \hat{C}_P)_B} \left( \frac{\text{Pr}}{\text{Sc}} \right)_B^{2/3} \quad (7)$$

*where the properties  $\rho$ ,  $\hat{C}_P$ , Pr and Sc belong to air, species  $B$ . The concentration of species  $A$  at the interface,  $c_{A_w}$ , is given by*

$$c_{A_w} = \frac{P_A^{\text{sat}}}{\mathcal{R} T_w} \quad (8)$$

It should be remembered that the quantities  $c_{A_w}$  and  $\tilde{\lambda}_A$  must be evaluated at  $T_w$ , whereas  $\rho_B$ ,  $\hat{C}_{P_B}$ ,  $\text{Pr}_B$  and  $\text{Sc}_B$  must be evaluated at  $T_f = (T_w + T_\infty)/2$ . Since  $T_w$  is unknown, a trial-and-error procedure will be used in order to determine  $T_w$  as follows:

**Step 1:** Assume  $T_w = 15^\circ\text{C}$

**Step 2:** Determine the physical properties:

$$\text{For water at } 15^\circ\text{C (288 K)} : \begin{cases} P_A^{\text{sat}} = 0.01703 \text{ bar} \\ \tilde{\lambda}_A = 2466 \times 18 = 44,388 \text{ kJ/kmol} \end{cases}$$

The saturation concentration is

$$c_{A_w} = \frac{P_A^{\text{sat}}}{\mathcal{R}T_w} = \frac{0.01703}{(8.314 \times 10^{-2})(15 + 273)} = 7.11 \times 10^{-4} \text{ kmol/m}^3$$

The film temperature is  $T_f = (35 + 15)/2 = 25^\circ\text{C}$ .

$$\text{For air at } 25^\circ\text{C (298 K)} : \begin{cases} \rho = 1.1845 \text{ kg/m}^3 \\ \nu = 15.54 \times 10^{-6} \text{ m}^2/\text{s} \\ \hat{C}_P = 1.005 \text{ kJ/kg}\cdot\text{K} \\ \text{Pr} = 0.712 \end{cases}$$

The diffusion coefficient of water in air is

$$\mathcal{D}_{AB} = (2.88 \times 10^{-5}) \left( \frac{298}{313} \right)^{3/2} = 2.68 \times 10^{-5} \text{ m}^2/\text{s}$$

The Schmidt number is

$$\begin{aligned} \text{Sc} &= \frac{\nu}{\mathcal{D}_{AB}} \\ &= \frac{15.54 \times 10^{-6}}{2.68 \times 10^{-5}} = 0.58 \end{aligned}$$

**Step 3:** Substitute the values into Eq. (7) and check whether the right and left sides are equal to each other:

$$T_\infty - T_w = 35 - 15 = 20$$

$$\frac{c_{A_w} \tilde{\lambda}_A}{(\rho \hat{C}_P)_B} \left( \frac{\text{Pr}}{\text{Sc}} \right)_B^{2/3} = \frac{(7.11 \times 10^{-4})(44,388)}{(1.1845)(1.005)} \left( \frac{0.712}{0.58} \right)^{2/3} = 30.4$$

Since the left- and right-hand sides of Eq. (7) are quite different from each other, another value of  $T_w$  should be assumed.

Assume  $T_w = 11^\circ\text{C}$

$$\text{For water at } 11^\circ\text{C (284 K)} : \begin{cases} P_A^{\text{sat}} = 0.01308 \text{ bar} \\ \tilde{\lambda}_A = 2475.4 \times 18 = 44,557 \text{ kJ/kmol} \end{cases}$$

The saturation concentration is

$$\begin{aligned} c_{A_w} &= \frac{P_A^{\text{sat}}}{R T_w} \\ &= \frac{0.01308}{(8.314 \times 10^{-2})(11 + 273)} = 5.54 \times 10^{-4} \text{ kmol/m}^3 \end{aligned}$$

The film temperature is  $T_f = (35 + 11)/2 = 23^\circ\text{C}$ .

$$\text{For air at } 23^\circ\text{C (296 K)} : \begin{cases} \rho = 1.1926 \text{ kg/m}^3 \\ \nu = 15.36 \times 10^{-6} \text{ m}^2/\text{s} \\ \hat{C}_P = 1.005 \text{ kJ/kg}\cdot\text{K} \\ \text{Pr} = 0.713 \end{cases}$$

The diffusion coefficient of water in air is

$$D_{AB} = (2.88 \times 10^{-5}) \left( \frac{296}{313} \right)^{3/2} = 2.65 \times 10^{-5} \text{ m}^2/\text{s}$$

The Schmidt number is

$$\begin{aligned} \text{Sc} &= \frac{\nu}{D_{AB}} \\ &= \frac{15.36 \times 10^{-6}}{2.65 \times 10^{-5}} = 0.58 \end{aligned}$$

The left- and right-hand sides of Eq. (7) now become

$$\begin{aligned} T_\infty - T_w &= 35 - 11 = 24 \\ \frac{c_{A_w} \tilde{\lambda}_A}{(\rho \hat{C}_P)_B} \left( \frac{\text{Pr}}{\text{Sc}} \right)_B^{2/3} &= \frac{(5.54 \times 10^{-4})(44,557)}{(1.1926)(1.005)} \left( \frac{0.713}{0.58} \right)^{2/3} = 23.6 \end{aligned}$$

Therefore, the steady-state temperature is  $11^\circ\text{C}$ .

**Comment:** Whenever a gas flows over a liquid, the temperature of the liquid decreases as a result of evaporation. This process is known as evaporative cooling. The resulting steady-state temperature, on the other hand, is called the wet-bulb temperature.

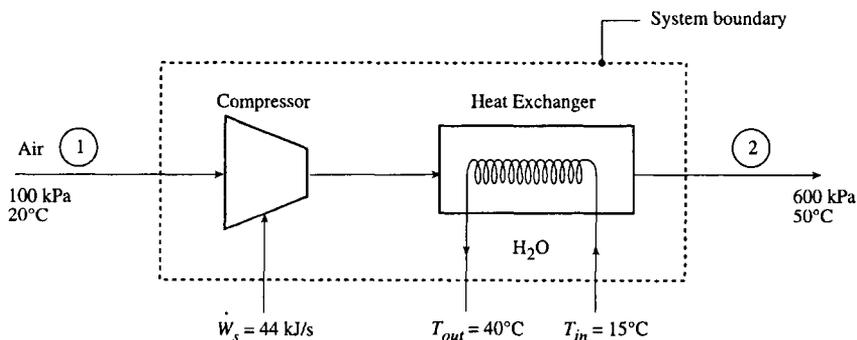
### 6.3.1.3 Variable pressure and no phase change

Enthalpy of an ideal gas is dependent only on temperature and is expressed by Eq. (6.3-18). Therefore, in problems involving ideal gases, variation in pressure has no effect on the enthalpy change. In the case of incompressible fluids, Eq. (6.3-12) reduces to

$$\hat{H} = \int_{T_{ref}}^T \hat{C}_P dT + \hat{V}(P - P_{ref}) \quad (6.3-22)$$

in which the enthalpy is taken zero at the reference temperature and pressure. At low and moderate pressures, the second term on the right-side of Eq. (6.3-22) is usually considered negligible.

**Example 6.5** *A certain process requires a steady supply of compressed air at 600 kPa and 50°C at the rate of 0.2 kg/s. For this purpose, air at ambient conditions of 100 kPa and 20°C is first compressed to 600 kPa in an adiabatic compressor, then it is fed to a heat exchanger where it is cooled to 50°C at constant pressure. As cooling medium, water is used and it enters the heat exchanger at 15°C and leaves at 40°C. Determine the mass flow rate of water if the rate of work done on the compressor is 44 kJ/s.*



## Solution

### Assumptions

1. *Steady-state conditions prevail.*
2. *Changes in kinetic and potential energies are negligible.*
3. *There is no heat loss from the heat exchanger to the surroundings.*
4. *Heat capacities of air and water remain essentially constant at the values of 1 kJ/kg·K and 4.178 kJ/kg·K, respectively.*

**Analysis**

*System: Compressor and heat exchanger*

*Conservation of total mass, Eq. (6.2-1), reduces to*

$$\dot{m}_1 = \dot{m}_2 = \dot{m} \quad (1)$$

*Therefore, Eq. (6.3-15) becomes*

$$\dot{m}_{air}(\hat{H}_1 - \hat{H}_2)_{air} - \dot{Q}_{int} + \dot{W}_s = 0 \quad (2)$$

*in which the enthalpy change of the air and the interphase heat transfer rate are given by*

$$(\hat{H}_1 - \hat{H}_2)_{air} = (\hat{C}_P)_{air}(T_1 - T_2)_{air} \quad (3)$$

$$\dot{Q}_{int} = (\dot{m}\hat{C}_P)_{H_2O}(T_{out} - T_{in})_{H_2O} \quad (4)$$

*Substitution of Eqs. (3) and (4) into Eq. (2) and rearrangement gives*

$$\begin{aligned} \dot{m}_{H_2O} &= \frac{(\dot{m}\hat{C}_P)_{air}(T_1 - T_2)_{air} + \dot{W}_s}{(\hat{C}_P)_{H_2O}(T_{out} - T_{in})_{H_2O}} \\ &= \frac{(0.2)(1)(20 - 50) + 44}{(4.178)(40 - 15)} = 0.364 \text{ kg/s} \end{aligned} \quad (5)$$

**Comment:** *Defining of a system plays a crucial role in the solution of the problem. Note that there is no need to find out the temperature and pressure at the exit of the compressor. If, however, one chooses the compressor and heat exchanger as two separate systems, then the pressure and temperature at the exit of the compressor must be calculated.*

## 6.3.2 Energy Equation With Chemical Reaction

### 6.3.2.1 Thermochemistry

Thermochemistry deals with the changes of energy in chemical reactions. The difference between the enthalpy of one mole of a pure compound and the total enthalpy of the elements from which it is composed is called the *heat of formation*,  $\Delta\hat{H}_f$ , of the compound. The *standard heat of formation*,  $\Delta\hat{H}_f^\circ$ , is the heat of formation when both the compound and its elements are at standard conditions as shown in Figure 6.4. The superscript  $^\circ$  implies the *standard state*. Since enthalpy is a state function, it is immaterial whether or not the reaction could take place at standard conditions.

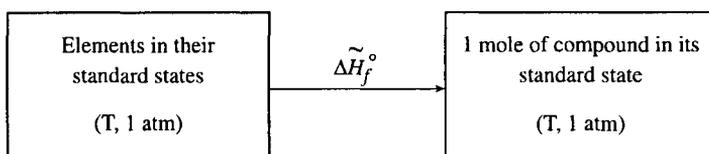
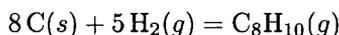


Figure 6.4 Calculation of the standard heat of formation,  $\Delta\tilde{H}_f^\circ$ .

The standard state is usually taken as the stable form of the element or compound at the temperature of interest,  $T$ , and under 1 atm (1.013 bar). Therefore, the word *standard* refers not to any particular temperature, but to unit pressure of 1 atm. The elements in their standard states are taken as the reference state and are assigned an enthalpy of zero. The standard heat of formation of many compounds are usually tabulated at 25°C and can readily be found in the Perry's Chemical Engineers' Handbook (1997) and thermodynamics textbooks. For example, the standard heat of formation of ethyl benzene,  $C_8H_{10}$ , in the gaseous state is 29,790 J/mol at 298 K. Consider the formation of ethyl benzene from its elements by the reaction



The standard heat of formation is given by

$$(\Delta\tilde{H}_f^\circ)_{C_8H_{10}} = \tilde{H}_{C_8H_{10}}^\circ - 8\tilde{H}_C^\circ - 5\tilde{H}_{H_2}^\circ = 29,790 \text{ J/mol}$$

Since  $\tilde{H}_C^\circ = \tilde{H}_{H_2}^\circ = 0$ , it follows that

$$(\Delta\tilde{H}_f^\circ)_{C_8H_{10}} = \tilde{H}_{C_8H_{10}}^\circ = 29,790 \text{ J/mol}$$

It is possible to generalize this result in the form

$$\left(\Delta\tilde{H}_f^\circ\right)_i = \tilde{H}_i^\circ \quad (6.3-23)$$

The standard heat of formation of a substance is just the standard heat of reaction in which one mole of it is formed from elementary species. Therefore, the *standard heat of reaction*,  $\Delta H_{rxn}^\circ$ , is the difference between the total enthalpy of the pure product mixture and that of the pure reactant mixture at standard conditions as shown in Figure 6.5.

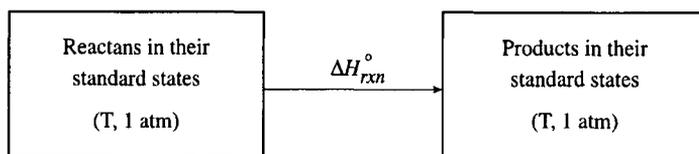


Figure 6.5 Calculation of the standard heat of reaction,  $\Delta H_{rxn}^\circ$ .

The standard heat of reaction can be calculated as

$$\Delta H_{rxn}^o = \sum_i \alpha_i \tilde{H}_i^o \quad (6.3-24)$$

Substitution of Eq. (6.3-23) into Eq. (6.3-24) gives

$$\Delta H_{rxn}^o = \sum_i \alpha_i (\Delta \tilde{H}_f^o)_i \quad (6.3-25)$$

Note that the standard heat of formation of an element is zero.

If heat is evolved in the reaction, the reaction is called *exothermic*. If heat is absorbed, the reaction is called *endothermic*. Therefore,

$$\Delta H_{rxn}^o \begin{cases} > 0 & \text{for an endothermic reaction} \\ < 0 & \text{for an exothermic reaction} \end{cases} \quad (6.3-26)$$

If the standard heat of reaction is known at 298 K, then its value at any other temperature can be found as follows: The variation of the standard heat of reaction as a function of temperature under constant pressure is given by

$$d\Delta H_{rxn}^o = \left( \frac{\partial \Delta H_{rxn}^o}{\partial T} \right)_{P=1} dT \quad (6.3-27)$$

The term  $(\partial \Delta H_{rxn}^o / \partial T)_P$  can be expressed as

$$\begin{aligned} \left( \frac{\partial \Delta H_{rxn}^o}{\partial T} \right)_P &= \frac{\partial}{\partial T} \left( \sum_i \alpha_i \tilde{H}_i^o \right) = \sum_i \alpha_i \left( \frac{\partial \tilde{H}_i^o}{\partial T} \right)_P \\ &= \sum_i \alpha_i \tilde{C}_{P_i}^o = \Delta \tilde{C}_P^o \end{aligned} \quad (6.3-28)$$

Substitution of Eq. (6.3-28) into Eq. (6.3-27) and integration gives

$$\boxed{\Delta H_{rxn}^o(T) = \Delta H_{rxn}^o(T = 298 \text{ K}) + \int_{298}^T \Delta \tilde{C}_P^o dT} \quad (6.3-29)$$

### 6.3.2.2 Energy balance around a continuous stirred tank reactor

An energy balance in a continuous stirred tank reactor (CSTR) with the following assumptions is a good example to the energy balance with chemical reaction:

1. Steady-state conditions prevail.
2. Stirring does not contribute much energy to the system, i.e.,  $\dot{W}_s \simeq 0$ .
3. Volume of the system is constant, i.e., inlet and outlet volumetric flow rates are equal.

4. As a result of perfect mixing, temperature and concentration of the system are uniform, i.e.,  $c_{out} = c_{sys}$  and  $T_{out} = T_{sys}$ .
5. Changes in kinetic and potential energies are negligible.

Since chemical reaction is involved in this case, it is more appropriate to work on molar basis. Therefore, Eq. (6.3-17) simplifies to

$$(\tilde{H} \dot{n})_{in} - (\tilde{H} \dot{n})_{out} + \dot{Q}_{int} = 0 \quad (6.3-30)$$

Any molar quantity of a mixture,  $\tilde{\psi}$ , can be expressed in terms of partial molar quantities<sup>2</sup>,  $\bar{\psi}_i$ , as

$$\tilde{\psi} = \sum_i x_i \bar{\psi}_i \quad (6.3-31)$$

Multiplication of Eq. (6.3-31) by molar flow rate,  $\dot{n}$ , gives

$$\tilde{\psi} \dot{n} = \sum_i \dot{n}_i \bar{\psi}_i \quad (6.3-32)$$

Therefore, Eq. (6.3-30) is expressed as

$$\left[ \sum_i \dot{n}_i \bar{H}_i(T_{in}) \right]_{in} - \left[ \sum_i \dot{n}_i \bar{H}_i(T) \right]_{out} + \dot{Q}_{int} = 0 \quad (6.3-33)$$

On the other hand, macroscopic mole balance for species  $i$ , Eq. (6.1-6), is

$$(\dot{n}_i)_{in} - (\dot{n}_i)_{out} + V_{sys} \sum_j \alpha_{ij} r_j = 0 \quad (6.3-34)$$

Multiplication of Eq. (6.3-34) by  $\bar{H}_i(T)$  and summation over all species gives

$$\left[ \sum_i \dot{n}_i \bar{H}_i(T) \right]_{in} - \left[ \sum_i \dot{n}_i \bar{H}_i(T) \right]_{out} - V_{sys} \sum_j r_j (-\Delta H_{rxn,j}) = 0 \quad (6.3-35)$$

where the heat of reaction is defined by

$$\Delta H_{rxn,j} = \sum_i \alpha_{ij} \bar{H}_i(T) \quad (6.3-36)$$

Subtraction of Eq. (6.3-35) from Eq. (6.3-33) yields

$$\left\{ \sum_i \dot{n}_i [\bar{H}_i(T_{in}) - \bar{H}_i(T)] \right\}_{in} + \dot{Q}_{int} + V_{sys} \sum_j r_j (-\Delta H_{rxn,j}) = 0 \quad (6.3-37)$$

---

<sup>2</sup>Partial molar quantities, unlike molar quantities of pure substances, depend also on the composition of the mixture.

Dividing Eq. (6.3-37) by the volumetric flow rate,  $Q$ , gives

$$\left\{ \sum_i c_i [\bar{H}_i(T_{in}) - \bar{H}_i(T)] \right\}_{in} + \frac{\dot{Q}_{int}}{Q} + \tau \sum_j r_j (-\Delta H_{rxn,j}) = 0 \quad (6.3-38)$$

where  $\tau$  is the residence time defined by

$$\tau = \frac{V_{sys}}{Q} \quad (6.3-39)$$

Partial molar heat capacity of species  $i$ ,  $\bar{C}_{P_i}$ , is related to the partial molar enthalpy as

$$\bar{C}_{P_i} = \left( \frac{\partial \bar{H}_i}{\partial T} \right)_P \quad (6.3-40)$$

If  $\bar{C}_{P_i}$  is independent of temperature, then integration of Eq. (6.3-40) gives

$$\bar{H}_i(T_{in}) - \bar{H}_i(T) = \bar{C}_{P_i}(T_{in} - T) \quad (6.3-41)$$

Substitution of Eqs. (6.3-40) and (6.3-41) into Eq. (6.3-38) yields

$$\boxed{(C_P)_{in}(T_{in} - T) + \frac{\dot{Q}_{int}}{Q} + \tau \sum_j r_j (-\Delta H_{rxn,j}) = 0} \quad (6.3-42)$$

where

$$(C_P)_{in} = \sum_i (c_i)_{in} \bar{C}_{P_i} \quad (6.3-43)$$

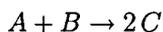
It should be noted that the reaction rate expression in Eq. (6.3-42) contains a reaction rate constant,  $k$ , expressed in the form

$$k = A e^{-\varepsilon/RT} \quad (6.3-44)$$

Therefore, Eq. (6.3-42) is highly nonlinear in temperature.

Once the feed composition, stoichiometry and order of the chemical reaction, heat of reaction, and reaction rate constant are known, conservation statements for chemical species and energy contain five variables, namely, inlet temperature,  $T_{in}$ , extent of reaction,  $\xi$ , reactor temperature,  $T$ , residence time,  $\tau$ , and interphase heat transfer rate,  $\dot{Q}_{int}$ . Therefore, three variables must be known while the remaining two can be calculated from the conservation of chemical species and energy. Among these variables  $T_{in}$  is the variable associated with the feed,  $\xi$  and  $T$  are the variables associated with the product,  $\tau$  and  $\dot{Q}_{int}$  are the variables of design.

**Example 6.6** A liquid feed to a jacketed CSTR consists of 2000 mol/m<sup>3</sup> A and 2400 mol/m<sup>3</sup> B. A second-order irreversible reaction takes place as



The rate of reaction is given by

$$r = k c_A c_B$$

where the reaction rate constant at 298 K is  $k = 8.4 \times 10^{-6} \text{ m}^3/\text{mol} \cdot \text{min}$ , and the activation energy is 50,000 J/mol. The reactor operates isothermally at 65°C. The molar heat capacity at constant pressure and the standard heat of formation of species A, B, and C at 298 K are given as follows:

Species	$\tilde{C}_P^\circ$ (J/mol.K)	$\Delta\tilde{H}_f^\circ$ (kJ/mol)
A	175	-60
B	130	-75
C	110	-90

- Calculate the residence time required to obtain 80% conversion of species A.
- What should be the volume of the reactor if species C are to be produced at a rate of 820 mol/min?
- If the feed enters the reactor at a temperature of 25°C, determine the rate of heat that must be removed from the reactor to maintain isothermal operation.
- If the heat transfer coefficient is 1050 W/m<sup>2</sup>.K and the average cooling fluid temperature is 15°C, estimate the required heat transfer area

### Solution

#### Assumptions

- As a result of perfect mixing, concentrations of the species within the reactor are uniform, i.e.,  $(c_i)_{out} = (c_i)_{sys}$ .
- Solution nonidealities are negligible, i.e.,  $\bar{C}_{P_i} = \tilde{C}_{P_i}$ ;  $\Delta H_{rxn} = \Delta H_{rxn}^\circ$
- There is no heat loss from the reactor.

#### Analysis

System: Contents of the reactor

- Since the reactor volume is constant, the inlet and outlet volumetric flow rates are the same and equal to  $Q$ . Therefore, the inventory rate equation for conservation of species A, Eq. (6.1-7), becomes

$$Q(c_A)_{in} - Q c_{A_{sys}} - (k c_{A_{sys}} c_{B_{sys}}) V_{sys} = 0 \quad (1)$$

where  $c_{A_{sys}}$  and  $c_{B_{sys}}$  represent the molar concentrations of species  $A$  and  $B$  in the reactor, respectively. Dropping the subscript "sys" and dividing Eq. (1) by the volumetric flow rate,  $Q$ , gives

$$\tau = \frac{(c_A)_{in} - c_A}{k c_A c_B} \quad (2)$$

Using Eq. (5.3-17), the extent of reaction can be calculated as

$$\begin{aligned} \xi &= \frac{(c_A)_{in}}{(-\alpha_A)} X_A \\ &= \frac{(2000)(0.8)}{1} = 1600 \text{ mol/m}^3 \end{aligned} \quad (3)$$

Therefore, the concentrations of species  $A$ ,  $B$ , and  $C$  in the reactor are

$$c_A = (c_A)_{in} + \alpha_A \xi = 2000 - 1600 = 400 \text{ mol/m}^3 \quad (4)$$

$$c_B = (c_B)_{in} + \alpha_B \xi = 2400 - 1600 = 800 \text{ mol/m}^3 \quad (5)$$

$$c_C = (c_C)_{in} + \alpha_C \xi = (2)(1600) = 3200 \text{ mol/m}^3 \quad (6)$$

If  $k_1$  and  $k_2$  represent the rate constants at temperatures of  $T_1$  and  $T_2$ , respectively, then

$$k_2 = k_1 \exp \left[ -\frac{\mathcal{E}}{\mathcal{R}} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \right] \quad (7)$$

Therefore, the reaction rate constant at 65 °C (338 K) is

$$\begin{aligned} k &= 8.4 \times 10^{-6} \exp \left[ -\frac{50,000}{8.314} \left( \frac{1}{338} - \frac{1}{298} \right) \right] \\ &= 9.15 \times 10^{-5} \text{ m}^3/\text{mol} \cdot \text{min} \end{aligned} \quad (8)$$

Substitution of numerical values into Eq. (2) gives

$$\tau = \frac{2000 - 400}{(9.15 \times 10^{-5})(400)(800)} = 54.6 \text{ min}$$

b) The reactor volume,  $V$ , is given by

$$V = \tau Q$$

The volumetric flow rate can be determined from the production rate of species  $C$ , i.e.,

$$c_C Q = 820 \quad \Rightarrow \quad Q = \frac{820}{3200} = 0.256 \text{ m}^3/\text{min}$$

Hence, the reactor volume is

$$V = (54.6)(0.256) = 14 \text{ m}^3$$

c) For this problem, Eq. (6.3-42) simplifies to

$$\dot{Q}_{int} = -Q(C_P)_{in}(T_{in} - T) - V(k c_A c_B)(-\Delta H_{rxn}^{\circ}) \quad (9)$$

The standard heat of reaction at 298 K is

$$\begin{aligned} \Delta H_{rxn}^{\circ}(298) &= \sum_i \alpha_i (\Delta \tilde{H}_f^{\circ})_i \\ &= (-1)(-60) + (-1)(-75) + (2)(-90) = -45 \text{ kJ/mol} \end{aligned}$$

The standard heat of reaction at 338 K is given by Eq. (6.3-29)

$$\Delta H_{rxn}^{\circ}(338) = \Delta H_{rxn}^{\circ}(298 \text{ K}) + \int_{298}^{338} \Delta \tilde{C}_P^{\circ} dT$$

where

$$\begin{aligned} \Delta \tilde{C}_P^{\circ} &= \sum_i \alpha_i \tilde{C}_{P_i}^{\circ} \\ &= (-1)(175) + (-1)(130) + (2)(110) = -85 \text{ J/mol} \cdot \text{K} \end{aligned}$$

Hence

$$\Delta H_{rxn}^{\circ}(338) = -45,000 + (-85)(338 - 298) = -48,400 \text{ J/mol}$$

On the other hand, the use of Eq. (6.3-43) gives

$$\begin{aligned} (C_P)_{in} &= \sum_i (c_i)_{in} \tilde{C}_{P_i}^{\circ} \\ &= (2000)(175) + (2400)(130) = 662,000 \text{ J/m}^3 \cdot \text{K} \end{aligned}$$

Therefore, substitution of the numerical values into Eq. (9) yields

$$\begin{aligned} \dot{Q}_{int} &= -(0.256)(662,000)(25 - 65) \\ &\quad - (14) [(9.15 \times 10^{-5})(400)(800)] (48,400) = -13 \times 10^6 \text{ J/min} \end{aligned}$$

The minus sign indicates that the system, i.e., reactor, loses energy to the surroundings.

d) The application of Newton's law of cooling gives

$$\left| \dot{Q}_{int} \right| = A_H \langle h \rangle (T_{reactor} - T_{coolant})$$

or,

$$A_H = \frac{13 \times 10^6}{(1050)(65 - 15)(60)} = 4.1 \text{ m}^2$$

## NOTATION

$A$	area, $\text{m}^2$
$A_H$	heat transfer area, $\text{m}^2$
$A_M$	mass transfer area, $\text{m}^2$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ}/\text{kg}\cdot\text{K}$
$c$	concentration, $\text{kmol}/\text{m}^3$
$D_{AB}$	diffusion coefficient for system $A$ - $B$ , $\text{m}^2/\text{s}$
$E$	total energy, $\text{J}$
$E_K$	kinetic energy, $\text{J}$
$E_P$	potential energy, $\text{J}$
$\dot{E}$	rate of energy, $\text{J}/\text{s}$
$\mathcal{E}$	activation energy, $\text{J}/\text{mol}$
$g$	acceleration of gravity, $\text{m}/\text{s}^2$
$H$	enthalpy, $\text{J}$
$h$	elevation, $\text{m}$
$k$	reaction rate constant
$k_c$	mass transfer coefficient, $\text{m}/\text{s}$
$\dot{m}$	mass flow rate, $\text{kg}/\text{s}$
$\mathcal{M}$	molecular weight, $\text{kg}/\text{kmol}$
$\dot{n}$	molar flow rate, $\text{kmol}/\text{s}$
$P$	pressure, $\text{Pa}$
$\dot{Q}$	heat transfer rate, $\text{W}$
$Q$	volumetric flow rate, $\text{m}^3/\text{s}$
$r$	rate of a chemical reaction, $\text{kmol}/\text{m}^3\cdot\text{s}$
$\mathcal{R}$	gas constant, $\text{J}/\text{mol}\cdot\text{K}$
$T$	temperature, $^\circ\text{C}$ or $\text{K}$
$t$	time, $\text{s}$
$U$	internal energy, $\text{J}$
$V$	volume, $\text{m}^3$
$v$	velocity, $\text{m}/\text{s}$
$\dot{W}$	rate of work, $\text{W}$
$\dot{W}_s$	rate of shaft work, $\text{W}$
$X$	fractional conversion
$x_i$	mole fraction of species $i$
$\alpha_i$	stoichiometric coefficient of species $i$
$\alpha_{ij}$	stoichiometric coefficient of $i^{\text{th}}$ species in the $j^{\text{th}}$ reaction
$\beta$	coefficient of volume expansion, Eq. (6.3-13), $\text{K}^{-1}$
$\Delta$	difference
$\Delta\tilde{H}_f$	heat of formation, $\text{J}/\text{mol}$
$\Delta H_{rxn}$	heat of reaction, $\text{J}$
$\lambda$	latent heat of vaporization, $\text{J}$
$\mu$	viscosity, $\text{kg}/\text{m}\cdot\text{s}$

$\nu$	kinematic viscosity, $\text{m}^2/\text{s}$
$\xi$	intensive extent of a reaction, $\text{kmol}/\text{m}^3$
$\rho$	density, $\text{kg}/\text{m}^3$
$\tau$	residence time, s

**Overlines**

$\sim$	per mole
$\hat{\phantom{a}}$	per unit mass
$\text{--}$	partial molar

**Bracket**

$\langle a \rangle$	average value of $a$
---------------------	----------------------

**Superscripts**

$o$	standard state
$sat$	saturation

**Subscripts**

$A, B$	species in binary systems
$ch$	characteristic
$f$	film
$i$	species in multicomponent systems
$in$	inlet
$int$	interphase
$j$	reaction number
$out$	out
$ref$	reference
$sys$	system

**Dimensionless Numbers**

$Pr$	Prandtl number
$Sc$	Schmidt number
$St_H$	Stanton number for heat transfer
$St_M$	Stanton number for mass transfer

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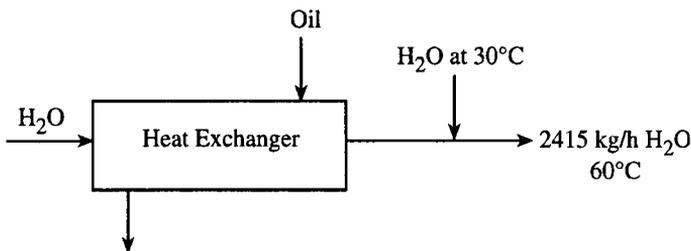
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## PROBLEMS

6.1 2520 kg/h of oil is to be cooled from 180 °C to 110 °C in a countercurrent heat exchanger as shown in the figure below. Calculate the flow rate of water passing through the heat exchanger for the following cases:

a) The cooling water, which enters the heat exchanger at 15 °C, is mixed with water at 30 °C at the exit of the heat exchanger to obtain 2415 kg/h of process water at 60 °C to be used in another location of the plant.

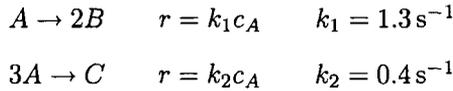
b) The cooling water, which enters the heat exchanger at 30 °C, is mixed with water at 30 °C at the exit of the heat exchanger to obtain 2415 kg/h of process water at 60 °C to be used in another location of the plant.



Assume that oil and water have constant heat capacities of 2.3 and 4.2 kJ/kg.K, respectively.

(Answer: a) 1610 kg/h)

**6.2** The following parallel reactions take place in an isothermal, constant-volume CSTR:



Pure  $\mathcal{A}$  is fed to the reactor at a concentration of 350 mol/m<sup>3</sup>.

a) Determine the residence time required to achieve 85% conversion of species  $\mathcal{A}$  under steady conditions.

b) Determine the concentrations of species  $\mathcal{B}$  and  $\mathcal{C}$ .

(Answer: a)  $\tau = 2.27 \text{ s}$  b)  $c_B = 309.9 \text{ mol/m}^3$ ,  $c_C = 47.7 \text{ mol/m}^3$ )

**6.3** Species  $\mathcal{A}$  undergoes the following consecutive first-order reactions in the liquid phase in an isothermal, constant-volume CSTR:



where  $k_1 = 1.5 \text{ s}^{-1}$  and  $k_2 = 0.8 \text{ s}^{-1}$ . If the feed to the reactor consists of pure  $\mathcal{A}$ , determine the residence time required to maximize the concentration of species  $\mathcal{B}$  under steady conditions.

(Answer: 0.913 s)

**6.4** An isomerization reaction



takes place in a constant-volume CSTR. The feed to the reactor consists of pure  $\mathcal{A}$ . The rate of the reaction is given by

$$r = k_1 c_A - k_2 c_B$$

For the maximum conversion of species  $\mathcal{A}$  at a given residence time, determine the reactor temperature.

$$\left( \text{Answer: } T = \frac{\mathcal{E}_2/\mathcal{R}}{\ln \{A_2 \tau [(\mathcal{E}_2/\mathcal{E}_1) - 1]\}} \right)$$

**6.5** Two electronic components ( $k = 190 \text{ W/m.K}$ ) are to be cooled by passing 0.2 m<sup>3</sup>/s of air at 25 °C between them. To enhance the rate of heat loss, it is proposed to install equally spaced rectangular aluminum plates between the electronic components as shown in Figure 6.6.

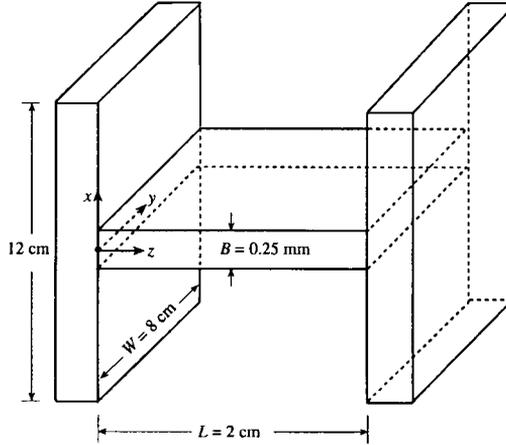


Figure 6.6 Schematic diagram for Problem 6.5.

The rate of heat loss from the electronic component at the left, i.e.,  $z = 0$ , must be 500 W and the temperature should not exceed  $80^\circ\text{C}$ ; while the other component must dissipate 2 kW with a maximum allowable temperature of  $90^\circ\text{C}$ . Determine the number of the plates that must be placed per cm between the electronic components (Use the temperature distribution given in Problem 4.6).

(Answer: One possible solution is 10 fins per cm)

6.6 As shown in Example 6.4, the wet-bulb temperature can be calculated from

$$T_\infty - T_w = \frac{c_{A_w} \tilde{\lambda}_A}{(\rho \hat{C}_P)_B} \left( \frac{\text{Pr}}{\text{Sc}} \right)_B^{2/3} \quad (1)$$

by a trial-and-error procedure because both  $c_{A_w}$  and  $\tilde{\lambda}_A$  must be evaluated at  $T_w$ , whereas  $\rho_B$ ,  $\hat{C}_{PB}$ ,  $\text{Pr}_B$  and  $\text{Sc}_B$  must be evaluated at the film temperature. In engineering applications, an approximate equation used to estimate the wet-bulb temperature is given by

$$T_w^2 - T_\infty T_w + \phi = 0 \quad (2)$$

where

$$\phi = \frac{P_A^{\text{sat}} T_\infty \mathcal{M}_A \tilde{\lambda}_A}{P_\infty \mathcal{M}_B \hat{C}_P} \left( \frac{\text{Pr}}{\text{Sc}} \right)_B^{2/3} \quad (3)$$

Develop Eq. (2) from Eq. (1) and indicate the assumptions involved in the derivation.

6.7 An exothermic, first-order, irreversible reaction



takes place in a constant-volume, jacketed CSTR.

a) Show that the conservation equations for chemical species  $\mathcal{A}$  and energy take the form

$$Q[(c_A)_{in} - c_A] - k c_A V = 0 \quad (1)$$

$$[Q(C_P)_{in} + A_H \langle h \rangle] (T_m - T) + V k c_A (-\Delta H_{rxn}) = 0 \quad (2)$$

where  $T_m$  is a weighted mean temperature defined by

$$T_m = \frac{Q(C_P)_{in} T_{in} + A_H \langle h \rangle T_c}{Q(C_P)_{in} + A_H \langle h \rangle} \quad (3)$$

in which  $\langle h \rangle$  is the average heat transfer coefficient,  $T_c$  is the cooling fluid temperature,  $A_H$  is the heat transfer area.

b) Show that the elimination of  $c_A$  between Eqs. (1) and (2) leads to

$$[Q(C_P)_{in} + A_H \langle h \rangle] (T_m - T) + \frac{k Q V (c_A)_{in}}{Q + k V} (-\Delta H_{rxn}) = 0 \quad (4)$$

c) In terms of the following dimensionless quantities

$$\begin{aligned} \theta &= \frac{\mathcal{E}}{\mathcal{R}} \left( \frac{1}{T_m} - \frac{1}{T} \right) \\ A_m &= A e^{-\mathcal{E}/\mathcal{R}T_m} \\ \chi &= \frac{[Q(C_P)_{in} + A_H \langle h \rangle] T_m}{Q(c_A)_{in} (-\Delta H_{rxn})} \\ \beta &= \frac{\mathcal{R} T_m}{\mathcal{E}} (1 + \chi) \\ \frac{1}{\gamma} &= \frac{\mathcal{R} T_m Q \chi}{\mathcal{E} V A_m} \end{aligned}$$

show that Eq. (4) takes the form

$$e^\theta = \frac{\theta}{\gamma(1 - \beta\theta)} \quad (5)$$

d) To determine the roots of Eq. (5) for given values of  $\gamma$  and  $\beta$ , it is more convenient to rearrange Eq. (5) in the form

$$F(\theta) = \ln \left[ \frac{\theta}{\gamma(1 - \beta\theta)} \right] \quad (6)$$

Examine the behavior of the function in Eq. (6) and conclude that

- At least one steady-state solution exists when  $\beta \geq 0.25$ ,

- Two steady-state solutions exist when  $\beta < 0.25$  and  $\gamma = \gamma_{\min} < \gamma_{\max}$  or,  $\gamma_{\min} < \gamma = \gamma_{\max}$ ,
- Three steady-state solutions exist when  $\beta < 0.25$  and  $\gamma_{\min} < \gamma < \gamma_{\max}$ ,

where  $\gamma_{\min}$  and  $\gamma_{\max}$  are defined by

$$\gamma_{\min} = \left( \frac{1 + \sqrt{1 - 4\beta}}{2\beta} \right)^2 \exp \left[ - \left( \frac{1 + \sqrt{1 - 4\beta}}{2\beta} \right) \right] \quad (7)$$

$$\gamma_{\max} = \left( \frac{2}{1 + \sqrt{1 - 4\beta}} \right)^2 \exp \left[ - \left( \frac{2}{1 + \sqrt{1 - 4\beta}} \right) \right] \quad (8)$$

The existence of more than one steady-state solution is referred to as multiple steady-states. For more detailed information on this problem see Kauschus *et al.* (1978).

# Chapter 7

## Unsteady-State Macroscopic Balances

In this chapter we will consider unsteady-state transfer processes between the phases by assuming no gradients within each phase. Since the dependent variables, such as temperature and concentration, are considered uniform within a given phase, the resulting macroscopic balances are ordinary differential equations in time.

The basic steps in the development of unsteady macroscopic balances are similar to those for steady-state balances given in Chapter 6. These can be briefly summarized as follows:

- Define your system.
- If possible, draw a simple sketch.
- List the assumptions.
- Write down the inventory rate equation for each of the basic concepts relevant to the problem at hand.
- Use engineering correlations to evaluate the transfer coefficients.
- Write down the initial conditions: The number of initial conditions must be equal to the sum of the order of differential equations written for the system.
- Solve the ordinary differential equations.

## 7.1 APPROXIMATIONS USED IN MODELLING OF UNSTEADY-STATE PROCESSES

### 7.1.1 Pseudo-Steady-State Approximation

As stated in Chapter 1, the general inventory rate equation can be expressed in the form

$$\left( \begin{array}{c} \text{Rate of} \\ \text{input} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{output} \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{generation} \end{array} \right) = \left( \begin{array}{c} \text{Rate of} \\ \text{accumulation} \end{array} \right) \quad (7.1-1)$$

Remember that the molecular and convective fluxes constitute the input and output terms. Among the terms appearing on the left side of Eq. (7.1-1), molecular transport is the slowest process. Therefore, in a given unsteady-state process, the term on the right side of Eq. (7.1-1) may be considered negligible if

$$\left( \begin{array}{c} \text{Rate of} \\ \text{molecular transport} \end{array} \right) \gg \left( \begin{array}{c} \text{Rate of} \\ \text{accumulation} \end{array} \right) \quad (7.1-2)$$

or,

$$(\text{Diffusivity}) \left( \begin{array}{c} \text{Gradient of} \\ \text{Quantity/Volume} \end{array} \right) (\text{Area}) \gg \frac{\text{Difference in quantity}}{\text{Characteristic time}} \quad (7.1-3)$$

Note that the "Gradient of Quantity/Volume" is expressed in the form

$$\text{Gradient of Quantity/Volume} = \frac{\text{Difference in Quantity/Volume}}{\text{Characteristic length}} \quad (7.1-4)$$

On the other hand, volume and area are expressed in terms of characteristic length as

$$\text{Volume} = (\text{Characteristic length})^3 \quad (7.1-5)$$

$$\text{Area} = (\text{Characteristic length})^2 \quad (7.1-6)$$

Substitution of Eqs. (7.1-4)-(7.1-6) into Eq. (7.1-3) gives

$$\boxed{\frac{(\text{Diffusivity})(\text{Characteristic time})}{(\text{Characteristic length})^2} \gg 1} \quad (7.1-7)$$

In engineering analysis, the neglect of the unsteady-state term is often referred to as the *pseudo-steady-state* (or, *quasi-steady-state*) approximation. However, it should be noted that the pseudo-steady-state approximation is only valid if the constraint given by Eq. (7.1-7) is satisfied.

**Example 7.1** We are testing a 2 cm thick insulating material. The density, thermal conductivity, and heat capacity of the insulating material are  $255 \text{ kg/m}^3$ ,  $0.07 \text{ W/m}\cdot\text{K}$ , and  $1300 \text{ J/kg}\cdot\text{K}$ , respectively. If our experiments take 10 min, is it possible to assume pseudo-steady-state behavior?

### Solution

For the pseudo-steady-state approximation to be valid, Eq. (7.1-7) must be satisfied, i.e.,

$$\frac{\alpha t_{ch}}{L_{ch}^2} \gg 1$$

The thermal diffusivity,  $\alpha$ , of the insulating material is

$$\begin{aligned} \alpha &= \frac{k}{\rho \hat{C}_P} \\ &= \frac{0.07}{(255)(1300)} = 2.11 \times 10^{-7} \text{ m}^2/\text{s} \end{aligned}$$

Hence,

$$\frac{\alpha t_{ch}}{L_{ch}^2} = \frac{(2.11 \times 10^{-7})(10)(60)}{(2 \times 10^{-2})^2} = 0.32 < 1$$

which indicates that we have an unsteady-state problem at hand.

### 7.1.2 No Variation of Dependent Variable Within the Phase of Interest

In engineering analysis it is customary to neglect spatial variations in either temperature or concentration within the solid. Although this approximation simplifies the mathematical problem, it is only possible under certain circumstances as will be shown in the following development.

Let us consider the transport of a quantity  $\varphi$  from the solid phase to the fluid phase through a solid-fluid interface. Under steady conditions without generation, the inventory rate equation, Eq. (1.1-1), for the interface takes the form

$$\left( \begin{array}{c} \text{Rate of transport of } \varphi \text{ from} \\ \text{the solid to the interface} \end{array} \right) = \left( \begin{array}{c} \text{Rate of transport of } \varphi \text{ from} \\ \text{the interface to the fluid} \end{array} \right) \quad (7.1-8)$$

Since the molecular flux of  $\varphi$  is dominant within the solid phase, Eq. (7.1-8) reduces to

$$\left( \begin{array}{c} \text{Molecular flux of } \varphi \text{ from} \\ \text{the solid to the interface} \end{array} \right) = \left( \begin{array}{c} \text{Flux of } \varphi \text{ from} \\ \text{the interface to the fluid} \end{array} \right) \quad (7.1-9)$$

or,

$$\left[ \left( \begin{array}{c} \text{Transport} \\ \text{property} \end{array} \right) \left( \begin{array}{c} \text{Gradient of} \\ \text{driving force} \end{array} \right) \right]_{solid} = \left[ \left( \begin{array}{c} \text{Transfer} \\ \text{coefficient} \end{array} \right) \left( \begin{array}{c} \text{Difference in} \\ \text{Quantity/Volume} \end{array} \right) \right]_{fluid} \quad (7.1-10)$$

The gradient of driving force is expressed in the form

$$\text{Gradient of driving force} = \frac{\text{Difference in driving force}}{\text{Characteristic length}} \quad (7.1-11)$$

On the other hand, "Difference in Quantity/Volume" can be expressed as

$$\left( \begin{array}{c} \text{Difference in} \\ \text{Quantity/Volume} \end{array} \right) = \left( \frac{\text{Transport property}}{\text{Diffusivity}} \right) \left( \begin{array}{c} \text{Difference in} \\ \text{driving force} \end{array} \right) \quad (7.1-12)$$

Substitution of Eqs. (7.1-11) and (7.1-12) to the left- and right-hand sides of Eq. (7.1-10), respectively, gives

$$\text{Bi} = \frac{\left( \begin{array}{c} \text{Characteristic} \\ \text{length} \end{array} \right)}{\left( \begin{array}{c} \text{Transport} \\ \text{property} \end{array} \right)_{solid}} \left[ \frac{\left( \begin{array}{c} \text{Transfer} \\ \text{coefficient} \end{array} \right) \left( \begin{array}{c} \text{Transport} \\ \text{property} \end{array} \right)}{\text{Diffusivity}} \right]_{fluid} \quad (7.1-13)$$

in which Bi designates the *Biot number* defined by

$$\text{Bi} = \frac{(\text{Difference in driving force})_{solid}}{(\text{Difference in driving force})_{fluid}} \quad (7.1-14)$$

Therefore, the Biot numbers for heat and mass transfer are defined as

$$\text{Bi}_H = \frac{\langle h \rangle L_{ch}}{k_{solid}} \quad (7.1-15)$$

$$\text{Bi}_M = \frac{\langle k_c \rangle L_{ch}}{(D_{AB})_{solid}} \quad (7.1-16)$$

It is important to distinguish the difference between the Biot and the Nusselt (or, the Sherwood) numbers. The transport properties in the Biot numbers, Eqs. (7.1-15) and (7.1-16), are referred to the solid, whereas the transport properties in the Nusselt and the Sherwood numbers, Eqs. (3.4-11) and (3.4-12), are referred to the fluid.

When the Biot number is small, one can conclude from Eq. (7.1-14) that

$$\left( \begin{array}{c} \text{Difference in} \\ \text{driving force} \end{array} \right)_{solid} \ll \left( \begin{array}{c} \text{Difference in} \\ \text{driving force} \end{array} \right)_{fluid} \quad (7.1-17)$$

Therefore, dependent variables may be considered uniform within the solid phase only if  $\text{Bi} \ll 1$ .

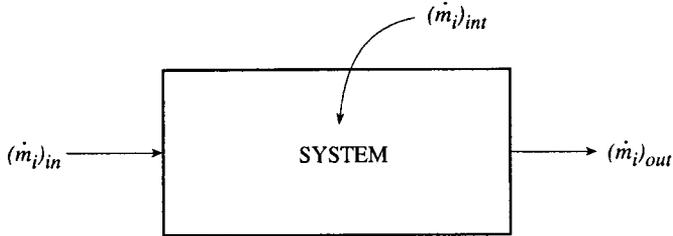
## 7.2 CONSERVATION OF CHEMICAL SPECIES

The conservation statement for the mass of the  $i^{\text{th}}$  chemical species is given by

$$\left( \begin{array}{c} \text{Rate of mass} \\ \text{of } i \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of mass} \\ \text{of } i \text{ out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of generation} \\ \text{of mass } i \end{array} \right) \\ = \left( \begin{array}{c} \text{Rate of accumulation} \\ \text{of mass } i \end{array} \right) \quad (7.2-1)$$

For a system with a single inlet and a single outlet stream as shown in Figure 7.1, Eq. (7.2-1) can be expressed as

$$\boxed{(\dot{m}_i)_{in} - (\dot{m}_i)_{out} \pm (\dot{m}_i)_{int} + V_{sys} \mathcal{M}_i \sum_j \alpha_{ij} r_j = \frac{d(m_i)_{sys}}{dt}} \quad (7.2-2)$$



**Figure 7.1** Unsteady-state flow system exchanging mass with the surroundings.

The interphase mass transfer rate,  $(\dot{m}_i)_{int}$ , is considered positive when mass is added to the system and is expressed by

$$(\dot{m}_i)_{int} = A_M \langle k_c \rangle (\Delta c_i)_{ch} \mathcal{M}_i \quad (7.2-3)$$

Substitution of Eq. (7.2-3) into Eq. (7.2-2) gives

$$\boxed{(\mathcal{Q} \rho_i)_{in} - (\mathcal{Q} \rho_i)_{out} \pm A_M \langle k_c \rangle (\Delta c_i)_{ch} \mathcal{M}_i + V_{sys} \mathcal{M}_i \sum_j \alpha_{ij} r_j = \frac{d(m_i)_{sys}}{dt}} \quad (7.2-4)$$

In terms of molar basis, Eqs. (7.2-2) and (7.2-4) take the form

$$\boxed{(\dot{n}_i)_{in} - (\dot{n}_i)_{out} \pm (\dot{n}_i)_{int} + V_{sys} \sum_j \alpha_{ij} r_j = \frac{d(n_i)_{sys}}{dt}} \quad (7.2-5)$$

and

$$\boxed{(\mathcal{Q}c_i)_{in} - (\mathcal{Q}c_i)_{out} \pm A_M \langle k_c \rangle (\Delta c_i)_{ch} + V_{sys} \sum_j \alpha_{ij} r_j = \frac{d(n_i)_{sys}}{dt}} \quad (7.2-6)$$

### 7.3 CONSERVATION OF TOTAL MASS

Summation of Eq. (7.2-2) over all species gives the total mass balance in the form

$$\boxed{\dot{m}_{in} - \dot{m}_{out} \pm \dot{m}_{int} = \frac{dm_{sys}}{dt}} \quad (7.3-1)$$

Note that the term  $\sum_i \alpha_{ij} \mathcal{M}_i$  is zero since mass is conserved. On the other hand, summation of Eq. (7.2-5) over all species gives the total mole balance as

$$\boxed{\dot{n}_{in} - \dot{n}_{out} \pm \dot{n}_{int} + V_{sys} \sum_j \bar{\alpha}_j r_j = \frac{dn_{sys}}{dt}} \quad (7.3-2)$$

where

$$\bar{\alpha}_j = \sum_i \alpha_{ij} \quad (7.3-3)$$

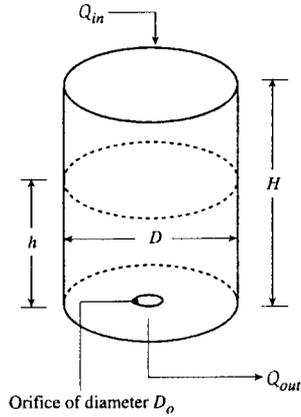
The generation term in Eq. (7.3-2) is not zero because moles are not conserved. This term vanishes only when  $\bar{\alpha}_j = 0$  for all values of  $j$ .

**Example 7.2** *An open cylindrical tank of height  $H$  and diameter  $D$  is initially half full of a liquid. At time  $t = 0$ , the liquid is fed into the tank at a constant volumetric flow rate of  $Q_{in}$ , and at the same time it is allowed to drain out through an orifice of diameter  $D_o$  at the bottom of the tank. Express the variation of the liquid height as a function of time.*

#### Solution

##### Assumptions

1. Rate of evaporation from the liquid surface is negligible.
2. Liquid is incompressible.
3. Pressure distribution in the tank is hydrostatic.



### Analysis

*System: Fluid in the tank*

The inventory rate equation for total mass, Eq. (7.3-1), reduces to

$$\rho Q_{in} - \rho \langle v_o \rangle A_o = \frac{d(Ah\rho)}{dt} \quad (1)$$

where  $\langle v_o \rangle$  is the average velocity through the orifice, i.e., the volumetric flow rate divided by the cross-sectional area;  $A_o$  and  $A$  are the cross-sectional areas of orifice and the tank, respectively. Since  $\rho$  and  $A$  are constant, Eq. (1) becomes

$$Q_{in} - \langle v_o \rangle A_o = A \frac{dh}{dt} \quad (2)$$

In order to proceed further,  $\langle v_o \rangle$  must be related to  $h$ .

For flow in a pipe of uniform cross-sectional area  $A$ , the pressure drop across an orifice is given by

$$\langle v_o \rangle = \frac{C_o}{\sqrt{1 - \beta^4}} \sqrt{\frac{2|\Delta P|}{\rho}} \quad (3)$$

where  $\beta$  is the ratio of the orifice diameter to the pipe diameter,  $|\Delta P|$  is the pressure drop across the orifice, and  $C_o$  is the orifice coefficient. The value of  $C_o$  is generally determined from experiments and given as a function of  $\beta$  and the Reynolds number,  $Re_o$ , defined by

$$Re_o = \frac{D_o \langle v_o \rangle \rho}{\mu} \quad (4)$$

For  $\beta < 0.25$ , the term  $\sqrt{1 - \beta^4}$  is almost unity. On the other hand, when  $Re_o > 20,000$ , experimental measurements show that  $C_o \simeq 0.61$ . Hence, Eq. (3) reduces

to

$$\langle v_o \rangle = 0.61 \sqrt{\frac{2|\Delta P|}{\rho}} \quad (5)$$

Since the pressure in the tank is hydrostatic,  $|\Delta P| \simeq \rho gh$  and Eq. (5) becomes

$$\langle v_o \rangle = 0.61 \sqrt{2gh} = 2.7\sqrt{h} \quad (6)$$

Substitution of Eq. (6) into Eq. (2) gives the governing differential equation for the liquid height in the tank as

$$2.7 \left( \frac{A_o}{A} \right) (\Omega - \sqrt{h}) = \frac{dh}{dt} \quad (7)$$

where

$$\Omega = \frac{Q_{in}}{2.7A_o} \quad (8)$$

Note that the system reaches steady-state when  $dh/dt = 0$  at which point the liquid height,  $h_s$ , is given by

$$h_s = \Omega^2 \quad (9)$$

Now, it is worthwhile to investigate two cases:

Case (i) Liquid level in the tank increases

At  $t = 0$ , the liquid level in the tank is  $H/2$ . Therefore, the liquid level increases, i.e.,  $dh/dt > 0$  in Eq. (7), if

$$\Omega^2 > H/2 \quad (10)$$

Rearrangement of Eq. (7) gives

$$\int_0^t dt = \frac{1}{2.7} \left( \frac{A}{A_o} \right) \int_{H/2}^h \frac{dh}{\Omega - \sqrt{h}} \quad (11)$$

Integration of Eq. (11) yields

$$t = 0.74 \left( \frac{A}{A_o} \right) \left[ \sqrt{\frac{H}{2}} - \sqrt{h} + \Omega \ln \left( \frac{\Omega - \sqrt{H/2}}{\Omega - \sqrt{h}} \right) \right] \quad (12)$$

Equations (9) and (10) indicate that  $h_s > H/2$ . When  $h_s > H$ , steady-state condition can never be achieved in the tank. The time required to fill the tank,  $t_f$ , is

$$t_f = 0.74 \left( \frac{A}{A_o} \right) \left[ \sqrt{\frac{H}{2}} - \sqrt{H} + \Omega \ln \left( \frac{\Omega - \sqrt{H/2}}{\Omega - \sqrt{H}} \right) \right] \quad (13)$$

If  $H/2 < h_s < H$ , then the time,  $t_\infty$ , required for the level of the tank to reach 99% of the steady-state value is

$$t_\infty = 0.74 \left( \frac{A}{A_o} \right) \left[ \sqrt{\frac{H}{2}} - \sqrt{0.99} \Omega + \Omega \ln \left( \frac{\Omega - \sqrt{H/2}}{\Omega - \sqrt{0.99} \Omega} \right) \right] \quad (14)$$

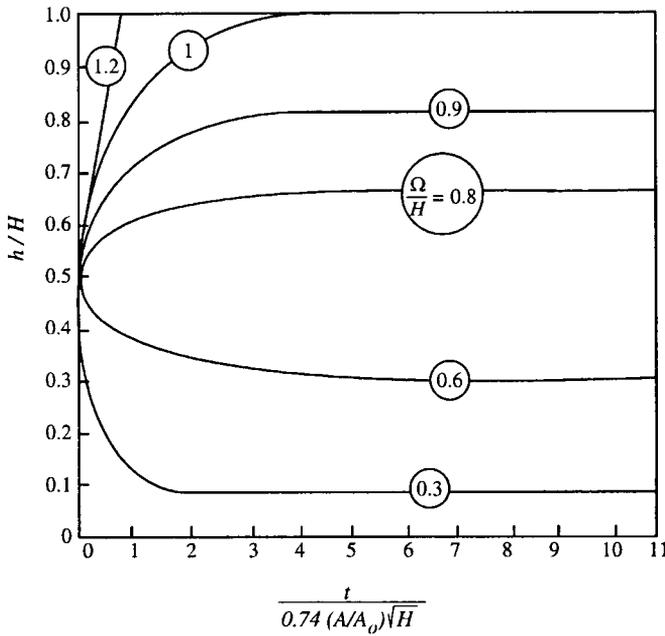
Case (ii) Liquid level in the tank decreases

The liquid level in the tank decreases, i.e.,  $dh/dt < 0$  in Eq. (7), if

$$\Omega^2 < H/2 \tag{15}$$

Equation (12) is also valid for this case. Equations (9) and (15) imply that  $h_s < H/2$ . Since  $h_s$  cannot be negative, this further implies that it is impossible to empty the tank under these circumstances. The time required for the level of the tank to reach 99% of the steady-state value is also given by Eq. (14).

The ratio  $h/H$  is plotted versus  $t/[0.74(A/A_o)\sqrt{H}]$  with  $\Omega/\sqrt{H}$  as a parameter in the figure below.



**Example 7.3** A liquid phase irreversible reaction



takes place in a CSTR of volume  $V_T$ . The reactor is initially empty. At  $t = 0$ , a solution of species  $A$  at concentration  $c_{A_0}$  flows into the reactor at a constant volumetric flow rate of  $Q_{in}$ . No liquid leaves the reactor until the liquid volume reaches a value of  $V_T$ . The rate of reaction is given by

$$r = k c_A$$

If the reaction takes place under isothermal conditions, express the concentration of species  $A$  within the reactor as a function of time.

**Solution****Assumptions**

1. *Well mixed system, i.e., the temperature and the concentration of the contents of the reactor are uniform.*
2. *The density of the reaction mixture is constant.*

**Analysis**

*System: Contents of the reactor*

*The problem should be considered in three parts: the filling period, the unsteady state period, and the steady-state period.*

*i) The filling period*

*During this period, there is no outlet stream from the reactor. Hence, the conservation of total mass, Eq. (7.3-1), is given by*

$$\rho Q_{in} = \frac{dm_{sys}}{dt} \quad (1)$$

*Since  $Q_{in}$  and  $\rho$  are constant, integration of Eq. (1) and the use of the initial condition,  $m_{sys} = 0$  at  $t = 0$ , gives*

$$m_{sys} = Q_{in}\rho t \quad (2)$$

*Since  $m_{sys} = \rho V_{sys}$ , Eq. (2) can also be expressed as*

$$V_{sys} = Q_{in} t \quad (3)$$

*From Eq. (3), the time required to fill the reactor,  $t^*$ , is calculated as  $t^* = V_T/Q_{in}$ , where  $V_T$  is the volume of the reactor.*

*The inventory rate equation based on the moles of species A, Eq. (7.2-6), reduces to*

$$Q_{in} c_{A_0} - k c_A V_{sys} = \frac{dn_A}{dt} \quad (4)$$

*where  $V_{sys}$ , the volume of the reaction mixture, is dependent on time. The molar concentration can be expressed in terms of the number of moles as*

$$c_A = \frac{n_A}{V_{sys}} \quad (5)$$

*such that Eq. (4) can be rearranged in the form*

$$\int_0^{n_A} \frac{dn_A}{Q_{in} c_{A_0} - k n_A} = \int_0^t dt \quad (6)$$

Integration gives

$$n_A = \frac{Q_{in} c_{A_0}}{k t} [1 - \exp(-k t)] \quad (7)$$

Substitution of Eq. (7) into Eq. (5) and the use of Eq. (3) gives the concentration as a function of time as

$$c_A = \frac{c_{A_0}}{k t} [1 - \exp(-k t)] \quad 0 \leq t \leq V_T/Q_{in} \quad (8)$$

The concentration  $c_A^*$  at the instant the tank is full, i.e., at  $t = t^* = V_T/Q_{in}$ , is

$$c_A^* = \frac{Q_{in} c_{A_0}}{k V_T} \left[ 1 - \exp\left(-\frac{k V_T}{Q_{in}}\right) \right] \quad (9)$$

ii) The unsteady-state period

Since the total volume of the reactor  $V_T$  is constant, then the inlet and outlet volumetric flow rates are the same, i.e.,

$$Q_{in} = Q_{out} = Q \quad (10)$$

The inventory rate equation on the moles of species A, Eq. (7.2-6), is

$$Q c_{A_0} - Q c_A - k c_A V_T = \frac{d(c_A V_T)}{dt} \quad (11)$$

Equation (11) can be rearranged in the form

$$\frac{1}{\tau} [c_{A_0} - c_A (1 + k\tau)] = \frac{dc_A}{dt} \quad (12)$$

where  $\tau$  is the residence time defined by

$$\tau = \frac{V_T}{Q} \quad (13)$$

Equation (12) is a separable equation and can be written in the form

$$\tau \int_{c_A^*}^{c_A} \frac{dc_A}{c_{A_0} - c_A (1 + k\tau)} = \int_{t^*}^t dt \quad (14)$$

Integration of Eq. (14) gives the concentration distribution as

$$c_A = \frac{c_{A_0}}{1 + k\tau} + \left( c_A^* - \frac{c_{A_0}}{1 + k\tau} \right) \exp \left[ -\frac{(1 + k\tau)(t - t^*)}{\tau} \right] \quad (15)$$

iii) *The steady-state period*

The concentration in the tank reaches its steady-state value,  $c_{A_s}$ , as  $t \rightarrow \infty$ . In this case, the exponential term in Eq. (15) vanishes and the result is

$$c_{A_s} = \frac{c_{A_0}}{1 + k\tau} \quad (16)$$

Note that Eq. (16) can also be obtained from Eq. (12) by letting  $dc_A/dt = 0$ . The time required for the concentration to reach 99% of its steady-state value,  $t_\infty$ , is

$$t_\infty = t^* + \frac{\tau}{1 + k\tau} \ln \left\{ 100 \left[ 1 - \left( \frac{1 + k\tau}{k\tau} \right) [1 - \exp(-k\tau)] \right] \right\} \quad (17)$$

When  $k\tau \ll 1$ , i.e., a slow first-order reaction, Eq. (17) simplifies to

$$t_\infty - t^* = 4.6\tau \quad (18)$$

**Example 7.4** A sphere of naphthalene, 2 cm in diameter, is suspended in air at 90 °C. Estimate the time required for the diameter of the sphere to be reduced to one-half its initial value if:

- The air is stagnant,
- The air is flowing past the naphthalene sphere with a velocity of 5 m/s.

**Solution**

**Physical properties**

$$\text{For naphthalene (species A) at } 90^\circ\text{C (363 K)} : \begin{cases} \rho_A^S = 1145 \text{ kg/m}^3 \\ \mathcal{M}_A = 128 \\ P_A^{sat} = 11.7 \text{ mmHg} \end{cases}$$

Diffusion coefficient of species A in air (species B):

$$(\mathcal{D}_{AB})_{363} = (0.62 \times 10^{-5}) \left( \frac{363}{300} \right)^{3/2} = 8.25 \times 10^{-6} \text{ m}^2/\text{s}$$

$$\text{For air at } 90^\circ\text{C (363 K)} : \nu = 21.95 \times 10^{-6} \text{ m}^2/\text{s}$$

The Schmidt number is

$$\begin{aligned} \text{Sc} &= \frac{\nu}{\mathcal{D}_{AB}} \\ &= \frac{21.95 \times 10^{-6}}{8.25 \times 10^{-6}} = 2.66 \end{aligned}$$

**Assumptions**

- Pseudo-steady-state behavior.

2. *Ideal gas behavior.*

### Analysis

*System: Naphthalene sphere*

*The terms appearing in the conservation of species A, Eq. (7.2-2), are*

$$\begin{aligned}(\dot{m}_A)_{in} &= (\dot{m}_A)_{out} = 0 \\(\dot{m}_A)_{int} &= -(\pi D_P^2) \langle k_c \rangle (c_{A_w} - c_{A_\infty}) \mathcal{M}_A \\&\quad \tau = 0 \\(m_A)_{sys} &= V_{sys} \rho_A^S = (\pi D_P^3/6) \rho_A^S\end{aligned}$$

*Therefore, Eq. (7.2-2) reduces to*

$$-(\pi D_P^2) \langle k_c \rangle (c_{A_w} - c_{A_\infty}) \mathcal{M}_A = \frac{d}{dt} \left( \frac{\pi D_P^3}{6} \rho_A^S \right) \quad (1)$$

*Taking  $c_{A_\infty} = 0$  and rearrangement gives*

$$t = \frac{\rho_A^S}{2 \mathcal{M}_A c_{A_w}} \int_{D_o/2}^{D_o} \frac{dD_P}{\langle k_c \rangle} \quad (2)$$

*where  $D_o$  is the initial diameter of the naphthalene sphere.*

*The average mass transfer coefficient,  $\langle k_c \rangle$ , can be related to the diameter of the sphere,  $D_P$ , by using one of the mass transfer correlations given in Section 4.3.3. The use of the Ranz-Marshall correlation, Eq. (4.3-33), gives*

$$\text{Sh} = 2 + 0.6 \text{Re}_P^{1/2} \text{Sc}^{1/3} \quad (3)$$

a) *When air is stagnant, i.e.,  $\text{Re}_P = 0$ , Eq. (3) reduces to*

$$\text{Sh} = \frac{\langle k_c \rangle D_P}{\mathcal{D}_{AB}} = 2 \quad \Rightarrow \quad \langle k_c \rangle = \frac{2 \mathcal{D}_{AB}}{D_P} \quad (4)$$

*Substitution of Eq. (4) into Eq. (2) and integration gives*

$$t = \frac{3}{32} \frac{\rho_A^S D_o^2}{\mathcal{M}_A c_{A_w} \mathcal{D}_{AB}} \quad (5)$$

*The saturation concentration of naphthalene,  $c_{A_w}$ , is*

$$\begin{aligned}c_{A_w} &= \frac{P_A^{\text{sat}}}{\mathcal{R}T} \\&= \frac{11.7/760}{(0.08205)(90 + 273)} = 5.17 \times 10^{-4} \text{ kmol/m}^3\end{aligned} \quad (6)$$

Substitution of the values into Eq. (5) gives the required time as

$$t = \frac{3}{32} \frac{(1145)(0.02)^2}{(128)(5.17 \times 10^{-4})(8.25 \times 10^{-6})} = 2.59 \times 10^5 \text{ s} \simeq 3 \text{ days}$$

b) When air flows with a certain velocity, the Ranz-Marshall correlation can be expressed as

$$\frac{\langle k_c \rangle D_P}{\mathcal{D}_{AB}} = 2 + 0.6 \left( \frac{D_P v_\infty}{\nu} \right)^{1/2} \text{Sc}^{1/3}$$

or,

$$\langle k_c \rangle = \frac{1}{D_P} \left( \alpha + \beta \sqrt{D_P} \right) \quad (7)$$

where the coefficients  $\alpha$  and  $\beta$  are defined by

$$\alpha = 2 \mathcal{D}_{AB} = 2(8.25 \times 10^{-6}) = 1.65 \times 10^{-5} \quad (8)$$

$$\begin{aligned} \beta &= 0.6 \mathcal{D}_{AB} (v_\infty/\nu)^{1/2} \text{Sc}^{1/3} \\ &= (0.6)(8.25 \times 10^{-6}) \left( \frac{5}{21.95 \times 10^{-6}} \right)^{1/2} (2.66)^{1/3} = 3.27 \times 10^{-3} \end{aligned} \quad (9)$$

Substitution of Eqs. (7)-(9) into Eq. (2) gives

$$t = \frac{1145}{(2)(128)(5.17 \times 10^{-4})} \int_{0.01}^{0.02} \left( \frac{D_P}{1.65 \times 10^{-5} + 3.27 \times 10^{-3} \sqrt{D_P}} \right) dD_P$$

Analytical evaluation of the above integral is possible and the result is

$$t = 3097 \text{ s} \simeq 52 \text{ min}$$

**Verification of the pseudo-steady-state approximation**

$$\frac{\mathcal{D}_{AB} t}{D_P^2} = \frac{(8.25 \times 10^{-6})(3097)}{(2 \times 10^{-2})^2} = 64 \gg 1$$

## 7.4 CONSERVATION OF MOMENTUM

According to Newton's second law of motion, the conservation statement for linear momentum is expressed as

$$\left( \begin{array}{c} \text{Time rate of change of} \\ \text{linear momentum of a body} \end{array} \right) = \left( \begin{array}{c} \text{Forces acting} \\ \text{on a body} \end{array} \right) \quad (7.4-1)$$

In Section 4.3, we considered the balance of forces acting on a single spherical particle of diameter  $D_P$ , falling in a stagnant fluid with a constant terminal velocity

$v_t$ . In the case of an accelerating sphere an additional force, called *fluid inertia force*, acts besides the gravitational, the buoyancy, and the drag forces. This force arises from the fact that the fluid around the sphere is also accelerated from the rest, resulting in a change in the momentum of the fluid. The rate of change of fluid momentum shows up as an additional force acting on the sphere, pointing in the direction opposite to the motion of the sphere. This additional force has a magnitude equal to one-half the rate of change of momentum of a sphere of liquid moving at the same velocity as the solid sphere. Therefore, Eq. (7.4-1) is written in the form

$$\left( \begin{array}{c} \text{Time rate of change of} \\ \text{linear momentum of a sphere} \end{array} \right) = \left( \begin{array}{c} \text{Gravitational} \\ \text{force} \end{array} \right) - \left( \begin{array}{c} \text{Buoyancy} \\ \text{force} \end{array} \right) - \left( \begin{array}{c} \text{Drag} \\ \text{force} \end{array} \right) - \left( \begin{array}{c} \text{Fluid inertia} \\ \text{force} \end{array} \right) \quad (7.4-2)$$

and can be expressed as

$$\frac{\pi D_P^3}{6} \rho_P \frac{dv}{dt} = \frac{\pi D_P^3}{6} \rho_P g - \frac{\pi D_P^3}{6} \rho g - \left( \frac{\pi D_P^2}{4} \right) \left( \frac{1}{2} \rho v^2 \right) f - \frac{\pi D_P^3}{12} \rho \frac{dv}{dt} \quad (7.4-3)$$

where  $\rho_P$  and  $D_P$  represent the density and diameter of the solid sphere, respectively, and  $\rho$  is the fluid density. Simplification of Eq. (7.4-3) gives

$$D_P (\rho_P + 0.5 \rho) \frac{dv}{dt} = D_P (\rho_P - \rho) g - \frac{3}{4} \rho v^2 f \quad (7.4-4)$$

The friction factor  $f$  is usually given as a function of the Reynolds number,  $\text{Re}_P$ , defined by

$$\text{Re}_P = \frac{D_P v \rho}{\mu} \quad (7.4-5)$$

Therefore, it is much more convenient to express the velocity,  $v$ , in terms of  $\text{Re}_P$ . Thus, Eq. (7.4-4) takes the form

$$(\rho_P + 0.5 \rho) \frac{D_P^2}{\mu} \frac{d\text{Re}_P}{dt} = \text{Ar} - \frac{3}{4} f \text{Re}_P^2 \quad (7.4-6)$$

where Ar is the Archimedes number defined by Eq. (4.3-6). Note that when the particle reaches its terminal velocity, i.e.,  $d\text{Re}_P/dt = 0$ , Eq. (7.4-6) reduces to Eq. (4.3-4). Integration of Eq. (7.4-6) gives

$$t = \frac{(\rho_P + 0.5 \rho) D_P^2}{\mu} \int_0^{\text{Re}_P} \left( \text{Ar} - \frac{3}{4} f \text{Re}_P^2 \right)^{-1} d\text{Re}_P \quad (7.4-7)$$

A friction factor – Reynolds number relationship is required to carry out the integration. Substitution of the Turton-Levenspiel correlation, Eq. (4.3-10), into

Eq. (7.4-7) gives

$$t = \frac{(\rho_P + 0.5 \rho) D_P^2}{\mu} \times \int_0^{\text{Re}_P} \left( \text{Ar} - 18 \text{Re}_P - 3.114 \text{Re}_P^{1.657} - \frac{0.31 \text{Re}_P^2}{1 + 16,300 \text{Re}_P^{-1.09}} \right)^{-1} d\text{Re}_P \quad (7.4-8)$$

Equation (7.4-8) should be evaluated numerically.

**Example 7.5** Calculate the time required for a spherical lead particle, 1.5 mm in diameter, to reach 60% of its terminal velocity in air at 50°C.

**Solution**

**Physical properties**

$$\text{For air at } 50^\circ\text{C (323 K)} : \begin{cases} \rho = 1.0928 \text{ kg/m}^3 \\ \mu = 19.57 \times 10^{-6} \text{ kg/m}\cdot\text{s} \end{cases}$$

$$\text{For lead at } 50^\circ\text{C} : \rho = 11,307 \text{ kg/m}^3$$

**Analysis**

When the particle reaches its terminal velocity, the value of the Reynolds number can be calculated from Eq. (4.3-12). The Archimedes number is

$$\begin{aligned} \text{Ar} &= \frac{D_P^3 g \rho (\rho_P - \rho)}{\mu^2} \\ &= \frac{(1.5 \times 10^{-3})^3 (9.8)(1.0928)(11,307)}{(19.57 \times 10^{-6})^2} = 1.067 \times 10^6 \end{aligned}$$

Substitution of this value into Eq. (4.3-12) gives the Reynolds number under steady conditions as

$$\begin{aligned} \text{Re}_P|_{v=v_t} &= \frac{\text{Ar}}{18} (1 + 0.0579 \text{Ar}^{0.412})^{-1.214} \\ &= \frac{1.067 \times 10^6}{18} \left[ 1 + 0.0579 (1.067 \times 10^6)^{0.412} \right]^{-1.214} = 1701 \end{aligned}$$

In this problem it is required to calculate the time for the particle to reach a Reynolds number of

$$\text{Re}_P = (0.6)(1701) = 1021$$

Therefore, the required time can be calculated from Eq. (7.4-8) as

$$t = \frac{(11,307)(1.5 \times 10^{-3})^2}{19.57 \times 10^{-6}} I \quad (1)$$

where

$$I = \int_0^{\text{Re}_P} \left( 1.067 \times 10^6 - 18 \text{Re}_P - 3.114 \text{Re}_P^{1.657} - \frac{0.31 \text{Re}_P^2}{1 + 16,300 \text{Re}_P^{-1.09}} \right)^{-1} d\text{Re}_P$$

The value of  $I$  can be determined by using one of the numerical techniques given in Section A.8-4 in Appendix A. The use of the Gauss-Legendre quadrature is shown below. According to Eq. (A.8-13)

$$\text{Re}_P = \frac{1021}{2} (u + 1)$$

and the five-point quadrature is given by

$$I = \frac{1021}{2} \sum_{i=0}^4 w_i F(u_i) \tag{2}$$

where the function  $F(u)$  is given by

$$F(u) = \frac{1}{1.067 \times 10^6 - 9189(u + 1) - 95602(u + 1)^{1.657} - \frac{80,789(u + 1)^2}{1 + 18.22(u + 1)^{-1.09}}}$$

The values of  $w_i$  and  $F(u_i)$  are given up to three decimals in the following table:

$i$	$u_i$	$w_i$	$F(u_i) \times 10^6$	$w_i F(u_i) \times 10^6$
0	0.000	0.569	1.044	0.594
1	+0.538	0.479	1.187	0.569
2	-0.538	0.479	0.966	0.463
3	+0.906	0.237	1.348	0.319
4	-0.906	0.237	0.940	0.223
$\sum_{i=0}^4 w_i F(u_i) = 2.17 \times 10^{-6}$				

Therefore, the value of  $I$  can be calculated from Eq. (2) as

$$I = \frac{1021}{2} (2.17 \times 10^{-6}) = 1.11 \times 10^{-3}$$

Substitution of this value into Eq. (1) gives

$$t = \frac{(11,307)(1.5 \times 10^{-3})^2 (1.11 \times 10^{-3})}{19.57 \times 10^{-6}} = 1.44 \text{ s}$$

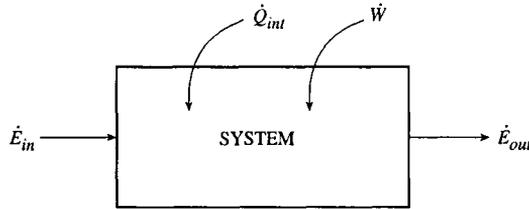
## 7.5 CONSERVATION OF ENERGY

The conservation statement for total energy under unsteady-state conditions is given by

$$\left( \begin{array}{c} \text{Rate of} \\ \text{energy in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{energy out} \end{array} \right) = \left( \begin{array}{c} \text{Rate of energy} \\ \text{accumulation} \end{array} \right) \quad (7.5-1)$$

For a system shown in Figure 7.2, following the discussion explained in Section 6.3, Eq. (7.5-1) is written as

$$\begin{aligned} \left[ (\hat{U} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{in} - \left[ (\hat{U} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{out} + \dot{Q}_{int} + \dot{W} \\ = \frac{d}{dt} \left[ (\hat{U} + \hat{E}_K + \hat{E}_P) m \right]_{sys} \end{aligned} \quad (7.5-2)$$



**Figure 7.2** Unsteady-state flow system exchanging energy in the form of heat and work with the surroundings.

Note that, contrary to the steady-state flow system, the boundaries of this system are not fixed in space. Therefore, besides shaft and flow works, work associated with the expansion or compression of the system boundaries must be included in  $\dot{W}$  so that it takes the form

$$\dot{W} = \underbrace{-P_{sys} \frac{dV_{sys}}{dt}}_A + \underbrace{\dot{W}_s}_B + \underbrace{\left( P\hat{V}\dot{m} \right)_{in} - \left( P\hat{V}\dot{m} \right)_{out}}_C \quad (7.5-3)$$

where terms  $A$ ,  $B$ , and  $C$  represent, respectively, work associated with the expansion or compression of the system boundaries, shaft work, and flow work.

Substitution of Eq. (7.5-3) into Eq. (7.5-2) and the use of the definition of enthalpy, i.e.,  $\hat{H} = \hat{U} + P\hat{V}$ , gives

$$\begin{aligned} \left[ (\hat{H} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{in} - \left[ (\hat{H} + \hat{E}_K + \hat{E}_P) \dot{m} \right]_{out} + \dot{Q}_{int} - P_{sys} \frac{dV_{sys}}{dt} + \dot{W}_s \\ = \frac{d}{dt} \left[ (\hat{U} + \hat{E}_K + \hat{E}_P) m \right]_{sys} \end{aligned} \quad (7.5-4)$$

which is known as the *general energy equation*. Note that under steady conditions, Eq. (7.5-4) reduces to Eq. (6.3-9). In terms of molar quantities, Eq. (7.5-4) is written as

$$\begin{aligned} \left[ (\tilde{H} + \tilde{E}_K + \tilde{E}_P) \dot{n} \right]_{in} - \left[ (\tilde{H} + \tilde{E}_K + \tilde{E}_P) \dot{n} \right]_{out} + \dot{Q}_{int} - P_{sys} \frac{dV_{sys}}{dt} + \dot{W}_s \\ = \frac{d}{dt} \left[ (\tilde{U} + \tilde{E}_K + \tilde{E}_P) n \right]_{sys} \end{aligned} \quad (7.5-5)$$

When the changes in the kinetic and potential energies between the inlet and outlet of the system as well as within the system are negligible, Eq. (7.5-4) reduces to

$$(\hat{H}\dot{m})_{in} - (\hat{H}\dot{m})_{out} + \dot{Q}_{int} - P_{sys} \frac{dV_{sys}}{dt} + \dot{W}_s = \frac{d}{dt} (\hat{U}m)_{sys} \quad (7.5-6)$$

The accumulation term in Eq. (7.5-6) can be expressed in terms of enthalpy as

$$\begin{aligned} \frac{d}{dt} (\hat{U}m)_{sys} &= \frac{d}{dt} \left[ (\hat{H} - P\hat{V}) m \right]_{sys} \\ &= \frac{d}{dt} (\hat{H}m)_{sys} - P_{sys} \frac{dV_{sys}}{dt} - V_{sys} \frac{dP_{sys}}{dt} \end{aligned} \quad (7.5-7)$$

Substitution of Eq. (7.5-7) into Eq. (7.5-6) gives

$$\boxed{(\hat{H}\dot{m})_{in} - (\hat{H}\dot{m})_{out} + \dot{Q}_{int} + V_{sys} \frac{dP_{sys}}{dt} + \dot{W}_s = \frac{d}{dt} (\hat{H}m)_{sys}} \quad (7.5-8)$$

On molar basis, Eq. (7.5-8) can be expressed as

$$\boxed{(\tilde{H}\dot{n})_{in} - (\tilde{H}\dot{n})_{out} + \dot{Q}_{int} + V_{sys} \frac{dP_{sys}}{dt} + \dot{W}_s = \frac{d}{dt} (\tilde{H}n)_{sys}} \quad (7.5-9)$$

**Example 7.6** Air at atmospheric pressure and 25°C is flowing at a velocity of 5 m/s over a copper sphere, 1.5 cm in diameter. The sphere is initially at a temperature of 50°C. How long will it take to cool the sphere to 30°C? How much heat is transferred from the sphere to the air?

### Solution

#### Physical properties

$$\text{For air at 25°C (298 K)} : \begin{cases} \mu = 18.41 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ \nu = 15.54 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 25.96 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ \text{Pr} = 0.712 \end{cases}$$

For air at 40°C (313 K) :  $\mu = 19.11 \times 10^{-6} \text{ kg/m}\cdot\text{s}$

For copper at 40°C (313 K) :  $\begin{cases} \rho = 8924 \text{ kg/m}^3 \\ \hat{C}_P = 387 \text{ J/kg}\cdot\text{K} \\ k = 397 \text{ W/m}\cdot\text{K} \end{cases}$

### Assumptions

1. No temperature gradients exist within the sphere, i.e.,  $\text{Bi} \ll 1$ .
2. The average heat transfer coefficient on the surface of the sphere is constant.
3. The physical properties of copper are independent of temperature.
4. Pseudo-steady-state behavior.

### Analysis

System: Copper sphere

For the problem at hand, the terms in Eq. (7.5-8) are

$$\begin{aligned} \dot{m}_{in} &= \dot{m}_{out} = 0 \\ \dot{W}_s &= 0 \\ \dot{Q}_{int} &= -(\pi D_P^2 \langle h \rangle)(T - T_\infty) \\ \frac{dP_{sys}}{dt} &= 0 \\ m_{sys} &= (\pi D_P^3 / 6) \rho_{Cu} \\ \hat{H}_{sys} &= (\hat{C}_P)_{Cu}(T - T_{ref}) \end{aligned}$$

where  $T$  is the copper sphere temperature at any instant and  $T_\infty$  is the air temperature.

Therefore, Eq. (7.5-8) becomes

$$-\pi D_P^2 \langle h \rangle (T - T_\infty) = \left( \frac{\pi D_P^3}{6} \right) (\rho \hat{C}_P)_{Cu} \frac{dT}{dt} \quad (1)$$

Integration of Eq. (1) with the initial condition that  $T = T_i$  at  $t = 0$  gives

$$t = \frac{D_P}{6 \langle h \rangle} (\rho \hat{C}_P)_{Cu} \ln \left( \frac{T_i - T_\infty}{T - T_\infty} \right) \quad (2)$$

To determine the average heat transfer coefficient,  $\langle h \rangle$ , first it is necessary to calculate the Reynolds number:

$$\begin{aligned} \text{Re}_P &= \frac{D_P v_\infty}{\nu} \\ &= \frac{(0.015)(5)}{15.54 \times 10^{-6}} = 4826 \end{aligned}$$

The use of the Whitaker correlation, Eq. (4.3-30), gives

$$\begin{aligned} \text{Nu} &= 2 + \left(0.4 \text{Re}_P^{1/2} + 0.06 \text{Re}_P^{2/3}\right) \text{Pr}^{0.4} (\mu_\infty/\mu_w)^{1/4} \\ &= 2 + \left[0.4(4826)^{1/2} + 0.06(4826)^{2/3}\right] (0.712)^{0.4} \left(\frac{18.41 \times 10^{-6}}{19.11 \times 10^{-6}}\right)^{1/4} \\ &= 40.9 \end{aligned}$$

The average heat transfer coefficient is

$$\begin{aligned} \langle h \rangle &= \text{Nu} \left(\frac{k}{D_P}\right) \\ &= (40.9) \left(\frac{25.96 \times 10^{-3}}{0.015}\right) = 71 \text{ W/m}^2 \cdot \text{K} \end{aligned}$$

Therefore, the time required for cooling is

$$t = \frac{(0.015)(8924)(387)}{(6)(71)} \ln\left(\frac{50 - 25}{30 - 25}\right) = 196 \text{ s}$$

The amount of energy transferred from the sphere to the air can be calculated from

$$Q_{int} = \int_0^t \dot{Q}_{int} dt = \pi D_P^2 \langle h \rangle \int_0^t (T - T_\infty) dt \quad (3)$$

Substitution of Eq. (2) into Eq. (3) and integration yields

$$Q_{int} = \left(\frac{\pi D_P^3}{6}\right) (\rho \hat{C}_P)_{Cu} (T_i - T_\infty) \left\{ 1 - \exp\left[-\frac{6 \langle h \rangle t}{D_P (\rho \hat{C}_P)_{Cu}}\right] \right\} \quad (4)$$

Note that from Eq. (2)

$$\exp\left[-\frac{6 \langle h \rangle t}{D_P (\rho \hat{C}_P)_{Cu}}\right] = \frac{T - T_\infty}{T_i - T_\infty} \quad (5)$$

Substitution of Eq. (5) into Eq. (4) gives

$$\begin{aligned} Q_{int} &= \left(\frac{\pi D_P^3}{6}\right) (\rho \hat{C}_P)_{Cu} (T_i - T) \\ &= \left[\frac{\pi(0.015)^3}{6}\right] [(8924)(387)] (50 - 30) = 122 \text{ J} \end{aligned} \quad (6)$$

### Verification of assumptions

- Assumption # 1

$$\begin{aligned} \text{Bi} &= \frac{\langle h \rangle D_P}{k_{Cu}} \\ &= \frac{(71)(0.015)}{397} = 0.0027 \ll 1 \end{aligned}$$

- Assumption # 4

$$\frac{\alpha t}{D_P^2} = \left[ \frac{397}{(8924)(387)} \right] \frac{(196)}{(0.015)^2} = 100 \gg 1$$

**Comment:** Note that Eq. (6) can simply be obtained from the first-law of thermodynamics written for a closed system. Considering the copper sphere as a system,

$$\Delta U = Q_{int} + W \quad \Rightarrow \quad Q_{int} = \Delta U = m \hat{C}_V \Delta T \simeq m \hat{C}_P \Delta T$$

**Example 7.7** A solid sphere at a uniform temperature of  $T_1$  is suddenly immersed in a well-stirred fluid of temperature  $T_o$  in an insulated tank ( $T_1 > T_o$ ).

- Determine the temperatures of the sphere and the fluid as a function of time.
- Determine the steady-state temperatures of the sphere and the fluid.

### Solution

#### Assumptions

- The physical properties of the sphere and the fluid are independent of temperature.
- The average heat transfer coefficient on the surface of the sphere is constant.
- The sphere and the fluid have uniform but unequal temperatures at any instant, i.e.,  $Bi \ll 1$  and mixing is perfect.

#### Analysis

a) Since the fluid and the sphere are at different temperatures at a given instant, it is necessary to write two differential equations: one for the fluid, and one for the sphere.

System: Solid sphere

The terms in Eq. (7.5-8) are

$$\begin{aligned} \dot{m}_{in} &= \dot{m}_{out} = 0 \\ \dot{W}_s &= 0 \\ \dot{Q}_{int} &= -(\pi D_P^2)(h)(T_s - T_f) \\ \frac{dP_{sys}}{dt} &= 0 \\ m_{sys} &= (\pi D_P^3/6) \rho_s \\ \hat{H}_{sys} &= \hat{C}_{P_s}(T_s - T_{ref}) \end{aligned}$$

where  $D_P$  is the diameter of the sphere, subscripts  $s$  and  $f$  stand for the sphere and the fluid, respectively. Therefore, Eq. (7.5-8) becomes

$$-\phi_s (T_s - T_f) = \frac{dT_s}{dt} \quad (1)$$

where

$$\phi_s = \frac{6 \langle h \rangle}{D_P \hat{C}_{P_s} \rho_s} \quad (2)$$

*System: Fluid in the tank*

The terms in Eq. (7.5-8) are

$$\begin{aligned} \dot{m}_{in} &= \dot{m}_{out} = 0 \\ \dot{W}_s &= 0 \\ \dot{Q}_{int} &= (\pi D_P^2) \langle h \rangle (T_s - T_f) \\ \frac{dP_{sys}}{dt} &= 0 \\ m_{sys} &= m_f \\ \dot{H}_{sys} &= \hat{C}_{P_f} (T_f - T_{ref}) \end{aligned}$$

Hence, Eq. (7.5-8) reduces to

$$\phi_f (T_s - T_f) = \frac{dT_f}{dt} \quad (3)$$

where

$$\phi_f = \frac{\langle h \rangle \pi D_P^2}{m_f \hat{C}_{P_f}} \quad (4)$$

From Eq. (1), the fluid temperature,  $T_f$ , is given in terms of the sphere temperature,  $T_s$ , as

$$T_f = T_s + \frac{1}{\phi_s} \frac{dT_s}{dt} \quad (5)$$

Substitution of Eq. (5) into Eq. (3) gives

$$\frac{d^2 T_s}{dt^2} + \phi \frac{dT_s}{dt} = 0 \quad (6)$$

where

$$\phi = \phi_f + \phi_s \quad (7)$$

Two initial conditions are necessary to solve this second-order ordinary differential equation. One of the initial conditions is

$$\text{at } t = 0 \quad T_s = T_1 \quad (8)$$

The other initial condition can be obtained from Eq. (5) as

$$\text{at } t = 0 \quad \frac{dT_s}{dt} = \phi_s(T_o - T_1) \quad (9)$$

The solution of Eq. (6) subject to the initial conditions defined by Eqs. (8) and (9) is

$$T_s = T_1 - \frac{\phi_s}{\phi}(T_1 - T_o)[1 - \exp(-\phi t)] \quad (10)$$

The use of Eq. (10) in Eq. (5) gives the fluid temperature in the form

$$T_f = T_1 - \frac{T_1 - T_o}{\phi} [\phi_s + \phi_f \exp(-\phi t)] \quad (11)$$

b) Under steady conditions, i.e.,  $t \rightarrow \infty$ , Eqs. (10) and (11) reduce to

$$T_s = T_f = T_\infty = \frac{\phi_f T_1 + \phi_s T_o}{\phi} \quad (12)$$

**Comment:** Note that the final steady-state temperature,  $T_\infty$ , can simply be obtained by the application of the first law of thermodynamics. Taking the sphere and the fluid together as a system, we get

$$\Delta U = \frac{\pi D_P^3}{6} \rho_s \hat{C}_{P_s} (T_\infty - T_1) + m_f \hat{C}_{P_f} (T_\infty - T_o) = 0 \quad (13)$$

Noting that

$$\frac{\phi_f}{\phi_s} = \frac{\pi D_P^3}{6} \frac{\rho_s \hat{C}_{P_s}}{m_f \hat{C}_{P_f}} \quad (14)$$

Equation (13) reduces to

$$\frac{\phi_f}{\phi_s} (T_\infty - T_1) + (T_\infty - T_o) = 0 \quad (15)$$

Solution of Eq. (15) results in Eq. (12).

**Example 7.8** A spherical steel tank of volume  $0.5 \text{ m}^3$  initially contains air at 7 bar and  $50^\circ\text{C}$ . A relief valve is opened and air is allowed to escape at a constant flow rate of 12 mol/min.

a) If the tank is well insulated, estimate the temperature and pressure of air within the tank after 5 minutes.

b) If heating coils are placed in the tank to maintain the air temperature constant at  $50^\circ\text{C}$ , estimate the pressure of air and the amount of heat transferred after 5 minutes.

Air may be assumed an ideal gas with a constant  $\tilde{C}_P$  of  $29 \text{ J/mol}\cdot\text{K}$ .

**Solution**

a) *System: Contents of the tank*

**Assumptions**

1. *Properties of the tank contents are uniform, i.e.,  $\tilde{H}_{out} = \tilde{H}_{sys}$ .*
2. *Heat transfer between the system and its surroundings is almost zero. Note that the insulation around the tank does not necessarily imply that  $\tilde{Q}_{int} = 0$ . Since the tank wall is in the surroundings, there will be heat transfer between the tank wall and air remaining in the tank during the evacuation process. Heat transfer may be considered negligible when (i) the mass of the wall is small, (ii) process takes place rapidly (remember that heat transfer is a slow process).*

**Analysis**

Since  $\dot{n}_{in} = \dot{n}_{int} = 0$  and there is no chemical reaction, Eq. (7.3-2) reduces to

$$-\dot{n}_{out} = \frac{dn_{sys}}{dt} \quad \Rightarrow \quad -12 = \frac{dn_{sys}}{dt} \quad (1)$$

Integration of Eq. (1) yields

$$n_{sys} = n_o - 12t \quad (2)$$

where  $n_o$  is the number of moles of air initially present in the tank, i.e.,

$$n_o = \frac{P_o V}{\mathcal{R} T_o} = \frac{(7)(0.5)}{(8.314 \times 10^{-5})(50 + 273)} = 130.3 \text{ mol}$$

On the other hand, the inventory rate equation for energy, Eq. (7.5-5), takes the form

$$\begin{aligned} -\tilde{H}_{out} \dot{n}_{out} &= \frac{d(n\tilde{U})_{sys}}{dt} \\ &= n_{sys} \frac{d\tilde{U}_{sys}}{dt} + \tilde{U}_{sys} \frac{dn_{sys}}{dt} \end{aligned} \quad (3)$$

Substitution of Eqs. (1) and (2) into Eq. (3) gives

$$-12(\tilde{H}_{out} - \tilde{U}_{sys}) = (n_o - 12t) \frac{d\tilde{U}_{sys}}{dt} \quad (4)$$

Since  $\tilde{H} = \tilde{U} + P\tilde{V} = \tilde{U} + \mathcal{R}T$ , the use of the first assumption enables us to express the left-hand side of Eq. (4) as

$$\begin{aligned} \tilde{H}_{out} - \tilde{U}_{sys} &= \tilde{H}_{sys} - \tilde{U}_{sys} \\ &= (\tilde{U}_{sys} + \mathcal{R}T_{sys}) - \tilde{U}_{sys} = \mathcal{R}T_{sys} \end{aligned} \quad (5)$$

On the other hand, the right-hand side of Eq. (4) is expressed in terms of temperature as

$$\frac{d\tilde{U}_{sys}}{dt} = \tilde{C}_V \frac{dT_{sys}}{dt} \quad (6)$$

Hence, substitution of Eqs. (5) and (6) into Eq. (4) gives

$$-12 \mathcal{R} T_{sys} = (n_o - 12t) \tilde{C}_V \frac{dT_{sys}}{dt} \quad (7)$$

For an ideal gas

$$\tilde{C}_P = \tilde{C}_V + \mathcal{R} \quad \Rightarrow \quad \frac{\tilde{C}_V}{\mathcal{R}} = \gamma - 1 \quad (8)$$

where

$$\gamma = \frac{\tilde{C}_P}{\tilde{C}_V} = \frac{29}{29 - 8.314} = 1.4 \quad (9)$$

Note that Eq. (7) is a separable equation. Substitution of Eq. (8) into Eq. (7) and rearrangement yields

$$-12(\gamma - 1) \int_0^t \frac{dt}{n_o - 12t} = \int_{T_o}^{T_{sys}} \frac{dT_{sys}}{T_{sys}} \quad (10)$$

Integration gives

$$T_{sys} = T_o \left( \frac{n_o - 12t}{n_o} \right)^{\gamma-1} \quad (11)$$

The variation of pressure as a function of time can be estimated by using the ideal gas law, i.e.,

$$P_{sys} = \frac{n_{sys} \mathcal{R} T_{sys}}{V} \quad (12)$$

Substitution of Eqs. (2) and (11) into Eq. (12) gives

$$P_{sys} = \frac{\mathcal{R} T_o}{V} (n_o - 12t) \left( \frac{n_o - 12t}{n_o} \right)^{\gamma-1} \quad (13)$$

Since  $\mathcal{R} T_o / V = P_o / n_o$ , Eq. (13) reduces to

$$P_{sys} = P_o \left( \frac{n_o - 12t}{n_o} \right)^{\gamma} \quad (14)$$

Substitution of the numerical values into Eqs. (11) and (14) gives  $T_{sys}$  and  $P_{sys}$ , respectively, after 5 minutes as

$$T_{sys} = (50 + 273) \left[ \frac{130.3 - (12)(5)}{130.3} \right]^{1.4-1} = 252.4 \text{ K}$$

$$P_{sys} = 7 \left[ \frac{130.3 - (12)(5)}{130.3} \right]^{1.4} = 2.95 \text{ bar}$$

**Comment:** Note that Eq. (11) can be rearranged in the form

$$\frac{T_{sys}}{T_o} = \left( \frac{n_{sys}}{n_o} \right)^{\gamma-1} \quad (15)$$

The use of the ideal gas law to express the number of moles gives

$$\frac{T_{sys}}{T_o} = \left( \frac{P_{sys}}{P_o} \right)^{\gamma-1} \left( \frac{T_o}{T_{sys}} \right)^{\gamma-1} \Rightarrow \frac{T_{sys}}{T_o} = \left( \frac{P_{sys}}{P_o} \right)^{(\gamma-1)/\gamma} \quad (16)$$

which is a well-known equation for a closed system undergoing a reversible adiabatic (or, isentropic) process. Therefore, the gas remaining in the tank undergoes a reversible adiabatic expansion throughout the process.

b) System: Contents of the tank

### Assumption

1. Properties of the tank contents are uniform, i.e.,  $\tilde{H}_{out} = \tilde{H}_{sys}$ .

### Analysis

Equation (7.3-2) becomes

$$-\dot{n}_{out} = \frac{dn_{sys}}{dt} \Rightarrow -12 = \frac{dn_{sys}}{dt} \quad (17)$$

Integration of Eq. (17) yields

$$n_{sys} = n_o - 12t \quad (18)$$

where  $n_o$  is the number of moles of air initially present in the tank, i.e.,

$$n_o = \frac{P_o V}{\mathcal{R} T_o} = \frac{(7)(0.5)}{(8.314 \times 10^{-5})(50 + 273)} = 130.3 \text{ mol}$$

In this case the process is isothermal and, as a result, the pressure of the system can be directly calculated from the ideal gas law, i.e.,

$$P_{sys} = \left( \frac{\mathcal{R} T_{sys}}{V} \right) n_{sys} \quad (19)$$

The use of Eq. (18) in Eq. (19) results in

$$\begin{aligned} P_{sys} &= \left( \frac{\mathcal{R} T_{sys}}{V} \right) (n_o - 12t) \\ &= P_o - 12 \left( \frac{\mathcal{R} T_{sys}}{V} \right) t \end{aligned} \quad (20)$$

Substitution of the numerical values gives

$$P = 7 - \frac{(12)(8.314 \times 10^{-5})(50 + 273)(5)}{0.5} = 3.78 \text{ bar}$$

The amount of heat supplied by the heating coils is determined from the inventory rate equation for energy, Eq. (7.5-5). Simplification of this equation is

$$\begin{aligned} -\tilde{H}_{out} \dot{n}_{out} + \dot{Q}_{int} &= \frac{d(n\tilde{U})_{sys}}{dt} \\ &= \tilde{U}_{sys} \frac{dn_{sys}}{dt} \end{aligned} \quad (21)$$

Since the process is isothermal,  $\tilde{U}_{sys}$  remains constant. Substituting Eq. (17) into Eq. (21) and using the fact that  $\tilde{H}_{out} = \tilde{H}_{sys}$  yields

$$\begin{aligned} \dot{Q}_{int} &= 12(\tilde{H}_{sys} - \tilde{U}_{sys}) = 12 \mathcal{R} T_{sys} \\ &= (12)(8.314)(50 + 273) = 32,225 \text{ J/min} \end{aligned}$$

Therefore, the amount of heat transferred is

$$Q_{int} = \dot{Q}_{int} t = (32,225)(5) = 161,125 \text{ J}$$

### 7.5.1 Unsteady-State Energy Balance Around a Continuous Stirred Tank Reactor

An unsteady-state energy balance in a continuous stirred tank reactor (CSTR) follows the same line as the steady-state case given in Section 6.3.2.2. Using the same assumptions, the resulting energy balance becomes

$$\left[ \sum_i \dot{n}_i \bar{H}_i(T_{in}) \right]_{in} - \left[ \sum_i \dot{n}_i \bar{H}_i(T) \right]_{out} + \dot{Q}_{int} = \frac{d}{dt} \left[ \sum_i n_i \bar{H}_i(T) \right]_{sys} \quad (7.5-10)$$

On the other hand, the macroscopic mole balance for species  $i$ , Eq. (7.2-5), is

$$(\dot{n}_i)_{in} - (\dot{n}_i)_{out} + V_{sys} \sum_j \alpha_{ij} r_j = \frac{d(n_i)_{sys}}{dt} \quad (7.5-11)$$

Multiplication of Eq. (7.5-11) by  $\bar{H}_i(T)$  and summation over all species gives

$$\begin{aligned} \left[ \sum_i \dot{n}_i \bar{H}_i(T) \right]_{in} - \left[ \sum_i \dot{n}_i \bar{H}_i(T) \right]_{out} - V_{sys} \sum_j r_j (-\Delta H_{rxn,j}) \\ = \left[ \sum_i \bar{H}_i(T) \frac{dn_i}{dt} \right]_{sys} \end{aligned} \quad (7.5-12)$$

Subtraction of Eq. (7.5-12) from Eq. (7.5-10) yields

$$\begin{aligned} \sum_i (\dot{n}_i)_{in} [\bar{H}_i(T_{in}) - \bar{H}_i(T)] + \dot{Q}_{int} + V_{sys} \sum_j r_j (-\Delta H_{rxn,j}) \\ = \left[ \sum_i n_i(T) \frac{d\bar{H}_i(T)}{dt} \right]_{sys} \end{aligned} \quad (7.5-13)$$

Dividing Eq. (7.5-13) by the volumetric flow rate,  $Q$ , gives

$$\begin{aligned} \sum_i (c_i)_{in} [\bar{H}_i(T_{in}) - \bar{H}_i(T)] + \frac{\dot{Q}_{int}}{Q} + \tau \sum_j r_j (-\Delta H_{rxn,j}) \\ = \tau \left[ \sum_i c_i(T) \frac{d\bar{H}_i(T)}{dt} \right]_{sys} \end{aligned} \quad (7.5-14)$$

where  $\tau$  is the residence time. Expressing the partial molar enthalpy of species  $i$  in terms of the partial molar heat capacity by Eq. (6.3-41) gives

$$\boxed{(C_P)_{in}(T_{in} - T) + \frac{\dot{Q}_{int}}{Q} + \tau \sum_j r_j (-\Delta H_{rxn,j}) = \tau (C_P)_{sys} \frac{dT}{dt}} \quad (7.5-15)$$

where

$$(C_P)_{in} = \sum_i (c_i)_{in} \bar{C}_{P_i} \quad (7.5-16)$$

$$(C_P)_{sys} = \sum_i (c_i)_{sys} \bar{C}_{P_i} \quad (7.5-17)$$

Note that Eq. (7.5-15) reduces to Eq. (6.3-42) under steady conditions. On the other hand, for a batch reactor, i.e., no inlet and outlet streams, Eq. (7.5-15) takes the form

$$\boxed{\dot{Q}_{int} + V_{sys} \sum_j r_j (-\Delta H_{rxn,j}) = V_{sys} (C_P)_{sys} \frac{dT}{dt}} \quad (7.5-18)$$

It is important to note that Eqs. (7.5-15) and (7.5-18) are valid for systems in which pressure remains constant.

**Example 7.9** *The reaction described in Example 6.6 is to be carried out in a batch reactor which operates adiabatically. The reactor is initially charged with 2000 moles of species A and 2400 moles of species B at a temperature of 25°C. Determine the time required for 80% conversion of A if the reactor volume is 1 m<sup>3</sup>.*

**Solution**

*System: Contents of the reactor*

*The conservation statement for species A, Eq. (7.2-5), is*

$$-k c_A c_B V = \frac{dn_A}{dt} \quad (1)$$

*or,*

$$-k n_A n_B = V \frac{dn_A}{dt} \quad (2)$$

*The number of moles of species A and B in terms of the molar extent of the reaction,  $\varepsilon$ , is given by*

$$n_A = n_{A_o} + \alpha_A \varepsilon = 2000 - \varepsilon \quad (3)$$

$$n_B = n_{B_o} + \alpha_B \varepsilon = 2400 - \varepsilon \quad (4)$$

*The molar extent of the reaction can be calculated from Eq. (5.3-12) as*

$$\begin{aligned} \varepsilon &= \frac{n_{A_o}}{(-\alpha_A)} X_A \\ &= \frac{(2000)(0.8)}{1} = 1600 \text{ mol} \end{aligned} \quad (5)$$

*Substitution of Eqs. (3) and (4) into Eq. (2) and rearrangement gives*

$$t = V \int_0^{1600} \frac{d\varepsilon}{k(2000 - \varepsilon)(2400 - \varepsilon)} \quad (6)$$

*Note that Eq. (6) cannot be integrated directly since the reaction rate constant,  $k$ , is dependent on  $\varepsilon$  via temperature.*

*The energy equation must be used to determine the variation of temperature as a function of the molar extent of the reaction. For an adiabatic reactor, i.e.,  $\dot{Q}_{int} = 0$ , Eq. (7.5-18) reduces to*

$$r(-\Delta H_{rxn}^o) = (C_P)_{sys} \frac{dT}{dt} \quad (7)$$

*Substitution of Eqs. (5.3-22) and (7.5-17) into Eq. (7) yields*

$$(-\Delta H_{rxn}^o) \frac{d\varepsilon}{dt} = \left[ \left( \sum_i n_{i_o} \tilde{C}_{P_i} \right) + \Delta \tilde{C}_P^o \varepsilon \right] \frac{dT}{dt} \quad (8)$$

*In this problem*

$$\Delta \tilde{C}_P^o = -85 \text{ J/mol.K} \quad (9)$$

$$\sum_i n_{i_o} \tilde{C}_{P_i} = (2000)(175) + (2400)(130) = 662,000 \quad (10)$$

$$\Delta H_{rxn}^o = -45,000 - 85(T - 298) \quad (11)$$

Substitution of Eqs. (9)-(11) into Eq. (8) and rearrangement gives

$$\int_0^\varepsilon \frac{d\varepsilon}{662,000 - 85\varepsilon} = \int_{298}^T \frac{dT}{45,000 + 85(T - 298)} \quad (12)$$

Integration gives

$$T = 298 + \frac{45,000\varepsilon}{662,000 - 85\varepsilon} \quad (13)$$

Now it is possible to evaluate Eq. (6) numerically. The use of Simpson's rule with  $n = 8$ , i.e.,  $\Delta\varepsilon = 200$ , gives

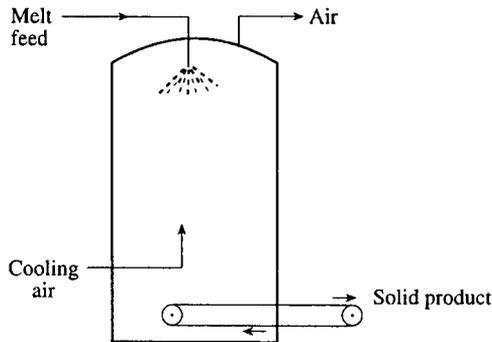
$\varepsilon$ (mol/m <sup>3</sup> )	$T$ (K)	$[k(2000 - \varepsilon)(2400 - \varepsilon)]^{-1} \times 10^4$
0	298	248
200	312	121.9
400	326.7	63.3
600	342.2	34.9
800	358.6	20.5
1000	376	12.9
1200	394.4	8.9
1400	414	6.9
1600	434.9	6.5

The application of Eq. (A.8-12) in Appendix A reduces Eq. (6) to

$$t = \frac{200}{3} [248 + 4(121.9 + 34.9 + 12.9 + 6.9) + 2(63.3 + 20.5 + 8.9) + 6.5] \times 10^{-4} = 7.64 \text{ min} \quad (14)$$

## 7.6 DESIGN OF A SPRAY TOWER FOR THE GRANULATION OF MELT

The purpose of this section is to apply the concepts covered in this chapter to a practical design problem. A typical tower for melt granulation is shown in Figure 7.3. The dimensions of the tower must be determined such that the largest melt particles solidify before striking the walls or the floor of the tower. Mathematical modelling of this tower can be accomplished by considering the unsteady-state macroscopic energy balances for the melt particles in conjunction with their settling velocities. This enables one to determine the cooling time and thus, the dimensions of the tower.



**Figure 7.3** Schematic diagram of a spray cooling tower.

It should be remembered that mathematical modeling is a highly interactive process. It is customary to build the initial model as simple as possible by making assumptions. Experience gained in working through this simplified model gives a feeling and confidence for the problem. The process is repeated several times, each time relaxing one of the assumptions and thus making the model more realistic. In the design procedure presented below, the following assumptions are made:

1. The particle falls at a constant terminal velocity.
2. Energy losses from the tower are negligible.
3. Particles do not shrink or expand during solidification, i.e., solid and melt densities are almost the same.
4. The temperature of the melt particle is uniform at any instant, i.e.,  $Bi \ll 1$ .
5. The physical properties are independent of temperature.
6. Solid particles at the bottom of the tower are at a temperature  $T_s$ , the solidification temperature.

### 7.6.1 Determination of Tower Diameter

The mass flow rate of air can be calculated from the energy balance around the tower:

$$\left( \begin{array}{c} \text{Rate of energy} \\ \text{gained by air} \end{array} \right) = \left( \begin{array}{c} \text{Rate of energy lost} \\ \text{by the melt particles} \end{array} \right) \quad (7.6-1)$$

or,

$$\dot{m}_a \langle \hat{C}_{P_a} \rangle [(T_a)_{out} - (T_a)_{in}] = \dot{m}_m \left\{ \hat{C}_{P_m} [(T_m)_{in} - T_s] + \hat{\lambda} \right\} \quad (7.6-2)$$

where the subscripts  $a$  and  $m$  stand for the air and the melt particle, respectively, and  $\hat{\lambda}$  is the latent heat of fusion per unit mass.

Once the air mass flow rate,  $\dot{m}_a$ , is calculated from Eq. (7.6-2), the diameter of the tower is calculated as

$$\dot{m}_a = \left( \frac{\pi D^2}{4} \right) v_a \rho_a \quad \Rightarrow \quad D = \sqrt{\frac{4 \dot{m}_a}{\pi \rho_a v_a}} \quad (7.6-3)$$

## 7.6.2 Determination of Tower Height

Tower height,  $H$ , is determined from

$$H = v_t t \quad (7.6-4)$$

The terminal velocity of the falling particle,  $v_t$ , is determined by using the formulas given in Section 4.3. The required cooling time,  $t$ , is determined from the unsteady-state energy balance around the melt particle.

### 7.6.2.1 Terminal velocity

The Turton-Clark correlation is an explicit relationship between the Archimedes and the Reynolds numbers as given by Eq. (4.3-12), i.e.,

$$\text{Re}_P = \frac{\text{Ar}}{18} [1 + 0.0579 \text{Ar}^{0.412}]^{-1.214} \quad (7.6-5)$$

The Archimedes number,  $\text{Ar}$ , can be calculated directly when the particle diameter and the physical properties of the fluid are known. The use of Eq. (7.6-5) then determines the Reynolds number. In this case, however, the definition of the Reynolds number involves the relative velocity,  $v_r$ , rather than the terminal velocity of the melt particle, i.e.,

$$\text{Re}_P = \frac{D_P v_r \rho_a}{\mu_a} \quad (7.6-6)$$

Since the air and the melt particle flow in countercurrent direction to each other, the relative velocity,  $v_r$ , is

$$v_r = v_t + v_a \quad (7.6-7)$$

### 7.6.2.2 Cooling time

The total cooling time consists of two parts: the cooling period during which the melt temperature decreases from the temperature at the inlet to  $T_s$  and, the solidification period during which the temperature of the melt remains at  $T_s$ .

*i) Cooling period:* Considering the melt particle as a system, the terms appearing

in Eq. (7.5-8) become

$$\begin{aligned}\dot{m}_{in} &= \dot{m}_{out} = 0 \\ \dot{W}_s &= 0 \\ \dot{Q}_{int} &= -(\pi D_P^2) \langle h \rangle (T_m - \langle T_a \rangle) \\ \frac{dP_{sys}}{dt} &= 0 \\ m_{sys} &= (\pi D_P^3 / 6) \rho_m \\ \hat{H}_{sys} &= \hat{C}_{P_m} (T_m - T_{ref})\end{aligned}$$

where  $\langle T_a \rangle$  is the average air temperature, i.e.,  $[(T_a)_{in} + (T_a)_{out}] / 2$ . Hence, Eq. (7.5-8) takes the form

$$-6 \langle h \rangle (T_m - \langle T_a \rangle) = D_P \rho_m \hat{C}_{P_m} \frac{dT_m}{dt} \quad (7.6-8)$$

Equation (7.6-8) is a separable equation and rearrangement yields

$$\int_0^{t_1} dt = -\frac{D_P \rho_m \hat{C}_{P_m}}{6 \langle h \rangle} \int_{(T_m)_{in}}^{T_s} \frac{dT_m}{T_m - \langle T_a \rangle} \quad (7.6-9)$$

Integration of Eq. (7.6-9) gives the cooling time,  $t_1$ , as

$$t_1 = \frac{D_P \rho_m \hat{C}_{P_m}}{6 \langle h \rangle} \ln \left[ \frac{(T_m)_{in} - \langle T_a \rangle}{T_s - \langle T_a \rangle} \right] \quad (7.6-10)$$

The average heat transfer coefficient,  $\langle h \rangle$  in Eq. (7.6-10) can be calculated from the Whitaker correlation, Eq. (4.3-30), i.e.,

$$\text{Nu} = 2 + \left( 0.4 \text{Re}_P^{1/2} + 0.06 \text{Re}_P^{2/3} \right) \text{Pr}^{0.4} (\mu_\infty / \mu_w)^{1/4} \quad (7.6-11)$$

*ii) Solidification period:* During the solidification process, solid and liquid phases coexist and temperature remains constant at  $T_s$ . Considering the particle as a system, the terms appearing in Eq. (7.5-8) become

$$\begin{aligned}\dot{m}_{in} &= \dot{m}_{out} = 0 \\ \dot{W}_s &= 0 \\ \dot{Q}_{int} &= -(\pi D_P^2) \langle h \rangle (T_s - \langle T_a \rangle) \\ \frac{dP_{sys}}{dt} &= 0 \\ m_{sys} &= m_l + m_s \\ T_{ref} = T_s &\Rightarrow \begin{cases} \hat{H}_l = 0 \\ \hat{H}_s = -\hat{\lambda} \end{cases} \Rightarrow (m\hat{H})_{sys} = m_l \hat{H}_l + m_s \hat{H}_s = -\hat{\lambda} m_s\end{aligned}$$

where  $m_l$  and  $m_s$  represent the liquid and solidified portions of the particle, respectively. Therefore, Eq. (7.5-8) reduces to

$$\pi D_P^2 \langle h \rangle (T_s - \langle T_a \rangle) = \hat{\lambda} \frac{dm_s}{dt} \quad (7.6-12)$$

Integration of Eq. (7.6-12) gives the time required for solidification,  $t_2$ , as

$$t_2 = \frac{\hat{\lambda} \rho_m D_P}{6 \langle h \rangle (T_s - \langle T_a \rangle)} \quad (7.6-13)$$

Therefore, the total time,  $t$ , in Eq. (7.6-4) is

$$t = t_1 + t_2 \quad (7.6-14)$$

**Example 7.10** Determine the dimensions of the spray cooling tower for the following conditions:

$$\text{Production rate} = 3000 \text{ kg/h}$$

$$D_P = 2 \text{ mm}$$

$$\rho_m = 1700 \text{ kg/m}^3$$

$$v_a = 2 \text{ m/s}$$

$$(T_a)_{in} = 10^\circ \text{C}$$

$$(T_a)_{out} = 20^\circ \text{C}$$

$$(T_m)_{in} = 110^\circ \text{C}$$

$$T_s = 70^\circ \text{C}$$

$$\hat{\lambda} = 186 \text{ kJ/kg}$$

$$\hat{C}_{P,m} = 1.46 \text{ kJ/kg}\cdot\text{K}$$

### Solution

#### Physical properties

The average air temperature is  $(10 + 20)/2 = 15^\circ \text{C}$ .

$$\text{For air at } 15^\circ \text{C (288 K)} : \begin{cases} \rho = 1.2 \text{ kg/m}^3 \\ \mu = 17.93 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ k = 25.22 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ \hat{C}_P = 1.004 \\ \text{Pr} = 0.714 \end{cases}$$

**Analysis**

The mass flow rate of air,  $\dot{m}_a$ , is calculated from Eq. (7.6-2) as

$$\begin{aligned}\dot{m}_a &= \frac{\dot{m}_m \left\{ \hat{C}_{P_m} [(T_m)_{in} - T_s] + \hat{\lambda} \right\}}{(\hat{C}_{P_a}) [(T_a)_{out} - (T_a)_{in}]} \\ &= \frac{(3000) [(1.46)(110 - 70) + 186]}{(1.004)(20 - 10)} = 73,028 \text{ kg/h}\end{aligned}$$

The use of Eq. (7.6-3) gives the tower diameter as

$$\begin{aligned}D &= \sqrt{\frac{4\dot{m}_a}{\pi\rho_a v_a}} \\ &= \sqrt{\frac{(4)(73,028)}{\pi(1.2)(2)(3600)}} = 3.3 \text{ m}\end{aligned}$$

The use of Eq. (4.3-6) gives the Archimedes number as

$$\begin{aligned}\text{Ar} &= \frac{D_P^3 g \rho_a (\rho_m - \rho_a)}{\mu_a^2} \\ &= \frac{(2 \times 10^{-3})^3 (9.8)(1.2)(1700 - 1.2)}{(17.93 \times 10^{-6})^2} = 4.97 \times 10^5\end{aligned}$$

Hence, the Reynolds number and the relative velocity are

$$\begin{aligned}\text{Re}_P &= \frac{\text{Ar}}{18} [1 + 0.0579 \text{Ar}^{0.412}]^{-1.214} \\ &= \frac{4.97 \times 10^5}{18} [1 + 0.0579 (4.97 \times 10^5)^{0.412}]^{-1.214} = 1134\end{aligned}$$

$$\begin{aligned}v_r &= \frac{\mu_a \text{Re}_P}{\rho_a D_P} \\ &= \frac{(17.93 \times 10^{-6})(1134)}{(1.2)(2 \times 10^{-3})} = 8.5 \text{ m/s}\end{aligned}$$

Therefore, the terminal velocity of the particle is

$$v_t = v_r - v_a = 8.5 - 2 = 6.5 \text{ m/s}$$

The use of the Whitaker correlation, Eq. (7.6-11), with  $\mu_\infty/\mu_w \approx 1$ , gives

$$\begin{aligned}\text{Nu} &= 2 + \left( 0.4 \text{Re}_P^{1/2} + 0.06 \text{Re}_P^{2/3} \right) \text{Pr}^{0.4} (\mu_\infty/\mu_w)^{1/4} \\ &= 2 + \left[ 0.4 (1134)^{1/2} + 0.06 (1134)^{2/3} \right] (0.714)^{0.4} = 19.5\end{aligned}$$

Hence, the average heat transfer coefficient is

$$\begin{aligned}\langle h \rangle &= \text{Nu} \left( \frac{k}{D_P} \right) \\ &= (19.5) \left( \frac{25.22 \times 10^{-3}}{2 \times 10^{-3}} \right) = 246 \text{ W/m}^2 \cdot \text{K}\end{aligned}$$

The time required for cooling and solidification can be calculated from Eqs. (7.6-10) and (7.6-13), respectively:

$$\begin{aligned}t_1 &= \frac{D_P \rho_m \hat{C}_{P_m}}{6 \langle h \rangle} \ln \left[ \frac{(T_m)_{in} - \langle T_a \rangle}{T_s - \langle T_a \rangle} \right] \\ &= \frac{(2 \times 10^{-3})(1700)(1460)}{(6)(246)} \ln \left( \frac{110 - 15}{70 - 15} \right) = 1.8 \text{ s} \\ t_2 &= \frac{\hat{\lambda} \rho_m D_P}{6 \langle h \rangle (T_s - \langle T_a \rangle)} \\ &= \frac{(186,000)(1700)(2 \times 10^{-3})}{(6)(246)(70 - 15)} = 7.8 \text{ s}\end{aligned}$$

Therefore, the tower height is

$$H = (6.5)(1.8 + 7.8) = 62.4 \text{ m}$$

## NOTATION

$A$	area, $\text{m}^2$
$A_M$	mass transfer area, $\text{m}^2$
$\hat{C}_V$	heat capacity at constant volume, $\text{kJ/kg} \cdot \text{K}$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ/kg} \cdot \text{K}$
$c$	concentration, $\text{kmol/m}^3$
$\mathcal{D}_{AB}$	diffusion coefficient for system $\mathcal{A}\text{-}\mathcal{B}$ , $\text{m}^2/\text{s}$
$E_K$	kinetic energy, $\text{J}$
$E_P$	potential energy, $\text{J}$
$\dot{E}$	rate of energy, $\text{J/s}$
$\mathcal{E}$	activation energy, $\text{J/mol}$
$f$	friction factor
$g$	acceleration of gravity, $\text{m/s}^2$
$H$	enthalpy, $\text{J}$
$h$	elevation, $\text{m}$ ; heat transfer coefficient, $\text{W/m}^2 \cdot \text{K}$
$k$	thermal conductivity, $\text{W/m} \cdot \text{K}$
$k_c$	mass transfer coefficient, $\text{m/s}$

$L$	length, m
$\dot{m}$	mass flow rate, kg/s
$\mathcal{M}$	molecular weight, kg/kmol
$\dot{n}$	molar flow rate, kmol/s
$P$	pressure, Pa
$\dot{Q}$	heat transfer rate, W
$Q$	volumetric flow rate, m <sup>3</sup> /s
$r$	rate of a chemical reaction, kmol/m <sup>3</sup> ·s
$\mathcal{R}$	gas constant, J/mol·K
$T$	temperature, °C or K
$t$	time, s
$U$	internal energy, J
$V$	volume, m <sup>3</sup>
$v$	velocity, m/s
$\dot{W}$	rate of work, W
$\dot{W}_s$	rate of shaft work, W
$X$	fractional conversion
$x_i$	mole fraction of species $i$
$\alpha$	thermal diffusivity, m <sup>2</sup> /s
$\alpha_{ij}$	stoichiometric coefficient of $i^{\text{th}}$ species in the $j^{\text{th}}$ reaction
$\gamma$	$\tilde{C}_P/\tilde{C}_V$
$\Delta$	difference
$\Delta H_{rxn}$	heat of reaction, J
$\varepsilon$	molar extent of a reaction, kmol
$\lambda$	latent heat, J
$\nu$	kinematic viscosity (or, momentum diffusivity), m <sup>2</sup> /s
$\rho$	density, kg/m <sup>3</sup>
$\tau$	residence time, s

**Overlines**

$\sim$	per mole
$\hat{\phantom{x}}$	per unit mass
$\bar{\phantom{x}}$	partial molar

**Bracket**

$\langle a \rangle$	average value of $a$
---------------------	----------------------

**Superscripts**

$o$	standard state
$S$	solid
$sat$	saturation

**Subscripts**

<i>A, B</i>	species in binary systems
<i>a</i>	air
<i>ch</i>	characteristic
<i>i</i>	species in multicomponent systems
<i>in</i>	inlet
<i>int</i>	interphase
<i>j</i>	reaction number
<i>m</i>	melt
<i>out</i>	out
<i>P</i>	particle
<i>sys</i>	system
<i>w</i>	surface or wall
$\infty$	free-stream

**Dimensionless Numbers**

Ar	Archimedes number
$Bi_H$	Biot number for heat transfer
$Bi_M$	Biot number for mass transfer
Pr	Prandtl number
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number

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## PROBLEMS

7.1 Two perfectly stirred tanks with capacities of 1.5 and 0.75 m<sup>3</sup> are connected in such a way that the effluent from the first passes to the second. Both tanks are initially filled with salt solution of 0.5 kg/L in concentration. If pure water is fed to the first tank at a rate of 75 L/min, determine the salt concentration in the second tank after 10 minutes?

(Answer: 0.423 kg/L)

7.2 Two vertical tanks placed on a platform are connected by a horizontal pipe 5 cm in diameter as shown in Figure 7.4. Each tank is 2 m deep and 1 m in diameter. At first, the valve on the pipe is closed and one tank is full while the other one is empty. When the valve is opened, the average velocity through the pipe is given by

$$\langle v \rangle = 2\sqrt{h}$$

where  $\langle v \rangle$  is the average velocity in m/s and  $h$  is the difference between the levels in the two tanks in meter. Calculate the time for the levels in the two tanks to become equal.

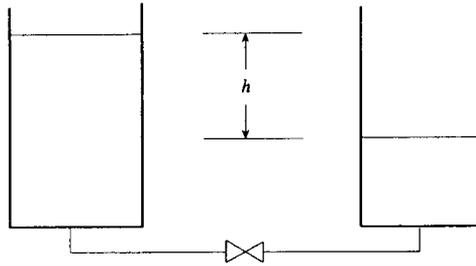


Figure 7.4 Schematic diagram for Problem 7.2

(Answer: 4.7 min)

7.3 a) A stream containing 10% species  $A$  by weight starts to flow at a rate of 2 kg/min into a tank, originally holding 300 kg of pure  $B$ . Simultaneously, a valve at the bottom of the tank is opened and the tank contents are also withdrawn at a rate of 2 kg/min. Considering perfect mixing within the tank, determine the time required for the exit stream to contain 5% species  $A$  by weight.

b) Consider the problem in part (a). As a result of the malfunctioning of the exit valve, tank contents are withdrawn at a rate of 2.5 kg/min instead of 2 kg/min. How long does it take for the exit stream to contain 5% species  $A$  in this case?

(Answer: a) 104 min b) 95.5 min)

7.4 The following levels were measured for the flow system shown in Figure 7.5. The cross-sectional area of each tank is  $1.5 \text{ m}^2$ .

$t$ (min)	$h_1$ (cm)	$h_2$ (cm)
0	50	30
1	58	35
2	67	40
3	74	46
4	82	51
5	89	58
6	96	64

a) Determine the value of  $Q_{in}$ .

b) If the flow rate of the stream leaving the first tank,  $Q$ , is given as

$$Q = \beta \sqrt{h_1}$$

determine the value of  $\beta$ .

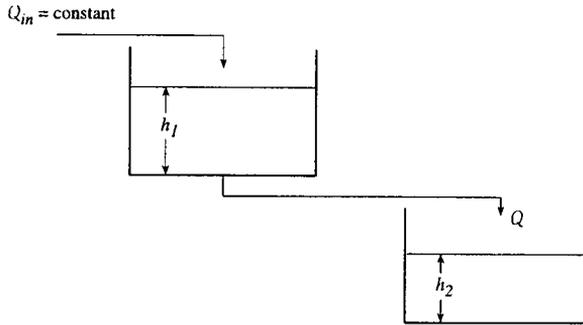


Figure 7.5 Schematic diagram for Problem 7.4

(Answer: a)  $0.2 \text{ m}^3/\text{min}$  b)  $0.17 \text{ m}^{5/2}/\text{min}$ )

7.5 Time required to empty a vessel is given for four common tank geometries by Foster (1981) as shown in Table 7.1. In each case, the liquid leaves the tank through an orifice of cross-sectional area  $A_o$ . The orifice coefficient is  $C_o$ . Assume that the pressure in each tank is atmospheric. Verify the formulas in Table 7.1.

7.6 For steady flow of an incompressible fluid through a control volume whose boundaries are stationary in space, show that Eq. (6.3-9) reduces to

$$\frac{\Delta P}{\rho} + \frac{\Delta \langle v \rangle^2}{2} + g \Delta h + (\Delta \hat{U} - \hat{Q}_{int}) = \hat{W}_s \quad (1)$$

where  $\Delta$  represents a difference between the outlet and inlet values.

a) Using the thermodynamic relations

$$d\hat{U} = T d\hat{S} - P d\hat{V} \quad (2)$$

and

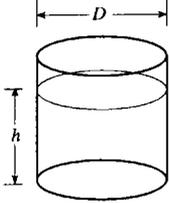
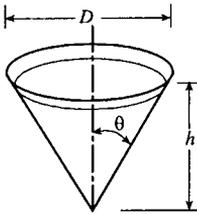
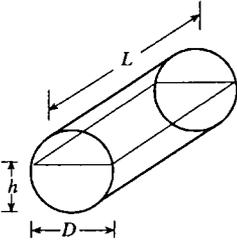
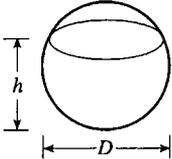
$$d\hat{S} = \frac{d\hat{Q}_{int}}{T} + d\hat{S}_{gen} \quad (3)$$

show that

$$d\hat{E}_v = T d\hat{S}_{gen} = d\hat{U} - d\hat{Q}_{int} \quad (4)$$

where  $\hat{E}_v$ , the friction loss per unit mass, represents the irreversible degradation of mechanical energy into thermal energy, and  $\hat{S}_{gen}$  is the entropy generation per unit mass.

**Table 7.1** Time required to empty tanks of different geometries.

Geometry	Time
	$t = \frac{\pi D^2 \sqrt{h}}{\sqrt{8g} C_o A_o}$
	$t = \sqrt{\frac{2}{g}} \frac{\pi h^{5/2} \tan^2 \theta}{5 C_o A_o}$
	$t = \sqrt{\frac{8}{g}} L \frac{[D^{3/2} - (D - h)^{3/2}]}{3 C_o A_o}$
	$t = \sqrt{\frac{2}{g}} \frac{\pi h^{3/2} (D - 0.6h)}{3 C_o A_o}$

b) Substitute Eq. (4) into Eq. (1) to obtain the engineering Bernoulli equation (or, macroscopic mechanical energy equation) for an incompressible fluid as

$$\frac{\Delta P}{\rho} + \frac{\Delta \langle v \rangle^2}{2} + g \Delta h + \hat{E}_v - \hat{W}_s = 0 \tag{5}$$

c) To estimate the friction loss for flow in a pipe, consider steady flow of an incompressible fluid in a horizontal pipe of circular cross-section. Simplify Eq. (5)

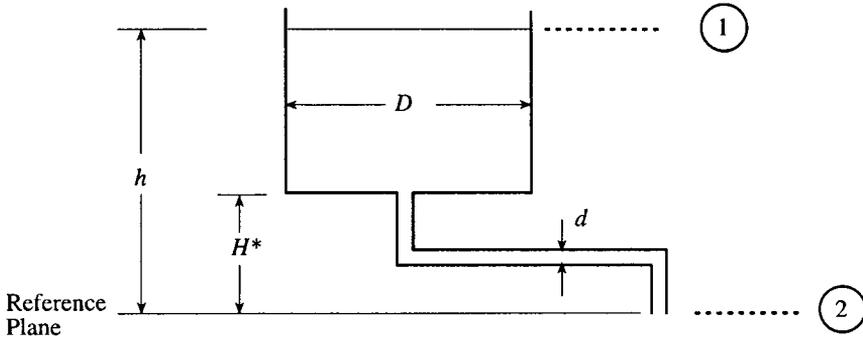
for this case to get

$$\hat{E}_v = \frac{|\Delta P|}{\rho} \quad (6)$$

Compare Eq. (6) with Eq. (4.5-6) and show that the friction loss per unit mass,  $\hat{E}_v$ , for pipe flow is given by

$$\hat{E}_v = \frac{2fL\langle v \rangle^2}{D} \quad (7)$$

**7.7** A cylindrical tank, 5 m in diameter, discharges through a mild steel pipe system ( $\varepsilon = 4.6 \times 10^{-5}$  m) connected to the tank base as shown in the figure below. The drain pipe system has an equivalent length of 100 m and a diameter of 23 cm. The tank is initially filled with water to an elevation of  $H$  with respect to the reference plane.



a) Apply the Bernoulli equation, Eq. (5) in Problem 7.6, to the region between planes "1" and "2" and show that

$$\langle v_2 \rangle^2 = \frac{2gh}{1 + \frac{4fL_{eq}}{d}}$$

where  $L_{eq}$  is the equivalent length of the drain pipe.

b) Consider the tank as a system and show that the application of the unsteady-state macroscopic mass balance gives

$$dt = - \left( \frac{D}{d} \right)^2 \sqrt{\frac{1}{2g} \left( 1 + \frac{4fL_{eq}}{d} \right)} \frac{dh}{\sqrt{h}} \quad (2)$$

Analytical integration of Eq. (2) is possible only if the friction factor  $f$  is constant.

c) At any instant, note that the pressure drop in the drain pipe system is equal to  $\rho g(h - H^*)$ . Use Eqs. (4.5-18)-(4.5-20) to determine  $f$  as a function of liquid height in the tank. Take  $H^* = 1$  m,  $H = 4$  m and the final value of  $h$  as 1.5 m.

d) If  $f$  remains almost constant, then show that the integration of Eq. (2) yields

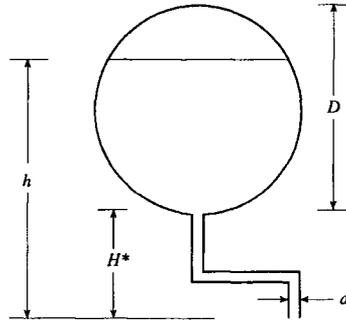
$$t = \left(\frac{D}{d}\right)^2 \sqrt{\frac{2}{g} \left(1 + \frac{4fL_{eq}}{d}\right)} (\sqrt{H} - \sqrt{h}) \quad (3)$$

Calculate the time required for  $h$  to drop from 4 m to 1.5 m.

e) Plot the variations of  $\langle v_2 \rangle$  and  $h$  as a function of time on the same plot. Show that  $dh/dt$  is negligible at all times in comparison with the liquid velocity through the drain pipe system.

(Answer: c) 0.0039 d) 7.7 min)

7.8 Consider draining of a spherical tank of diameter  $D$  with associated drain piping as shown in the figure below. The tank is initially filled with water to an elevation of  $H$  with respect to the reference plane.



a) Repeat the procedure given in Problem 7.7 and show that

$$t = \frac{4}{d^2} \sqrt{\frac{2}{g} \left(1 + \frac{4fL_{eq}}{d}\right)} \left[ \sqrt{h} \left( \frac{h^2}{5} - \frac{2}{3} X_1 h + X_2 \right) - \sqrt{H} \left( \frac{H^2}{5} - \frac{2}{3} X_1 H + X_2 \right) \right]$$

where

$$X_1 = H^* + R$$

$$X_2 = X_1^2 - R^2$$

b) A spherical tank, 4 m in diameter, discharges through a mild steel pipe system ( $\varepsilon = 4.6 \times 10^{-5}$  m) with an equivalent length of 100 m and a diameter of 23 cm. Determine the time to drain the tank if  $H^* = 1$  m and  $H = 4.5$  m.

(Answer: b) 4.9 min)

**7.9** Suspended particles in agitated vessels are frequently encountered in the chemical process industries. Some examples are mixer-settler extractors, catalytic slurry reactors and crystallizers. The design of such equipment requires the mass transfer coefficient to be known. For this purpose, solid particles (species  $\mathcal{A}$ ) with a known external surface area,  $A_o$ , and total mass,  $M_o$ , are added to an agitated liquid of volume  $V$  and the concentration of species  $\mathcal{A}$  is recorded as a function of time.

a) Consider the liquid as a system and show that the unsteady-state macroscopic mass balance for species  $\mathcal{A}$  is

$$\langle k_c \rangle A_o \left( \frac{M}{M_o} \right)^{2/3} (c_A^{sat} - c_A) = V \frac{dc_A}{dt} \quad (1)$$

where  $M$  is the total mass of solid particles at any instant and  $c_A^{sat}$  is the equilibrium solubility. Rearrange Eq. (1) in the form

$$\langle k_c \rangle = - \frac{V}{A_o (M/M_o)^{2/3}} \frac{d \ln(c_A^{sat} - c_A)}{dt} \quad (2)$$

and show how one can obtain the average mass transfer coefficient from the experimental data.

b) Another way of calculating the mass transfer coefficient is to choose experimental conditions so that only a small fraction of the initial solids is dissolved during a run. Under these circumstances, show that the average mass transfer coefficient can be calculated from the following expression:

$$\langle k_c \rangle = \frac{V}{\langle A \rangle t} \ln \left( \frac{c_A^{sat}}{c_A^{sat} - c_A} \right) \quad (3)$$

where  $\langle A \rangle$  is the average surface area of the particles. Indicate the assumptions involved in the derivation of Eq. (3).

**7.10** Consider Problem 7.9 in which the average mass transfer coefficient of suspended particles is known. Estimate the time required for the dissolution of solid particles as follows:

a) Write down the total mass balance for species  $\mathcal{A}$  and relate the mass of the particles,  $M$ , to concentration of species  $\mathcal{A}$ ,  $c_A$ , as

$$\frac{M}{M_o} = 1 - \left( \frac{V}{M_o} \right) c_A \quad (1)$$

b) Substitute Eq. (1) into Eq. (1) in Problem 7.9 to get

$$dt = \alpha \frac{d\theta}{[1 - (1 + \beta^3)\theta]^{2/3} (1 - \theta)} \quad (2)$$

where

$$\theta = \frac{c_A}{c_A^{sat}} \quad \alpha = \frac{V}{(k_c)A_o} \quad \beta^3 = \frac{Vc_A^{sat}}{M_o} - 1 \quad (3)$$

c) Show that the integration of Eq. (2) leads to

$$t = \frac{1}{6\beta^2} \ln \left[ \left( \frac{u+\beta}{1+\beta} \right)^2 \left( \frac{1-\beta+\beta^2}{u^2-u\beta+\beta^2} \right) \right] + \frac{1}{\sqrt{3}\beta^2} \tan^{-1} \left\{ \frac{\sqrt{3}(u-1)}{2\beta-1+u[(2/\beta)-1]} \right\} \quad (4)$$

where

$$u^3 = 1 - (1 + \beta^3)\theta \quad (5)$$

**7.11** Rework Example 7.3 if the rate of reaction is given by

$$r = k c_A^2 \quad (1)$$

a) For the filling period show that the governing differential equation is given by

$$t \frac{dc_A}{dt} + k t c_A^2 + c_A = c_{A_o} \quad (2)$$

Using the substitution

$$c_A = \frac{1}{ku} \frac{du}{dt} \quad (3)$$

show that Eq. (1) reduces to

$$\frac{d}{dt} \left( t \frac{du}{dt} \right) - c_{A_o} k u = 0 \quad (4)$$

Solve Eq. (4) and obtain the solution as

$$c_A = \sqrt{\frac{c_{A_o}}{kt}} \frac{I_1(2\sqrt{c_{A_o}kt})}{I_o(2\sqrt{c_{A_o}kt})} \quad (5)$$

Note that Eq. (2) indicates that  $c_A = c_{A_o}$  at  $t = 0$ . Obtain the same result from Eq. (5).

b) Show that the governing differential equation for the unsteady-state period is given in the form

$$\frac{dc_A}{dt} + k c_A^2 + \frac{c_A}{\tau} = \frac{c_{A_o}}{\tau} \quad (6)$$

where  $\tau$  is the residence time. Using

$$c_A = c_{A_s} + \frac{1}{z} \quad (7)$$

show that Eq. (6) reduces to

$$\frac{dz}{dt} - \beta z = k \quad (8)$$

where

$$\beta = 2k c_{A_s} + \frac{1}{\tau} \quad (9)$$

Note that  $c_{A_s}$  in Eq. (7) represents the steady-state concentration satisfying the equation

$$k c_{A_s}^2 + \frac{c_{A_s}}{\tau} = \frac{c_{A_0}}{\tau} \quad (10)$$

Solve Eq. (8) and obtain

$$c_A = c_{A_s} + \frac{1}{\left[ (c_A^* - c_{A_s})^{-1} + (k/\beta) \right] \exp[\beta(t - t^*)] - (k/\beta)} \quad (11)$$

where  $c_A^*$  and  $t^*$  represent the concentration and time at the end of the filling period, respectively.

**7.12** For creeping flow, i.e.,  $\text{Re} \ll 1$ , a relationship between the friction factor and the Reynolds number is given by Stokes' law, Eq. (4.3-7).

a) Substitute Eq. (4.3-7) into Eq. (7.4-7) and show that

$$v = \frac{(\rho_P - \rho) g D_P^2}{18 \mu} \left\{ 1 - \exp \left[ - \frac{18 \mu t}{(\rho_P + 0.5 \rho) D_P^2} \right] \right\} \quad (1)$$

b) Show that the time required for the sphere to reach 99% of its terminal velocity,  $t_\infty$ , is given by

$$t_\infty = \frac{D_P^2}{3.9 \mu} (\rho_P + 0.5 \rho) \quad (2)$$

and investigate the cases under which initial acceleration period is negligible.

c) Show that the distance travelled by the particle during unsteady-state fall is given by

$$s = t v_t - v_t \frac{(\rho_P - \rho) D_P^2}{18 \mu} \left\{ 1 - \exp \left[ - \frac{18 \mu t}{(\rho_P + 0.5 \rho) D_P^2} \right] \right\} \quad (3)$$

where  $v_t$  is the terminal velocity of the falling particle and is defined by

$$v_t = \frac{(\rho_P - \rho) g D_P^2}{18 \mu} \quad (4)$$

**7.13** When Newton's law is applicable, the friction factor is constant and is given by Eq. (4.3-9).

a) Substitute Eq. (4.3-9) into Eq. (7.4-7) and show that

$$\frac{v}{v_t} = \frac{1 - \exp(-\gamma t)}{1 + \exp(-\gamma t)} \quad (1)$$

where the terminal velocity,  $v_t$ , and  $\gamma$  are given by

$$v_t = 1.74 \sqrt{\frac{(\rho_P - \rho) g D_P}{\rho}} \quad (2)$$

$$\gamma^{-1} = 1.51 \left( \frac{\rho_P + 0.5\rho}{\rho} \right) \frac{D_P}{v_t} \quad (3)$$

b) Show that the distance travelled is

$$s = t v_t + \frac{2 v_t}{\gamma} \ln \left[ \frac{1 + \exp(-\gamma t)}{2} \right] \quad (4)$$

**7.14** Consider two-dimensional motion of a spherical particle in a fluid. When the horizontal component of velocity is very large compared to the vertical component, the process can be modelled as a one-dimensional motion in the absence of a gravitational field. Using unsteady-state momentum balance show that

$$t = \frac{4 \rho_P D_P^2}{3 \mu} \int_{\text{Re}_P}^{\text{Re}_{P_0}} \frac{d \text{Re}_P}{f \text{Re}_P^2} \quad (1)$$

where  $\text{Re}_{P_0}$  is the value of the Reynolds number at  $t = 0$ .

a) When Stokes' law is applicable, show that the distance travelled by the particle is given by

$$s = \frac{v_o \rho_P D_P^2}{18 \mu} \left[ 1 - \exp \left( - \frac{18 \mu t}{\rho_P D_P^2} \right) \right] \quad (2)$$

where  $v_o$  is the value of velocity at  $t = 0$ .

b) When Newton's law is applicable, show that the distance travelled by the particle is given by

$$s = \frac{3.03 \rho_P D_P}{\rho} \ln \left( 1 + \frac{\rho v_o t}{3.03 \rho_P D_P} \right) \quad (3)$$

**7.15** Coming home with a friend to have a cold beer after work, you find out that you had left the beer on the kitchen counter. As a result of the sunlight coming from the kitchen window, it was too warm to drink.

One way of cooling the beer is obviously putting it into a freezer. However, your friend insists that placing a can of beer in a pot in the kitchen sink, and letting cold water run over it into the pot and then into the sink shortens the cooling time. He claims that the overall heat transfer coefficient for this process is much greater than that for a can of beer sitting idly in the freezer in still air. He supports this idea by presenting the following data of Horwitz (1981):

	Freezer	Tap Water
Cooling medium temperature ( $^{\circ}\text{C}$ )	- 21	13
Initial temperature of beer ( $^{\circ}\text{C}$ )	29	29
Final temperature of beer ( $^{\circ}\text{C}$ )	15	15
Time elapsed (min)	21.1	8.6
Surface area of can = $0.03 \text{ m}^2$		
Quantity of beer in can = $0.355 \text{ kg}$		
Heat capacity of beer = $4.2 \text{ kJ/kg}\cdot\text{K}$		

a) Do you think that your friend is right? Show your work by calculating the heat transfer coefficient in each case. Ignore the cost and availability of water.

b) Calculate the time required to cool the beer from  $29^{\circ}\text{C}$  to  $4^{\circ}\text{C}$  in the freezer.

c) Suppose that you first cool the beer to  $15^{\circ}\text{C}$  by the running water and then place the beer in the freezer. Calculate the time required to cool the beer from  $29^{\circ}\text{C}$  to  $4^{\circ}\text{C}$  in this case.

(Answer: a)  $\langle h \rangle$  (freezer) =  $12.9 \text{ W/m}^2\cdot\text{K}$ ,  $\langle h \rangle$  (tap water) =  $200 \text{ W/m}^2\cdot\text{K}$   
 b) 44.5 min c) 32 min)

**7.16**  $M$  kg of a liquid is to be heated from  $T_1$  to  $T_2$  in a well stirred, jacketed tank by steam condensing at  $T_s$  in the jacket. The heat transfer area,  $A$ , the heat capacity of tank contents per unit mass,  $\hat{C}_P$ , and the overall heat transfer coefficient,  $U$ , are known. Show that the required heating time is given by

$$t = \frac{M\hat{C}_P}{UA} \ln \left( \frac{T_s - T_1}{T_s - T_2} \right) \quad (1)$$

Indicate the assumptions involved in the derivation of Eq. (1).

**7.17** In Problem 7.16, assume that hot water, with a constant mass flow rate  $\dot{m}$  and inlet temperature  $T_{in}$ , is used as a heating medium instead of steam.

a) Show that the outlet temperature of hot water,  $T_{out}$ , is given by

$$T_{out} = T + \frac{T_{in} - T}{\Omega} \quad (1)$$

where

$$\Omega = \exp\left(\frac{UA}{\dot{m}C}\right) \quad (2)$$

in which  $T$  is the temperature of the tank contents at any instant and  $C$  is the heat capacity of hot water.

b) Write down the unsteady-state energy balance and show that the time required to increase the temperature of the tank contents from  $T_1$  to  $T_2$  is given by

$$t = \frac{M\hat{C}_P}{\dot{m}C} \left(\frac{\Omega}{\Omega - 1}\right) \ln\left(\frac{T_{in} - T_1}{T_{in} - T_2}\right) \quad (3)$$

c) Bondy and Lippa (1983) argued that when the difference between the outlet and inlet jacket temperatures is less than 10% of the  $\Delta T_{LM}$  between the average temperature of the jacket and the temperature of the tank contents, Eq. (1) in Problem 7.16 can be used instead of Eq. (3) by replacing  $T_s$  by the average jacket temperature. Do you agree? For more information on this problem see Tosun and Akşahin (1993).

**7.18** 600 kg of a liquid is to be heated from 15 °C to 150 °C in a well stirred, jacketed tank by steam condensing at 170 °C in the jacket. The heat transfer surface area of the jacket is 4.5 m<sup>2</sup> and the heat capacity of the liquid is 1850 J/kg·K. The overall heat transfer coefficient,  $U$ , varies with temperature as follows:

$T$ (°C)	$U$ (W/m <sup>2</sup> ·K)
15	390
30	465
60	568
90	625
120	664
150	680

- a) Calculate the required heating time.  
 b) Correlate the data in terms of the expression

$$U = A - \frac{B}{T}$$

where  $T$  is in degrees Kelvin, and calculate the required heating time.

(Answer: a) 11.7 min; b) 13.7 min)

**7.19** 500 kg of a liquid is to be heated from 15 °C to 150 °C in a well stirred, jacketed tank by steam condensing at 170 °C in the jacket. The heat transfer surface

area of the jacket is  $4.5 \text{ m}^2$  and the heat capacity of the liquid is  $1850 \text{ J/kg}\cdot\text{K}$ . Calculate the average overall heat transfer coefficient if the variation of liquid temperature as a function of time is recorded as follows:

$t$ (min)	$T$ ( $^{\circ}\text{C}$ )
0	15
2	59
4	90
6	112
8	129
10	140
12	150

(Answer:  $564 \text{ W/m}^2\cdot\text{K}$ )

**7.20** An insulated rigid tank of volume  $0.1 \text{ m}^3$  is connected to a large pipeline carrying air at 10 bar and  $120^{\circ}\text{C}$ . The valve between the pipeline and the tank is opened and air is admitted to the tank at a constant mass flow rate. The pressure in the tank is recorded as a function of time as follows:

$t$ (min)	$P$ (bar)
5	1.6
10	2.1
15	2.7
20	3.3
25	3.9
30	4.4

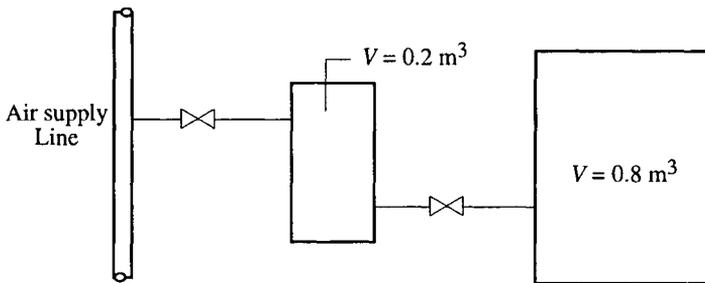
If the tank initially contains air at 1 bar and  $20^{\circ}\text{C}$ , determine the mass flow rate of air entering the tank. Air may be assumed an ideal gas with a constant  $\tilde{C}_P$  of  $29 \text{ J/mol}\cdot\text{K}$ .

(Answer:  $7.25 \text{ g/min}$ )

**7.21** An insulated rigid tank of volume  $0.2 \text{ m}^3$  is connected to a large pipeline carrying nitrogen at 10 bar and  $70^{\circ}\text{C}$ . The valve between the pipeline and the tank is opened and nitrogen is admitted to the tank at a constant mass flow rate of  $4 \text{ g/s}$ . Simultaneously, nitrogen is withdrawn from the tank, also at a constant mass flow rate of  $4 \text{ g/s}$ . Calculate the temperature and pressure within the tank after 1 minute if the tank initially contains nitrogen at 2 bar and  $35^{\circ}\text{C}$ . Nitrogen may be assumed an ideal gas with a constant  $\tilde{C}_P$  of  $30 \text{ J/mol}\cdot\text{K}$ .

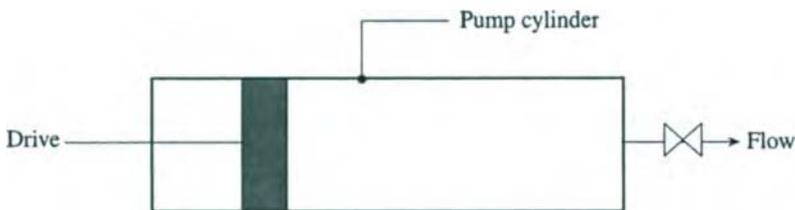
(Answer:  $326.8 \text{ K}$ ,  $2.12 \text{ bar}$ )

**7.22** A rigid tank of volume  $0.2\text{ m}^3$  initially contains air at 2 bar and  $35^\circ\text{C}$ . On one side it is connected to an air supply line at 10 bar and  $70^\circ\text{C}$ , on the other side it is connected to an empty rigid tank of  $0.8\text{ m}^3$  as shown in the figure below. Both tanks are insulated and initially both valves are closed. The valve between the pipeline and the tank is opened and air starts to flow into the tank at a constant flow rate of  $10\text{ mol/min}$ . Simultaneously, the valve between the tanks is also opened so as to provide a constant flow rate of  $6\text{ mol/min}$  to the larger tank. Determine the temperature and pressure of air in the larger tank after 2 minutes. Air may be assumed an ideal gas with a constant  $\tilde{C}_P$  of  $29\text{ J/mol}\cdot\text{K}$ .



(Answer: 482.3 K, 0.6 bar)

**7.23** Metering pumps provide a constant liquid mass flow rate for a wide variety of scientific, industrial and medical applications. A typical pump consists of a cylinder fitted with a piston as shown in Figure 7.19. The piston is generally located on the end of a long screw which itself is driven at a constant velocity by a synchronous electric motor.



a) Assume that the manufacturer has calibrated the pump at some reference temperature,  $T_{ref}$ . Write down the unsteady-state mass balance and show that the reference mass flow rate,  $\dot{m}_{ref}$ , delivered by the pump is given by

$$\dot{m}_{ref} = -\rho_{ref} \frac{dV_{ref}}{dt} \tag{1}$$

where  $\rho_{ref}$  and  $V_{ref}$  are the density and the volume of the liquid in the pump cylinder at the reference temperature, respectively. Integrate Eq. (1) and show

that the variation in the liquid volume as a function of time is given by

$$V_{ref} = V_{ref}^o - \left( \frac{\dot{m}_{ref}}{\rho_{ref}} \right) t \quad (2)$$

where  $V_{ref}^o$  is the volume of the cylinder at  $t = 0$ .

b) If the pump operates at a temperature different from the reference temperature, show that the mass flow rate provided by the pump is given by

$$\dot{m} = - \frac{d}{dt} (\rho V) \quad (3)$$

where  $\rho$  and  $V$  are the density and the volume of the pump liquid at temperature  $T$ , respectively. Expand  $\rho$  and  $V$  in a Taylor series in  $T$  about the reference temperature  $T_{ref}$  and show that

$$\rho V \simeq \rho_{ref} V_{ref} - \rho_{ref} V_{ref} (\beta_C - \beta_L) (T - T_{ref}) \quad (4)$$

where  $\beta$ , the coefficient of volume expansion, is defined by

$$\beta = \frac{1}{\hat{V}} \left( \frac{\partial \hat{V}}{\partial T} \right)_P = - \frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_P \quad (5)$$

in which the subscripts  $L$  and  $C$  represent the liquid and the cylinder, respectively. Indicate the assumptions involved in the derivation of Eq. (4).

c) Show that the substitution of Eq. (4) into Eq. (3) and making use of Eqs. (1) and (2) gives the fractional error in mass flow rate as

$$\frac{\dot{m} - \dot{m}_{ref}}{\dot{m}_{ref}} = - (\beta_L - \beta_C) (T - T_{ref}) + \left( \frac{V_{ref}^o}{R_o} - t \right) (\beta_L - \beta_C) \frac{dT}{dt} \quad (6)$$

where

$$R_o = - \frac{dV_{ref}}{dt} \quad (7)$$

Note that the first and the second terms on the right-side of Eq. (6) represent, respectively, the steady-state and the unsteady-state contributions to the error term.

d) Assume that at any instant the temperature of the pump liquid is uniform and equal to that of the surrounding fluid, i.e., the cylinder wall is diathermal, and determine the fractional error in mass flow rate for the following cases:

- The temperature of the fluid surrounding the pump,  $T_f$ , is constant. Take  $\beta_C = 4 \times 10^{-5} \text{ K}^{-1}$ ,  $\beta_L = 1.1 \times 10^{-3} \text{ K}^{-1}$ , and  $T_f - T_{ref} = 5 \text{ K}$ .
- The temperature of the surrounding fluid changes at a constant rate of  $1 \text{ K/h}$ . Take  $V_{ref}^o = 500 \text{ cm}^3$  and  $R_o = 25 \text{ cm}^3/\text{h}$ .

- The surrounding fluid temperature varies periodically with time, i.e.,

$$T_f = T_{ref} + A \sin \omega t \quad (8)$$

Take  $A = 1^\circ\text{C}$  and  $\omega = 8\pi \text{ h}^{-1}$ .

e) Now assume that the liquid temperature within the pump is uniform but different from the surrounding fluid temperature as a result of a finite rate of heat transfer. If the temperature of the surrounding fluid changes as

$$T_f = T_\infty + (T_{ref} - T_\infty)e^{-\tau t} \quad T_\infty < T_{ref} \quad (9)$$

where  $T_\infty$  is the asymptotic temperature and  $\tau$  is the time constant, show that the fractional error in mass flow rate is given by

$$f = \frac{\phi}{\phi - \tau} (e^{-\tau t} - e^{-\phi t}) + e^{-\phi t} - 1 + \left( \frac{V_{ref}^o}{R_o} - t \right) \frac{\phi\tau}{\phi - \tau} (e^{-\tau t} - e^{-\phi t}) \quad (10)$$

The terms  $f$  and  $\phi$  are defined as

$$f = - \frac{\dot{m} - \dot{m}_{ref}}{\dot{m}_{ref}} \frac{1}{(\beta_L - \beta_C)(T_{ref} - T_\infty)} \quad (11)$$

$$\phi = \frac{UA}{\rho V \hat{C}_P} \quad (12)$$

where  $A$  is the surface area of the liquid being pumped,  $U$  is the overall heat transfer coefficient, and  $\hat{C}_P$  is the heat capacity of the pump liquid.

f) Show that the time,  $t^*$ , at which the fractional error function  $f$  achieves its maximum absolute value is given by

$$t^* = \frac{\ln(\phi/\tau)}{\phi - \tau} \quad (13)$$

This problem is studied in detail by Eubank *et al.* (1985).

**7.24** A spherical salt, 5 cm in diameter, is suspended in a large, well-mixed tank containing a pure solvent at  $25^\circ\text{C}$ . If the percent decrease in the mass of the sphere is found to be 5% in 12 minutes, calculate the average mass transfer coefficient. The solubility of salt in the solvent is  $180 \text{ kg/m}^3$  and the density of the salt is  $2500 \text{ kg/m}^3$ .

(Answer:  $8.2 \times 10^{-6} \text{ m/s}$ )

**7.25** The phosphorous content of lakes not only depends on the external loading rate but also on the interactions between the sediments and the overlying waters. The model shown in Figure 7.6 is proposed by Chapra and Canale (1991) in which

the sediment layer gains phosphorous by settling and loses phosphorous by recycle and burial.

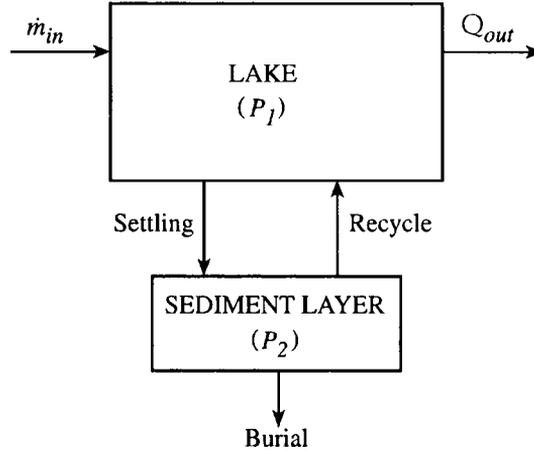


Figure 7.6 Schematic diagram for Problem 7.25

Show that the governing equations for the phosphorous concentrations in the lake,  $P_1$ , and in the sediment layer,  $P_2$ , are given as

$$\dot{m}_{in} - Q_{out}P_1 - v_s A_2 P_1 + A_2 \langle k_c \rangle_r P_2 = V_1 \frac{dP_1}{dt} \quad (1)$$

$$v_s A_2 P_1 - A_2 \langle k_c \rangle_r P_2 - A_2 \langle k_c \rangle_b P_2 = V_2 \frac{dP_2}{dt} \quad (2)$$

where

$\dot{m}_{in}$	= loading rate	= 2000 kg/year
$Q_{out}$	= outflow volumetric flow rate	= $80 \times 10^6 \text{ m}^3/\text{year}$
$v_s$	= settling velocity of phosphorous	= 40 m/year
$A_2$	= surface area of the sediment layer	= $4.8 \times 10^6 \text{ m}^2$
$\langle k_c \rangle_r$	= recycle mass transfer coefficient	= $2.5 \times 10^{-2} \text{ m/year}$
$\langle k_c \rangle_b$	= burial mass transfer coefficient	= $1 \times 10^{-3} \text{ m/year}$
$V_1$	= volume of the lake	= $53 \times 10^6 \text{ m}^3$
$V_2$	= volume of the sediment layer	= $4.8 \times 10^5 \text{ m}^3$

and determine the variation of  $P_1$  in  $\text{mg}/\text{m}^3$  as a function of time if the initial concentrations are given as  $P_1 = 60 \text{ mg}/\text{m}^3$  and  $P_2 = 500,000 \text{ mg}/\text{m}^3$ .

(Answer:  $P_1 = 22.9 - 165.4e^{-5.311t} + 202.5e^{-0.081t}$ )

## Chapter 8

# Steady-State Microscopic Balances Without Generation

So far we have considered macroscopic balances in which quantities such as temperature and concentration varied only with respect to time. As a result, the inventory rate equations are written by considering the total volume as a system and the resulting governing equations turn out to be the ordinary differential equations in time. If the dependent variables such as velocity, temperature and concentration change as a function of both position and time, then the inventory rate equations for the basic concepts are written over a differential volume element taken within the volume of the system. The resulting equations at the microscopic level are called the *equations of change*.

In this chapter we will consider steady-state microscopic balances without internal generation. Therefore, the governing equations will be either ordinary or partial differential equations in position. It should be noted that the treatment for heat and mass transport is different from the one for momentum transport. The main reasons for this are: (i) momentum is a vector quantity while heat and mass are scalar, (ii) in heat and mass transport the velocity appears only in the convective flux term, while it appears both in the molecular and convective flux terms for the case of momentum transfer.

## 8.1 MOMENTUM TRANSPORT

Momentum per unit mass, by definition, is the fluid velocity and changes in velocity can result in momentum transport. For *fully developed flow*<sup>1</sup> through conduits, velocity variations take place in the direction perpendicular to the flow since no-slip boundary conditions must be satisfied at the boundaries of the conduit. This results in the transfer of momentum in the direction perpendicular to the flow direction.

The inventory rate equation for momentum at the microscopic level is called the *equation of motion*. It is a vector equation with three components. For steady transfer of momentum without generation, the conservation statement for momentum reduces to

$$(\text{Rate of momentum in}) - (\text{Rate of momentum out}) = 0 \quad (8.1-1)$$

When there is no generation of momentum, this implies that both pressure and gravity terms are zero. Hence, flow can only be generated by the movement of surfaces enclosing the fluid and the resulting flow is called *Couette flow*. We will restrict our analysis to cases in which the following assumptions hold:

1. Incompressible Newtonian fluid,
2. One-dimensional<sup>2</sup>, fully developed laminar flow,
3. Constant physical properties.

The last assumption comes from the fact that temperature rise as a result of viscous dissipation during fluid motion, i.e., irreversible degradation of mechanical energy into thermal energy, is very small and cannot be detected by ordinary measuring devices in most of the cases. Hence, for all practical purposes the flow is assumed isothermal.

### 8.1.1 Plane Couette Flow

Consider a Newtonian fluid between two parallel plates that are separated by a distance  $B$  as shown in Figure 8.1. The lower plate is moved in the positive  $z$ -direction with a constant velocity of  $V$  while the upper plate is held stationary.

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<sup>1</sup> *Fully developed flow* means there is no variation of velocity in the axial direction. In this way, the flow development regions near the entrance and exit are not taken into consideration.

<sup>2</sup> *One-dimensional flow* indicates that there is only one non-zero velocity component.

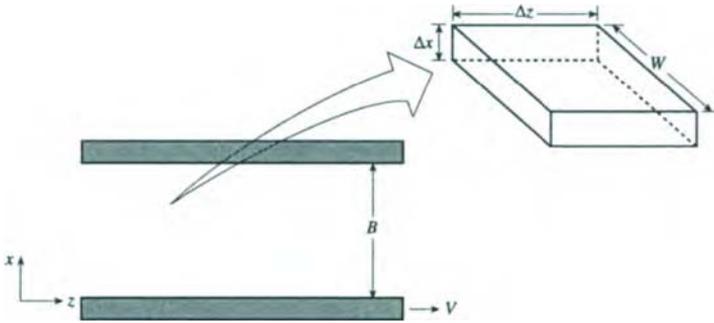


Figure 8.1 Couette flow between two parallel plates.

The first step in the translation of Eq. (8.1-1) into mathematical terms is to postulate the functional forms of the non-zero velocity components. This can be done by making reasonable assumptions and examining the boundary conditions. For the problem at hand, the simplification of the velocity components is shown in Figure 8.2.

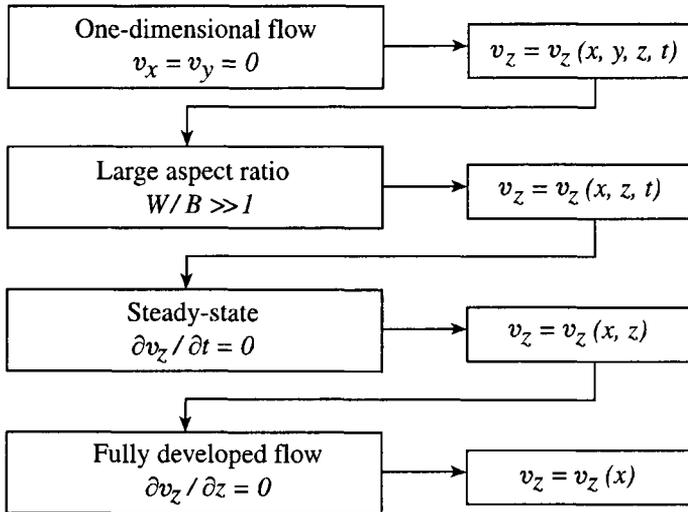


Figure 8.2 Simplification of the velocity components for Couette flow between two parallel plates.

Since  $v_z = v_z(x)$  and  $v_x = v_y = 0$ , Table C.1 in Appendix C indicates that the only non-zero shear-stress component is  $\tau_{xz}$ . Therefore, the components of the

total momentum flux are expressed as

$$\pi_{xz} = \tau_{xz} + (\rho v_z) v_x = \tau_{xz} = -\mu \frac{dv_z}{dx} \quad (8.1-2)$$

$$\pi_{yz} = \tau_{yz} + (\rho v_z) v_y = 0 \quad (8.1-3)$$

$$\pi_{zz} = \tau_{zz} + (\rho v_z) v_z = \rho v_z^2 \quad (8.1-4)$$

For a rectangular differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , as shown in Figure 8.1, Eq. (8.1-1) is expressed as

$$(\pi_{zz}|_z W \Delta x + \pi_{xz}|_x W \Delta z) - (\pi_{zz}|_{z+\Delta z} W \Delta x + \pi_{xz}|_{x+\Delta x} W \Delta z) = 0 \quad (8.1-5)$$

Following the notation introduced by Bird *et al.* (1960), “in” and “out” directions for the fluxes are taken in the direction of positive  $x$ - and  $z$ -axes. Dividing Eq. (8.1-5) by  $W \Delta x \Delta z$  and taking the limit as  $\Delta x \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{\pi_{zz}|_z - \pi_{zz}|_{z+\Delta z}}{\Delta z} + \lim_{\Delta x \rightarrow 0} \frac{\pi_{xz}|_x - \pi_{xz}|_{x+\Delta x}}{\Delta x} = 0 \quad (8.1-6)$$

or,

$$\frac{\partial \pi_{zz}}{\partial z} + \frac{d\pi_{xz}}{dx} = 0 \quad (8.1-7)$$

Substitution of Eqs. (8.1-2) and (8.1-4) into Eq. (8.1-7) and noting that  $\partial v_z / \partial z = 0$  yields

$$\frac{d}{dx} \left( \frac{dv_z}{dx} \right) = 0 \quad (8.1-8)$$

The solution of Eq. (8.1-8) is

$$v_z = C_1 x + C_2 \quad (8.1-9)$$

where  $C_1$  and  $C_2$  are constants of integration. The use of the boundary conditions

$$\text{at } x = 0 \quad v_z = V \quad (8.1-10)$$

$$\text{at } x = B \quad v_z = 0 \quad (8.1-11)$$

gives the velocity distribution as

$$\boxed{\frac{v_z}{V} = 1 - \frac{x}{B}} \quad (8.1-12)$$

The use of the velocity distribution, Eq. (8.1-12), in Eq. (8.1-2) indicates that the shear stress distribution is uniform across the cross-section of the plate, i.e.,

$$\boxed{\tau_{xz} = \frac{\mu V}{B}} \quad (8.1-13)$$

The volumetric flow rate can be determined by integrating the velocity distribution over the cross-sectional area, i.e.,

$$Q = \int_0^W \int_0^B v_z dx dy \quad (8.1-14)$$

Substitution of Eq. (8.1-12) into Eq. (8.1-14) gives the volumetric flow rate in the form

$$Q = \frac{WBV}{2} \quad (8.1-15)$$

Dividing the volumetric flow rate by the flow area gives the average velocity as

$$\langle v_z \rangle = \frac{Q}{WB} = \frac{V}{2} \quad (8.1-16)$$

### 8.1.2 Annular Couette Flow

Consider a Newtonian fluid in a concentric annulus as shown in Figure 8.3. The inner circular rod moves in the positive  $z$ -direction with a constant velocity of  $V$ .

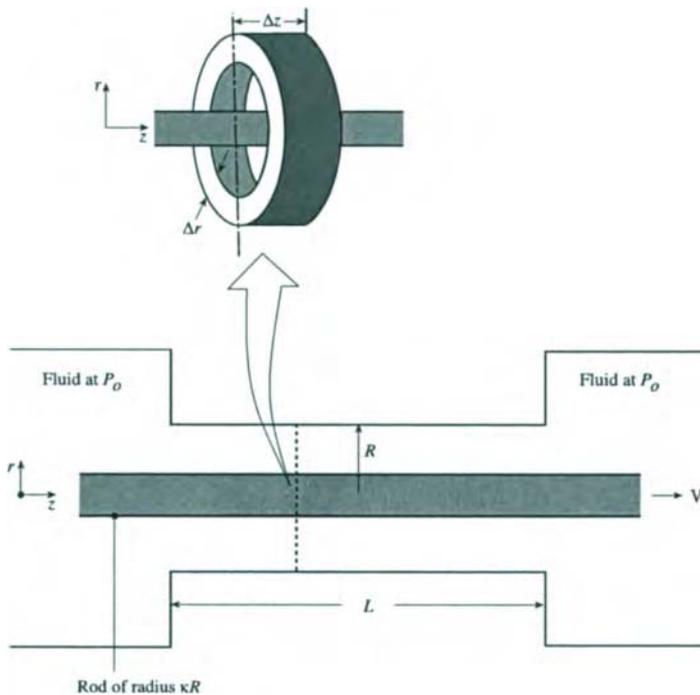


Figure 8.3 Couette flow in a concentric annulus.

For the problem at hand, the simplification of the velocity components is shown in Figure 8.4. Since  $v_z = v_z(r)$  and  $v_r = v_\theta = 0$ , Table C.2 in Appendix C indicates that the only non-zero shear-stress component is  $\tau_{rz}$ . Therefore, the components of the total momentum flux are given by

$$\pi_{rz} = \tau_{rz} + (\rho v_z) v_r = \tau_{rz} = -\mu \frac{dv_z}{dr} \quad (8.1-17)$$

$$\pi_{\theta z} = \tau_{\theta z} + (\rho v_z) v_\theta = 0 \quad (8.1-18)$$

$$\pi_{zz} = \tau_{zz} + (\rho v_z) v_z = \rho v_z^2 \quad (8.1-19)$$

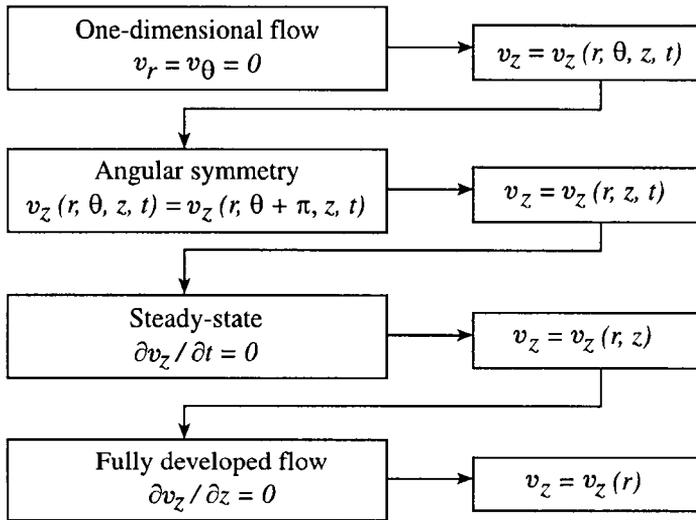


Figure 8.4 Simplification of the velocity components for Couette flow in a concentric annulus.

For a cylindrical differential volume element of thickness  $\Delta r$  and length  $\Delta z$ , as shown in Figure 8.3, Eq. (8.1-1) is expressed as

$$(\pi_{zz}|_z 2\pi r \Delta r + \pi_{rz}|_r 2\pi r \Delta z) - [\pi_{zz}|_{z+\Delta z} 2\pi r \Delta r + \pi_{rz}|_{r+\Delta r} 2\pi(r + \Delta r)\Delta z] = 0 \quad (8.1-20)$$

Dividing Eq. (8.1-20) by  $2\pi\Delta r\Delta z$  and taking the limit as  $\Delta r \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} r \left( \frac{\pi_{zz}|_z - \pi_{zz}|_{z+\Delta z}}{\Delta z} \right) + \lim_{\Delta r \rightarrow 0} \frac{(r\pi_{rz})|_r - (r\pi_{rz})|_{r+\Delta r}}{\Delta r} = 0 \quad (8.1-21)$$

or,

$$r \frac{\partial \pi_{zz}}{\partial z} + \frac{d(r\pi_{rz})}{dr} = 0 \quad (8.1-22)$$

Substitution of Eqs. (8.1-17) and (8.1-19) into Eq. (8.1-22) and noting that  $\partial v_z / \partial z = 0$  gives the governing equation for velocity as

$$\frac{d}{dr} \left[ r \left( \frac{dv_z}{dr} \right) \right] = 0 \quad (8.1-23)$$

The solution of Eq. (8.1-23) is

$$v_z = C_1 \ln r + C_2 \quad (8.1-24)$$

where  $C_1$  and  $C_2$  are integration constants. The use of the boundary conditions

$$\text{at } r = R \quad v_z = 0 \quad (8.1-25)$$

$$\text{at } r = \kappa R \quad v_z = V \quad (8.1-26)$$

gives the velocity distribution as

$$\boxed{\frac{v_z}{V} = \frac{\ln(r/R)}{\ln \kappa}} \quad (8.1-27)$$

The use of the velocity distribution, Eq. (8.1-27), in Eq. (8.1-17) gives the shear stress distribution as

$$\boxed{\tau_{rz} = - \left( \frac{\mu V}{\ln \kappa} \right) \frac{1}{r}} \quad (8.1-28)$$

The volumetric flow rate is obtained by integrating the velocity distribution over the annular cross-sectional area, i.e.,

$$Q = \int_0^{2\pi} \int_{\kappa R}^R v_z r \, dr \, d\theta \quad (8.1-29)$$

Substitution of Eq. (8.1-27) into Eq. (8.1-29) and integration gives

$$\boxed{Q = \frac{\pi R^2 V}{2} \left[ \frac{1 - \kappa^2}{\ln(1/\kappa)} - 2\kappa^2 \right]} \quad (8.1-30)$$

Dividing the volumetric flow rate by the flow area gives the average velocity as

$$\boxed{\langle v_z \rangle = \frac{Q}{\pi R^2 (1 - \kappa^2)} = \frac{V}{2} \left[ \frac{1}{\ln(1/\kappa)} - \frac{2\kappa^2}{1 - \kappa^2} \right]} \quad (8.1-31)$$

The drag force acting on the rod is

$$F_D = - \tau_{rz} |_{r=\kappa R} 2\pi \kappa R L \quad (8.1-32)$$

The use of Eq. (8.1-28) in Eq. (8.1-32) gives

$$\boxed{F_D = \frac{2\pi \mu L V}{\ln \kappa}} \quad (8.1-33)$$

## 8.1.2.1 Investigation of the limiting case

Once the solution to a given problem is obtained, it is always advisable to investigate the limiting cases if possible, and compare the results with the known solutions. If the results match, this does not necessarily mean that the solution is correct, however, the chances of it being correct are fairly high.

In this case, when the ratio of the radius of the inner pipe to that of the outer pipe is close to unity, i.e.,  $\kappa \rightarrow 1$ , a concentric annulus may be considered to be a thin-plane slit and its curvature can be neglected. Approximation of a concentric annulus as a parallel plate requires the width,  $W$ , and the length,  $L$ , of the plate to be defined as

$$W = \pi R(1 + \kappa) \quad (8.1-34)$$

$$B = R(1 - \kappa) \quad (8.1-35)$$

Therefore, the product  $WB$  is equal to

$$WB = \pi R^2(1 - \kappa^2) \quad \implies \quad \pi R^2 = \frac{WB}{1 - \kappa^2} \quad (8.1-36)$$

so that Eq. (8.1-30) becomes

$$Q = \frac{WBV}{2} \lim_{\kappa \rightarrow 1} \left[ -\frac{1}{\ln \kappa} - 2 \left( \frac{\kappa^2}{1 - \kappa^2} \right) \right] \quad (8.1-37)$$

Substitution of  $\psi = 1 - \kappa$  into Eq. (8.1-37) gives

$$Q = \frac{WBV}{2} \lim_{\psi \rightarrow 0} \left\{ -\frac{1}{\ln(1 - \psi)} - 2 \left[ \frac{(1 - \psi)^2}{1 - (1 - \psi)^2} \right] \right\} \quad (8.1-38)$$

The Taylor series expansion of the term  $\ln(1 - \psi)$  is

$$\ln(1 - \psi) = -\psi - \frac{1}{2}\psi^2 - \frac{1}{3}\psi^3 - \dots \quad -1 < \psi \leq 1 \quad (8.1-39)$$

Using Eq. (8.1-39) in Eq. (8.1-38) and carrying out the divisions yields

$$Q = \frac{WBV}{2} \lim_{\psi \rightarrow 0} \left[ \frac{1}{\psi} - \frac{1}{2} - \frac{\psi}{12} + \dots - 2 \left( \frac{1}{2\psi} - \frac{3}{4} - \frac{3\psi}{8} - \dots \right) \right] \quad (8.1-40)$$

or,

$$Q = \frac{WBV}{2} \lim_{\psi \rightarrow 0} \left( 1 + \frac{2}{3}\psi + \dots \right) = \frac{WBV}{2} \quad (8.1-41)$$

Note that Eq. (8.1-41) is equivalent to Eq. (8.1-15).

## 8.2 ENERGY TRANSPORT WITHOUT CONVECTION

The inventory rate equation for energy at the microscopic level is called the *equation of energy*. For a steady transfer of energy without generation, the conservation statement for energy reduces to

$$(\text{Rate of energy in}) = (\text{Rate of energy out}) \quad (8.2-1)$$

The rate of energy entering and leaving the system is determined from the energy flux. As stated in Chapter 2, the total energy flux is the sum of the molecular and convective fluxes. In this case we will restrict our analysis to cases in which convective energy flux is either zero or negligible compared with the molecular flux. This implies transfer of energy by conduction in solids and stationary liquids.

### 8.2.1 Conduction in Rectangular Coordinates

Consider the transfer of energy by conduction through a slightly tapered slab as shown in Figure 8.5. If the taper angle is small and the lateral surface is insulated, energy transport can be considered one-dimensional in the  $z$ -direction<sup>3</sup>, i.e.,  $T = T(z)$ .

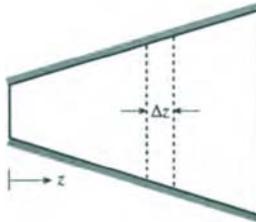


Figure 8.5 Conduction through a slightly tapered slab.

Table C.4 in Appendix C indicates that the only non-zero energy flux component is  $e_z$  and it is given by

$$e_z = q_z = -k \frac{dT}{dz} \quad (8.2-2)$$

The negative sign in Eq. (8.2-2) implies that positive  $z$ -direction is in the direction of decreasing temperature. If the answer turns out to be negative, this implies that the flux is in the negative  $z$ -direction

For a differential volume element of thickness  $\Delta z$ , as shown in Figure 8.5, Eq. (8.2-1) is expressed as

$$(Aq_z)|_z - (Aq_z)|_{z+\Delta z} = 0 \quad (8.2-3)$$

<sup>3</sup>The  $z$ -direction in the rectangular and cylindrical coordinate systems are equivalent to each other.

Dividing each term by  $\Delta z$  and taking the limit as  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{(Aq_z)|_z - (Aq_z)|_{z+\Delta z}}{\Delta z} = 0 \quad (8.2-4)$$

or,

$$\frac{d(Aq_z)}{dz} = 0 \quad (8.2-5)$$

Since flux times area gives the heat transfer rate,  $\dot{Q}$ , it is possible to conclude from Eq. (8.2-5) that

$$Aq_z = \text{constant} = \dot{Q} \quad (8.2-6)$$

in which the area  $A$  is perpendicular to the direction of energy flux. Substitution of Eq. (8.2-2) into Eq. (8.2-6) and integration gives

$$\boxed{\int_0^T k(T) dT = -\dot{Q} \int_0^z \frac{dz}{A(z)} + C} \quad (8.2-7)$$

where  $C$  is an integration constant. The determination of  $\dot{Q}$  and  $C$  requires two boundary conditions.

If the surface temperatures are specified, i.e.,

$$\begin{aligned} \text{at } z = 0 & \quad T = T_o \\ \text{at } z = L & \quad T = T_L \end{aligned} \quad (8.2-8)$$

the heat transfer rate as well as the temperature distribution as a function of position are given in Table 8.1.

On the other hand, if one surface is exposed to a constant heat flux while the other one is maintained at a constant temperature, i.e.,

$$\begin{aligned} \text{at } z = 0 & \quad -k \frac{dT}{dz} = q_o \\ \text{at } z = L & \quad T = T_L \end{aligned} \quad (8.2-9)$$

the resulting heat transfer rate and the temperature distribution as a function of position are given in Table 8.2. It should be noted that the boundary conditions given by Eqs. (8.2-8) and (8.2-9) are not the only boundary conditions available for energy transport. For different boundary conditions, Eq. (8.2-7) should be used to determine the constants.

**Table 8.1** Heat transfer rate and temperature distribution for one-dimensional conduction in a plane wall for the boundary conditions given by Eq. (8.2-8).

Constants	Heat Transfer Rate	Temperature Distribution
None	$\frac{\int_{T_L}^{T_o} k(T) dT}{\int_0^L \frac{dz}{A(z)}} \quad (\text{A})$	$\frac{\int_T^{T_o} k(T) dT}{\int_{T_L}^{T_o} k(T) dT} = \frac{\int_0^z \frac{dz}{A(z)}}{\int_0^L \frac{dz}{A(z)}} \quad (\text{E})$
$k$	$\frac{k(T_o - T_L)}{\int_0^L \frac{dz}{A(z)}} \quad (\text{B})$	$\frac{T_o - T}{T_o - T_L} = \frac{\int_0^z \frac{dz}{A(z)}}{\int_0^L \frac{dz}{A(z)}} \quad (\text{F})$
$A$	$\frac{A \int_{T_L}^{T_o} k(T) dT}{L} \quad (\text{C})$	$\frac{\int_T^{T_o} k(T) dT}{\int_{T_L}^{T_o} k(T) dT} = \frac{z}{L} \quad (\text{G})$
$\frac{k}{A}$	$\frac{k(T_o - T_L)A}{L} \quad (\text{D})$	$\frac{T_o - T}{T_o - T_L} = \frac{z}{L} \quad (\text{H})$

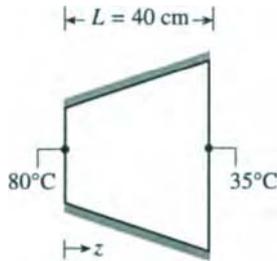
**Table 8.2** Heat transfer rate and temperature distribution for one-dimensional conduction in a plane wall for the boundary conditions given by Eq. (8.2-9).

Constants	Heat Transfer Rate	Temperature Distribution
None	$A _{z=0} q_o \quad (\text{A})$	$\int_{T_L}^T k(T) dT = A _{z=0} q_o \int_z^L \frac{dz}{A(z)} \quad (\text{E})$
$k$	$A _{z=0} q_o \quad (\text{B})$	$T - T_L = \frac{A _{z=0} q_o}{k} \int_z^L \frac{dz}{A(z)} \quad (\text{F})$
$A$	$A q_o \quad (\text{C})$	$\int_{T_L}^T k(T) dT = q_o L \left(1 - \frac{z}{L}\right) \quad (\text{G})$
$\frac{k}{A}$	$A q_o \quad (\text{D})$	$T - T_L = \frac{q_o L}{k} \left(1 - \frac{z}{L}\right) \quad (\text{H})$

**Example 8.1** Consider a solid cone of circular cross-section as shown in Figure 8.6. The diameter at  $z = 0$  is 8 cm and the diameter at  $z = L$  is 10 cm. Calculate the steady rate of heat transfer if the lateral surface is well insulated and the thermal conductivity of the solid material as a function of temperature is given by

$$k(T) = 400 - 0.07T$$

where  $k$  is in W/m.K and  $T$  is in degrees Celsius.



**Figure 8.6** Conduction through a solid cone.

### Solution

The diameter increases linearly in the  $z$ -direction, i.e.,

$$D(z) = 0.05z + 0.08$$

Therefore, the cross-sectional area perpendicular to the direction of heat flux is given as a function of position in the form

$$A(z) = \frac{\pi D^2}{4} = \frac{\pi}{4} (0.05z + 0.08)^2$$

The use of Eq. (A) in Table 8.1 with  $T_o = 80^\circ\text{C}$ ,  $T_L = 35^\circ\text{C}$  and  $L = 0.4$  m gives the heat transfer rate as

$$\dot{Q} = \frac{\int_{35}^{80} (400 - 0.07T) dT}{\int_0^{0.4} \frac{dz}{\pi(0.05z + 0.08)^2/4}} = 280 \text{ W}$$

**Example 8.2** Consider the problem given in Example 2.2. Determine the temperature distribution within the slab.

**Solution**

With  $T_L = 35^\circ\text{C}$ ,  $q_o = 100,000 \text{ W/m}^2$ ,  $k = 398 \text{ W/m}\cdot\text{K}$  and  $L = 0.04 \text{ m}$ , Eq. (H) in Table 8.2 gives the temperature distribution as

$$T - 35 = \frac{(100,000)(0.04)}{398} \left(1 - \frac{z}{0.04}\right)$$

or,

$$T = 45.1 - 251.3 z$$

**Example 8.3** In rivers ice begins to form when water is cooled to  $0^\circ\text{C}$  and continues to lose heat to the atmosphere. The presence of ice on rivers not only causes transportation problems but also floods on its melting. Once the ice cover is formed, its thickening depends on the rate of heat transferred from the water, through the ice cover, to the cold atmosphere. As an engineer you are asked to estimate the increase in the thickness of the ice block as a function of time.

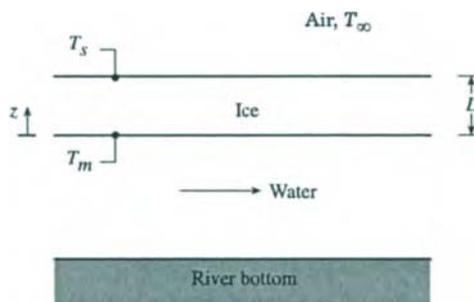
**Solution****Assumptions**

1. Pseudo-steady-state behavior.
2. River temperature is close to  $0^\circ\text{C}$  and the heat transferred from water to ice is negligible. This assumption implies that the major cause of ice thickening is the conduction of heat through the ice.

**Analysis**

System: Ice block

Since the density of ice is less than that of water, it floats on the river as shown in Figure 8.7. The temperatures  $T_m$  and  $T_s$  represent the melting temperature ( $0^\circ\text{C}$ ) and the top surface temperature, respectively.



**Figure 8.7** Ice block on a river.

The temperature distribution in the ice block under steady conditions can be determined from Eq. (H) in Table 8.1 as

$$\frac{T_m - T}{T_m - T_s} = \frac{z}{L} \quad (1)$$

Therefore, the steady heat flux through the ice block is given by

$$\begin{aligned} q_z &= -k \frac{dT}{dz} \\ &= \frac{k(T_m - T_s)}{L} \end{aligned} \quad (2)$$

For the ice block, the macroscopic inventory rate equation for energy is

$$- \text{Rate of energy out} = \text{Rate of energy accumulation} \quad (3)$$

If the enthalpy of liquid water at  $T_m$  is taken as zero, then the enthalpy of solid ice is

$$\hat{H}_{\text{ice}} = -\hat{\lambda} - \underbrace{\int_T^{T_m} \hat{C}_P dT}_{\text{Negligible}} \quad (4)$$

Therefore, Eq. (3) is expressed as

$$-q_z A = \frac{d}{dt} [AL\rho(-\hat{\lambda})] \quad (5)$$

For the unsteady-state problem at hand, pseudo-steady-state assumption implies that Eq. (2) holds at any given instant, i.e.,

$$q_z(t) = \frac{k(T_m - T_s)}{L(t)} \quad (6)$$

Substitution of Eq. (6) into Eq. (5) and rearrangement gives

$$\int_0^L L dL = \frac{k}{\rho \hat{\lambda}} \int_0^t (T_m - T_s) dt \quad (7)$$

Integration yields the thickness of the ice block in the form

$$L = \left[ \frac{2k}{\rho \hat{\lambda}} \int_0^t (T_m - T_s) dt \right]^{1/2} \quad (8)$$

### 8.2.1.1 Electrical circuit analogy

Using the analogy with Ohm's law, i.e., current = voltage/resistance, it is customary in the literature to express the rate equations in the form

$$\text{Rate} = \frac{\text{Driving force}}{\text{Resistance}} \quad (8.2-10)$$

Note that Eq. (D) in Table 8.1 is expressed as

$$\dot{Q} = \frac{T_o - T_L}{\frac{L}{kA}} \tag{8.2-11}$$

Comparison of Eq. (8.2-11) with Eq. (8.2-10) indicates that

$$\text{Driving force} = T_o - T_L \tag{8.2-12}$$

$\text{Resistance} = \frac{L}{kA} = \frac{\text{Thickness}}{(\text{Transport property})(\text{Area})}$	(8.2-13)
--	----------

Hence, the electric circuit analog of the plane wall can be represented as shown in Figure 8.8. Note that the electrical circuit analogy holds only if the thermal conductivity is constant. In the case of a composite plane wall, the resulting electrical circuit analogs are shown in Figure 8.9.

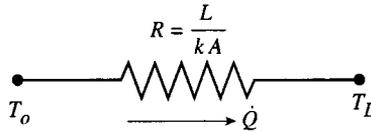


Figure 8.8 Electrical circuit analog of the plane wall.

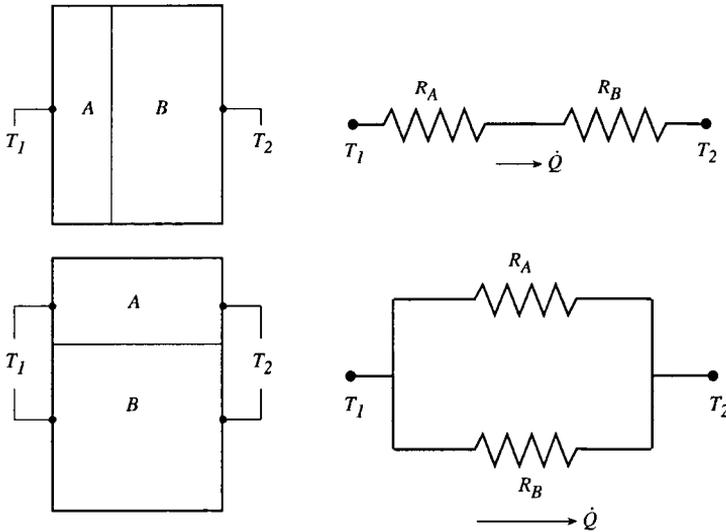


Figure 8.9 Electrical circuit analogs of composite plane walls in series and parallel arrangement.

**Example 8.4** For the composite wall shown in Figure 8.10, related thermal conductivities are given as  $k_A = 35 \text{ W/m.K}$ ,  $k_B = 12 \text{ W/m.K}$ ,  $k_C = 23 \text{ W/m.K}$ , and  $k_D = 5 \text{ W/m.K}$ .

- a) Determine the steady-state heat transfer rate.
- b) Determine the effective thermal conductivity for the composite walls. This makes it possible to consider the composite wall as a single material of thermal conductivity  $k_{eff}$ , rather than four different materials with four different thermal conductivities.

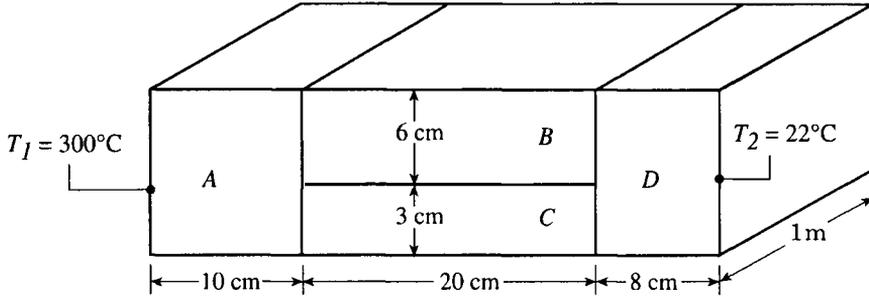
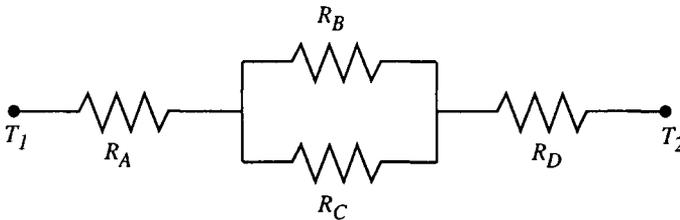


Figure 8.10 Heat conduction through a composite wall.

**Solution**

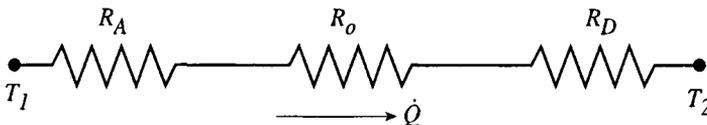
a) An analogous electrical circuit for this case is shown below:



The equivalent resistance,  $R_o$ , of the two resistances in parallel is

$$R_o = \left( \frac{1}{R_B} + \frac{1}{R_C} \right)^{-1}$$

Thus, the electrical analog for the heat transfer process through the composite wall can be represented as shown below:



Using Eq. (8.2-13) the resistances are calculated as follows:

$$R_A = \frac{L_A}{k_A A} = \frac{0.1}{(35)(0.09 \times 1)} = 0.032 \text{ K/W}$$

$$R_B = \frac{L_B}{k_B A} = \frac{0.2}{(12)(0.06 \times 1)} = 0.278 \text{ K/W}$$

$$R_C = \frac{L_C}{k_C A} = \frac{0.2}{(23)(0.03 \times 1)} = 0.290 \text{ K/W}$$

$$R_D = \frac{L_D}{k_D A} = \frac{0.08}{(5)(0.09 \times 1)} = 0.178 \text{ K/W}$$

$$R_o = \left( \frac{1}{R_B} + \frac{1}{R_C} \right)^{-1} = \left( \frac{1}{0.278} + \frac{1}{0.290} \right)^{-1} = 0.142 \text{ K/W}$$

The total resistance of the entire circuit is

$$\sum R = R_A + R_o + R_D = 0.032 + 0.142 + 0.178 = 0.352 \text{ K/W}$$

Hence, the heat transfer rate is

$$\dot{Q} = \frac{T_1 - T_2}{\sum R} = \frac{300 - 22}{0.352} = 790 \text{ W}$$

b) Note that

$$\sum R = \frac{\sum L}{k_{eff} A} \quad \Rightarrow \quad k_{eff} = \frac{\sum L}{A \sum R}$$

Therefore, the effective thermal conductivity is

$$k_{eff} = \frac{0.1 + 0.2 + 0.08}{(0.09 \times 1)(0.352)} = 12 \text{ W/m.K}$$

### 8.2.1.2 Transfer rate in terms of bulk fluid properties

Consider the transfer of thermal energy from fluid  $A$ , at a temperature  $T_A$  with an average heat transfer coefficient  $\langle h_A \rangle$ , through a solid plane wall with thermal conductivity  $k$ , to fluid  $B$ , at a temperature  $T_B$  with an average heat transfer coefficient  $\langle h_B \rangle$ , as shown in Figure 8.11.

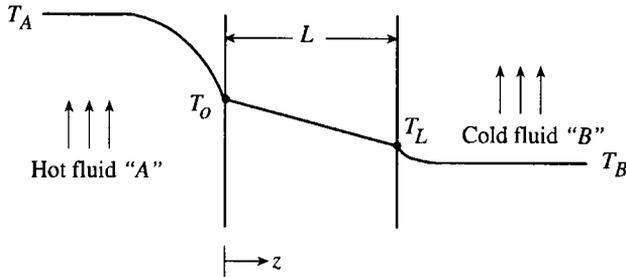


Figure 8.11 Heat transfer through a plane wall.

When the thermal conductivity and the area are constant, the heat transfer rate is calculated from Eq. (8.2-11). The use of this equation, however, requires the values of  $T_o$  and  $T_L$  be known or measured. In common practice, it is much easier to measure the bulk fluid temperatures,  $T_A$  and  $T_B$ . It is then necessary to relate  $T_o$  and  $T_L$  to  $T_A$  and  $T_B$ .

The heat transfer rates at the surfaces  $z = 0$  and  $z = L$  are given by Newton's law of cooling with appropriate heat transfer coefficients and expressed as

$$\dot{Q} = A\langle h_A \rangle (T_A - T_o) = A\langle h_B \rangle (T_L - T_B) \quad (8.2-14)$$

Equations (8.2-11) and (8.2-14) can be rearranged in the form

$$T_A - T_o = \dot{Q} \left( \frac{1}{A\langle h_A \rangle} \right) \quad (8.2-15)$$

$$T_o - T_L = \dot{Q} \left( \frac{L}{Ak} \right) \quad (8.2-16)$$

$$T_L - T_B = \dot{Q} \left( \frac{1}{A\langle h_B \rangle} \right) \quad (8.2-17)$$

Addition of Eqs. (8.2-15)-(8.2-17) gives

$$T_A - T_B = \dot{Q} \left( \frac{1}{A\langle h_A \rangle} + \frac{L}{Ak} + \frac{1}{A\langle h_B \rangle} \right) \quad (8.2-18)$$

or,

$$\dot{Q} = \frac{T_A - T_B}{\frac{1}{A\langle h_A \rangle} + \frac{L}{Ak} + \frac{1}{A\langle h_B \rangle}} \quad (8.2-19)$$

in which the terms in the denominator indicate that the resistances are in series. The electrical circuit analogy for this case is given in Figure 8.12.

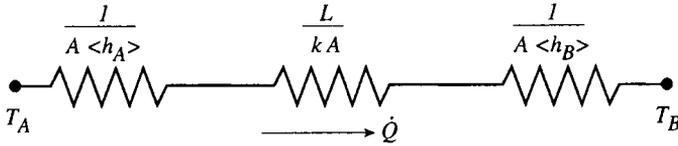


Figure 8.12 Electrical circuit analogy.

**Example 8.5** A plane wall separates hot air (A) at a temperature of  $50^\circ\text{C}$  from cold air (B) at  $-10^\circ\text{C}$  as shown in Figure 8.13. Calculate the steady rate of heat transfer through the wall if the thermal conductivity of the wall is

- a)  $k = 0.7 \text{ W/m}\cdot\text{K}$
- b)  $k = 20 \text{ W/m}\cdot\text{K}$

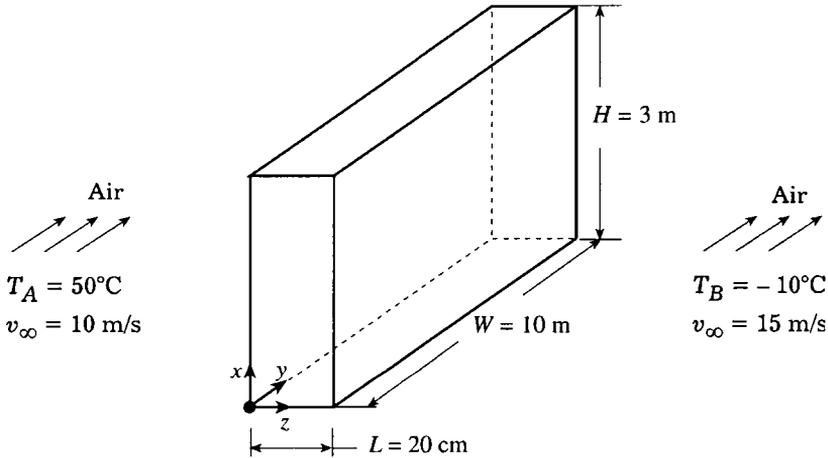


Figure 8.13 Conduction through a plane wall.

**Solution**

**Physical properties**

$$\text{For air at } 50^\circ\text{C (323 K)} : \begin{cases} \nu = 17.91 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 27.80 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ \text{Pr} = 0.708 \end{cases}$$

$$\text{For air at } -10^\circ\text{C (263 K)} : \begin{cases} \nu = 12.44 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 23.28 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ \text{Pr} = 0.72 \end{cases}$$

$$\begin{aligned} \text{For air at } 33.5^\circ\text{C (306.5 K)} : & \begin{cases} \nu = 16.33 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 26.59 \times 10^{-3} \text{ W/m.K} \\ \text{Pr} = 0.711 \end{cases} \\ \text{For air at } 0^\circ\text{C (273 K)} & : \begin{cases} \nu = 13.30 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 24.07 \times 10^{-3} \text{ W/m.K} \\ \text{Pr} = 0.717 \end{cases} \end{aligned}$$

### Analysis

The rate of heat loss can be calculated from Eq. (8.2-19), i.e.,

$$\dot{Q} = \frac{WH(T_A - T_B)}{\frac{1}{\langle h_A \rangle} + \frac{L}{k} + \frac{1}{\langle h_B \rangle}} \quad (1)$$

The average heat transfer coefficients,  $\langle h_A \rangle$  and  $\langle h_B \rangle$ , can be calculated from the correlations given in Table 4.2. However, the use of these equations require physical properties to be evaluated at the film temperature. Since the surface temperatures of the wall cannot be determined a priori, as a first approximation, the physical properties will be evaluated at the fluid temperatures.

### Left-side of the wall

Note that the characteristic length in the calculation of the Reynolds number is 10 m. The Reynolds number is

$$\begin{aligned} \text{Re} &= \frac{L_{ch} v_\infty}{\nu} \\ &= \frac{(10)(10)}{17.91 \times 10^{-6}} = 5.6 \times 10^6 \end{aligned} \quad (2)$$

Since this value is between  $5 \times 10^5$  and  $10^8$ , both laminar and turbulent conditions exist on the wall. The use of Eq. (E) in Table 4.2 gives the Nusselt number as

$$\begin{aligned} \langle \text{Nu} \rangle &= \left( 0.037 \text{Re}_L^{4/5} - 871 \right) \text{Pr}^{1/3} \\ &= \left[ 0.037 (5.6 \times 10^6)^{4/5} - 871 \right] (0.708)^{1/3} = 7480 \end{aligned} \quad (3)$$

Therefore, the average heat transfer coefficient is

$$\begin{aligned} \langle h_A \rangle &= \langle \text{Nu} \rangle \left( \frac{k}{L_{ch}} \right) \\ &= (7480) \left( \frac{27.80 \times 10^{-3}}{10} \right) = 20.8 \text{ W/m}^2 \cdot \text{K} \end{aligned} \quad (4)$$

**Right-side of the wall**

The Reynolds number is

$$\begin{aligned} \text{Re} &= \frac{L_{ch} v_{\infty}}{\nu} \\ &= \frac{(10)(15)}{12.44 \times 10^{-6}} = 12.1 \times 10^6 \end{aligned} \quad (5)$$

The use of Eq. (E) in Table 4.2 gives

$$\begin{aligned} \langle \text{Nu} \rangle &= (0.037 \text{Re}_L^{4/5} - 871) \text{Pr}^{1/3} \\ &= \left[ 0.037 (12.1 \times 10^6)^{4/5} - 871 \right] (0.72)^{1/3} = 14,596 \end{aligned} \quad (6)$$

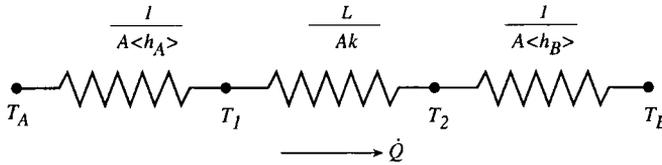
Therefore, the average heat transfer coefficient is

$$\begin{aligned} \langle h_B \rangle &= \langle \text{Nu} \rangle \left( \frac{k}{L_{ch}} \right) \\ &= (14,596) \left( \frac{23.28 \times 10^{-3}}{10} \right) = 34 \text{ W/m}^2 \cdot \text{K} \end{aligned} \quad (7)$$

a) Substitution of the numerical values into Eq. (1) gives

$$\dot{Q} = \frac{(10)(3) [50 - (-10)]}{\frac{1}{20.8} + \frac{0.2}{0.7} + \frac{1}{34}} = 4956 \text{ W} \quad (8)$$

Now we have to calculate the surface temperatures and check whether it is appropriate to evaluate physical properties at the fluid temperatures. The electrical circuit analogy for this problem is shown below:



The surface temperatures  $T_1$  and  $T_2$  can be calculated as

$$\begin{aligned} T_1 &= T_A - \frac{\dot{Q}}{A \langle h_A \rangle} \\ &= 50 - \frac{4956}{(30)(20.8)} \simeq 42^\circ \text{C} \end{aligned} \quad (9)$$

$$\begin{aligned} T_2 &= T_B + \frac{\dot{Q}}{A \langle h_B \rangle} \\ &= -10 + \frac{4956}{(30)(34)} \simeq -5^\circ \text{C} \end{aligned} \quad (10)$$

Therefore, the film temperatures at the left- and right-sides of the wall are  $(42 + 50)/2 = 46^\circ\text{C}$  and  $(-10 - 5)/2 = -7.5^\circ\text{C}$ , respectively. Since these temperatures are not very much different from the fluid temperatures, the heat transfer rate can be considered equal to 4956 W.

b) For  $k = 20\text{ W/m}\cdot\text{K}$ , the use of Eq. (1) gives

$$\dot{Q} = \frac{(10)(3)[50 - (-10)]}{\frac{1}{20.8} + \frac{0.2}{20} + \frac{1}{34}} = 20,574\text{ W} \quad (11)$$

The surface temperatures  $T_1$  and  $T_2$  can be calculated as

$$\begin{aligned} T_1 &= T_A - \frac{\dot{Q}}{A \langle h_A \rangle} \\ &= 50 - \frac{20,574}{(30)(20.8)} \simeq 17^\circ\text{C} \end{aligned} \quad (12)$$

$$\begin{aligned} T_2 &= T_B + \frac{\dot{Q}}{A \langle h_B \rangle} \\ &= -10 + \frac{20,574}{(30)(34)} \simeq 10^\circ\text{C} \end{aligned} \quad (13)$$

In this case, the film temperatures at the left- and right-sides are  $(17 + 50)/2 = 33.5^\circ\text{C}$  and  $(-10 + 10)/2 = 0^\circ\text{C}$ , respectively. Since these values are different from the fluid temperatures, it is necessary to recalculate the average heat transfer coefficients.

### Left-side of the wall

Using the physical properties evaluated at  $33.5^\circ\text{C}$ , the Reynolds number becomes

$$\begin{aligned} \text{Re} &= \frac{L_{ch} v_\infty}{\nu} \\ &= \frac{(10)(10)}{16.33 \times 10^{-6}} = 6.1 \times 10^6 \end{aligned} \quad (14)$$

The Nusselt number is

$$\begin{aligned} \langle \text{Nu} \rangle &= (0.037 \text{Re}_L^{4/5} - 871) \text{Pr}^{1/3} \\ &= \left[ 0.037 (6.1 \times 10^6)^{4/5} - 871 \right] (0.711)^{1/3} = 8076 \end{aligned} \quad (15)$$

Therefore, the average heat transfer coefficient is

$$\begin{aligned} \langle h_A \rangle &= \langle \text{Nu} \rangle \left( \frac{k}{L_{ch}} \right) \\ &= (8076) \left( \frac{26.59 \times 10^{-3}}{10} \right) = 21.5\text{ W/m}^2 \cdot \text{K} \end{aligned} \quad (16)$$

**Right-side of the wall**

Using the physical properties evaluated at 0°C, the Reynolds number becomes

$$\begin{aligned} \text{Re} &= \frac{L_{ch} v_{\infty}}{\nu} \\ &= \frac{(10)(15)}{13.30 \times 10^{-6}} = 11.3 \times 10^6 \end{aligned} \quad (17)$$

The use of Eq. (E) in Table 4.2 gives

$$\begin{aligned} \langle \text{Nu} \rangle &= (0.037 \text{Re}_L^{4/5} - 871) \text{Pr}^{1/3} \\ &= \left[ 0.037 (11.3 \times 10^6)^{4/5} - 871 \right] (0.717)^{1/3} = 13,758 \end{aligned} \quad (18)$$

Therefore, the average heat transfer coefficient is

$$\begin{aligned} \langle h_B \rangle &= \langle \text{Nu} \rangle \left( \frac{k}{L_{ch}} \right) \\ &= (13,758) \left( \frac{24.07 \times 10^{-3}}{10} \right) = 33.1 \text{ W/m}^2 \cdot \text{K} \end{aligned} \quad (19)$$

Substitution of the new values of the average heat transfer coefficients, Eqs. (16) and (19), into Eq. (1) gives the heat transfer rate as

$$\dot{Q} = \frac{(10)(3) [50 - (-10)]}{\frac{1}{21.5} + \frac{0.2}{20} + \frac{1}{33.1}} = 20,756 \text{ W} \quad (20)$$

The surface temperatures are

$$\begin{aligned} T_1 &= T_A - \frac{\dot{Q}}{A \langle h_A \rangle} \\ &= 50 - \frac{20,756}{(30)(21.5)} \simeq 18^\circ \text{C} \end{aligned} \quad (21)$$

$$\begin{aligned} T_2 &= T_B + \frac{\dot{Q}}{A \langle h_B \rangle} \\ &= -10 + \frac{20,756}{(30)(33.1)} \simeq 11^\circ \text{C} \end{aligned} \quad (22)$$

Since these values are almost equal to the previous values, then the rate of heat loss is 20,756 W.

**Comment:** The Biot numbers, i.e.,  $\langle h \rangle L_{ch}/k$ , for this problem are calculated as follows:

	Left Side	Right Side
Part (a)	5.9	9.7
Part (b)	0.2	0.3

Note that the physical significance of the Biot number was given by Eq. (7.1.14), i.e.,

$$\text{Bi} = \frac{(\text{Difference in driving force})_{\text{solid}}}{(\text{Difference in driving force})_{\text{fluid}}}$$

Therefore, when Bi is large, the temperature drop between the surface of the wall and the bulk temperature is small and the physical properties can be calculated at the bulk fluid temperature rather than the film temperature in engineering calculations. On the other hand, when Bi is small, the temperature drop between the surface of the wall and the bulk fluid temperature is large and the physical properties must be evaluated at the film temperature. Evaluation of the physical properties at the bulk fluid temperature for small values of Bi may lead to erroneous results especially if the physical properties of the fluid are strongly dependent on temperature.

## 8.2.2 Conduction in Cylindrical Coordinates

Consider a one-dimensional transfer of energy in the  $r$ -direction in a hollow cylindrical pipe with inner and outer radii of  $R_1$  and  $R_2$ , respectively, as shown in Figure 8.14. Since  $T = T(r)$ , Table C.5 in Appendix C indicates that the only non-zero energy flux component is  $e_r$  and it is given by

$$e_r = q_r = -k \frac{dT}{dr} \quad (8.2-20)$$

For a cylindrical differential volume element of thickness  $\Delta r$ , as shown in Figure 8.14, Eq. (8.2-1) is expressed in the form

$$(Aq_r)|_r - (Aq_r)|_{r+\Delta r} = 0 \quad (8.2-21)$$

Dividing Eq. (8.2-21) by  $\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

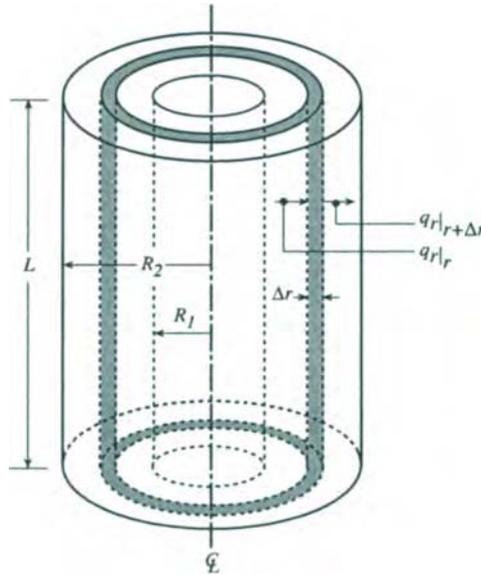
$$\lim_{\Delta r \rightarrow 0} \frac{(Aq_r)|_r - (Aq_r)|_{r+\Delta r}}{\Delta r} = 0 \quad (8.2-22)$$

or,

$$\frac{d(Aq_r)}{dr} = 0 \quad (8.2-23)$$

Since flux times area gives the heat transfer rate,  $\dot{Q}$ , it is possible to conclude that

$$Aq_r = \text{constant} = \dot{Q} \quad (8.2-24)$$



**Figure 8.14** Conduction in a hollow cylindrical pipe.

The area  $A$  in Eq. (8.2-24) is perpendicular to the direction of energy flux in the  $r$ -direction and is given by

$$A = 2\pi rL \quad (8.2-25)$$

Substitution of Eqs. (8.2-20) and (8.2-25) into Eq. (8.2-24) and integration gives

$$\int_0^T k(T) dT = - \left( \frac{\dot{Q}}{2\pi L} \right) \ln r + C \quad (8.2-26)$$

where  $C$  is an integration constant.

If the surface temperatures are specified, i.e.,

$$\begin{aligned} \text{at } r = R_1 \quad T &= T_1 \\ \text{at } r = R_2 \quad T &= T_2 \end{aligned} \quad (8.2-27)$$

the heat transfer rate as well as the temperature distribution as a function of position are given in Table 8.3.

On the other hand, if one surface is exposed to a constant heat flux while the other one is maintained at a constant temperature, i.e.,

$$\begin{aligned} \text{at } r = R_1 \quad -k \frac{dT}{dr} &= q_1 \\ \text{at } r = R_2 \quad T &= T_2 \end{aligned} \quad (8.2-28)$$

the resulting heat transfer rate and the temperature distribution as a function of position are given in Table 8.4.

**Table 8.3** Heat transfer rate and temperature distribution for one-dimensional conduction in a hollow cylinder for the boundary conditions given by Eq. (8.2-27).

Constants	Heat Transfer Rate	Temperature Distribution
None	$\frac{2\pi L \int_{T_1}^{T_2} k(T) dT}{\ln\left(\frac{R_1}{R_2}\right)} \quad (\text{A})$	$\frac{\int_T^{T_2} k(T) dT}{\int_{T_1}^{T_2} k(T) dT} = \frac{\ln\left(\frac{r}{R_2}\right)}{\ln\left(\frac{R_1}{R_2}\right)} \quad (\text{C})$
$k$	$\frac{2\pi L k (T_2 - T_1)}{\ln\left(\frac{R_1}{R_2}\right)} \quad (\text{B})$	$\frac{T_2 - T}{T_2 - T_1} = \frac{\ln\left(\frac{r}{R_2}\right)}{\ln\left(\frac{R_1}{R_2}\right)} \quad (\text{D})$

**Table 8.4** Heat transfer rate and temperature distribution for one-dimensional conduction in a hollow cylinder for the boundary conditions given by Eq. (8.2-28).

Constants	Heat Transfer Rate	Temperature Distribution
None	$2\pi R_1 L q_1 \quad (\text{A})$	$\int_T^{T_2} k(T) dT = q_1 R_1 \ln\left(\frac{r}{R_2}\right) \quad (\text{C})$
$k$	$2\pi R_1 L q_1 \quad (\text{B})$	$T_2 - T = \frac{q_1 R_1}{k} \ln\left(\frac{r}{R_2}\right) \quad (\text{D})$

### 8.2.2.1 Electrical circuit analogy

Equation (B) in Table 8.3 can be expressed as

$$\dot{Q} = \frac{T_1 - T_2}{\frac{\ln(R_2/R_1)}{2\pi L k}} \quad (8.2-29)$$

Comparison of Eq. (8.2-29) with Eq. (8.2-10) indicates that the resistance is given by

$$\text{Resistance} = \frac{\ln(R_2/R_1)}{2\pi L k} \quad (8.2-30)$$

At first, it looks as if the resistance expression for the rectangular and the cylindrical coordinate systems are different from each other. However, the similarities between these two expressions can be shown by the following analysis.

Note that the *logarithmic-mean area*,  $A_{LM}$ , can be defined as

$$A_{LM} = \frac{A_2 - A_1}{\ln(A_2/A_1)} = \frac{2\pi L(R_2 - R_1)}{\ln(R_2/R_1)} \tag{8.2-31}$$

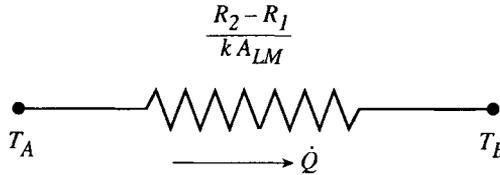
Substitution of Eq. (8.2-31) into Eq. (8.2-30) gives

$$\boxed{\text{Resistance} = \frac{R_2 - R_1}{k A_{LM}}} \tag{8.2-32}$$

Note that Eqs. (8.2-13) and (8.2-32) have the same general form of

$$\text{Resistance} = \frac{\text{Thickness}}{(\text{Transport property})(\text{Area})} \tag{8.2-33}$$

The electrical circuit analog of the cylindrical wall can be represented as shown in Figure 8.15.



**Figure 8.15** Electrical circuit analog of the cylindrical wall.

**Example 8.6** Heat flows through an annular wall of inside radius  $R_1 = 10$  cm and outside radius  $R_2 = 15$  cm. The inside and outside surface temperatures are  $60^\circ\text{C}$  and  $30^\circ\text{C}$ , respectively. The thermal conductivity of the wall is dependent on temperature as follows:

$$\begin{aligned} T = 30^\circ\text{C} & \quad k = 42 \text{ W/m}\cdot\text{K} \\ T = 60^\circ\text{C} & \quad k = 49 \text{ W/m}\cdot\text{K} \end{aligned}$$

Calculate the steady rate of heat transfer if the wall has a length of 2 m.

**Solution**

**Assumption**

1. The thermal conductivity varies linearly with temperature.

**Analysis**

The variation of the thermal conductivity with temperature can be estimated as

$$\begin{aligned} k &= 42 + \left( \frac{49 - 42}{60 - 30} \right) (T - 30) \\ &= 35 + 0.233 T \end{aligned}$$

The heat transfer rate is estimated from Eq. (A) in Table 8.3 with  $R_1 = 10$  cm,  $R_2 = 15$  cm,  $T_1 = 60^\circ\text{C}$  and  $T_2 = 30^\circ\text{C}$  :

$$\begin{aligned} \dot{Q} &= \frac{2\pi L \int_{T_1}^{T_2} k(T) dT}{\ln(R_1/R_2)} = \frac{2\pi L \int_{T_2}^{T_1} k(T) dT}{\ln(R_2/R_1)} \\ &= \frac{2\pi(2)}{\ln(15/10)} \int_{30}^{60} (35 + 0.233 T) dT = 42,291 \text{ W} \end{aligned}$$

**8.2.2.2 Transfer rate in terms of bulk fluid properties**

The use of Eq. (8.2-29) in the calculation of the heat transfer rate requires surface values  $T_1$  and  $T_2$  be known or measured. In common practice, the bulk temperatures of the adjoining fluids to the surfaces at  $R = R_1$  and  $R = R_2$ , i.e.,  $T_A$  and  $T_B$ , are known. It is then necessary to relate  $T_1$  and  $T_2$  to  $T_A$  and  $T_B$ .

The heat transfer rates at the surfaces  $R = R_1$  and  $R = R_2$  are expressed in terms of the heat transfer coefficients by Newton's law of cooling as

$$\dot{Q} = A_1 \langle h_A \rangle (T_A - T_1) = A_2 \langle h_B \rangle (T_2 - T_B) \quad (8.2-34)$$

The surface areas  $A_1$  and  $A_2$  are expressed in the form

$$A_1 = 2\pi R_1 L \quad \text{and} \quad A_2 = 2\pi R_2 L \quad (8.2-35)$$

Equations (8.2-29) and (8.2-34) can be rearranged in the form

$$T_A - T_1 = \dot{Q} \left( \frac{1}{A_1 \langle h_A \rangle} \right) \quad (8.2-36)$$

$$T_1 - T_2 = \dot{Q} \left( \frac{R_2 - R_1}{A_{LM} k} \right) \quad (8.2-37)$$

$$T_2 - T_B = \dot{Q} \left( \frac{1}{A_2 \langle h_B \rangle} \right) \quad (8.2-38)$$

Addition of Eqs. (8.2-36)-(8.2-38) gives

$$T_A - T_B = \dot{Q} \left( \frac{1}{A_1 \langle h_A \rangle} + \frac{R_2 - R_1}{A_{LM} k} + \frac{1}{A_2 \langle h_B \rangle} \right) \quad (8.2-39)$$

or,

$$\dot{Q} = \frac{T_A - T_B}{\frac{1}{A_1 \langle h_A \rangle} + \frac{R_2 - R_1}{A_{LM} k} + \frac{1}{A_2 \langle h_B \rangle}} \quad (8.2-40)$$

in which the terms in the denominator indicate that the resistances are in series. The electrical circuit analogy for this case is given in Figure 8.16.

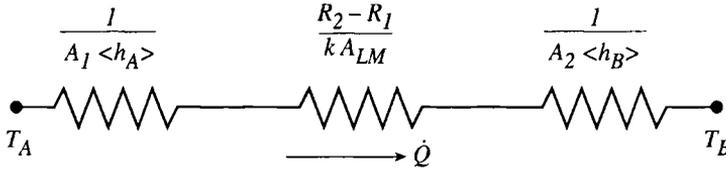


Figure 8.16 Electrical circuit analogy for Eq. (8.2-40).

In the literature, Eq. (8.2-40) is usually expressed in the form

$$\dot{Q} = A_1 U_A (T_A - T_B) = A_2 U_B (T_A - T_B) \quad (8.2-41)$$

where the terms  $U_A$  and  $U_B$  are called the *overall heat transfer coefficients*. Comparison of Eq. (8.2-41) with Eq. (8.2-40) gives  $U_A$  and  $U_B$  as

$$\begin{aligned} U_A &= \left[ \frac{1}{\langle h_A \rangle} + \frac{(R_2 - R_1) A_1}{A_{LM} k} + \frac{A_1}{\langle h_B \rangle A_2} \right]^{-1} \\ &= \left[ \frac{1}{\langle h_A \rangle} + \frac{R_1 \ln(R_2/R_1)}{k} + \frac{R_1}{\langle h_B \rangle R_2} \right]^{-1} \end{aligned} \quad (8.2-42)$$

and

$$\begin{aligned} U_B &= \left[ \frac{A_2}{\langle h_A \rangle A_1} + \frac{(R_2 - R_1) A_2}{A_{LM} k} + \frac{1}{\langle h_B \rangle} \right]^{-1} \\ &= \left[ \frac{R_2}{\langle h_A \rangle R_1} + \frac{R_2 \ln(R_2/R_1)}{k} + \frac{1}{\langle h_B \rangle} \right]^{-1} \end{aligned} \quad (8.2-43)$$

**Example 8.7** Consider a cylindrical pipe of length  $L$  with inner and outer radii of  $R_1$  and  $R_2$ , respectively, and investigate how the rate of heat loss changes as a function of insulation thickness.

### Solution

The immediate reaction of most students after reading the problem statement is "What's the point of discussing the rate of heat loss as a function of insulation thickness? Adding insulation thickness obviously decreases the rate of heat loss."

This conclusion is true only for planar surfaces. In the case of curved surfaces, however, close examination of Eq. (8.2-32) indicates that while addition of insulation increases the thickness, i.e.,  $R_2 - R_1$ , it also increases the heat transfer area, i.e.,  $A_{LM}$ . Hence, both numerator and denominator of Eq. (8.2-32) increase when the insulation thickness increases. If the increase in the heat transfer area is greater than the increase in thickness, then resistance decreases with a concomitant increase in the rate of heat loss.

For the geometry shown in Figure 8.17, the rate of heat loss is given by

$$\dot{Q} = \frac{T_A - T_B}{\frac{1}{2\pi R_1 L \langle h_A \rangle} + \frac{\ln(R_2/R_1)}{2\pi L k_w} + \underbrace{\frac{\ln(R_3/R_2)}{2\pi L k_i} + \frac{1}{2\pi R_3 L \langle h_B \rangle}}_X} \quad (1)$$

where  $k_w$  and  $k_i$  are the thermal conductivities of the wall and the insulating material, respectively.

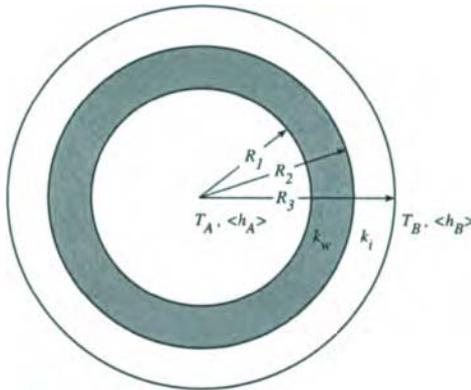


Figure 8.17 Conduction through an insulated cylindrical pipe.

Note that the term  $X$  in the denominator of Eq. (1) is dependent on the insulation thickness. Differentiation of  $X$  with respect to  $R_3$  gives

$$\frac{dX}{dR_3} = \frac{1}{2\pi L} \left( \frac{1}{R_3 k_i} - \frac{1}{\langle h_B \rangle R_3^2} \right) = 0 \quad \Rightarrow \quad R_3 = \frac{k_i}{\langle h_B \rangle} \quad (2)$$

To determine whether this point corresponds to a minimum or a maximum value, it is necessary to calculate the second derivative, i.e.,

$$\left. \frac{d^2 X}{dR_3^2} \right|_{R_3 = k_i / \langle h_B \rangle} = \frac{1}{2\pi L} \frac{\langle h_B \rangle^2}{k_i^3} > 0 \quad (3)$$

Therefore, at  $R_3 = k_i/\langle h_B \rangle$ ,  $X$  has the minimum value. This implies that the rate of heat loss will reach the maximum value at  $R_3 = R_{cr} = k_i/\langle h_B \rangle$ , where  $R_{cr}$  is called the critical thickness of insulation. For  $R_2 < R_3 \leq R_{cr}$ , addition of insulation causes an increase in the rate of heat loss rather than a decrease. A representative graph showing the variation of the heat transfer rate with insulation thickness is given in Figure 8.18.

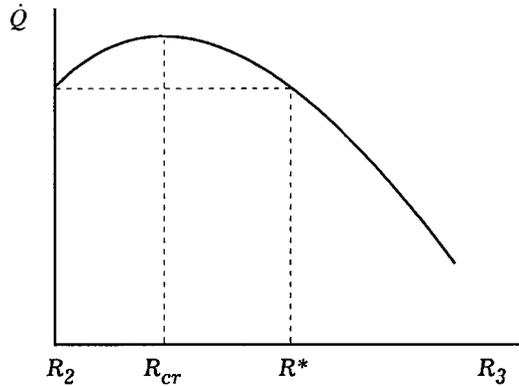


Figure 8.18 Rate of heat loss as a function of insulation thickness.

Another point of interest is to determine the value of  $R^*$ , the point at which the rate of heat loss is equal to that of the bare pipe. The rate of heat loss through the bare pipe,  $\dot{Q}_o$ , is

$$\dot{Q}_o = \frac{T_A - T_B}{\frac{1}{2\pi R_1 L \langle h_A \rangle} + \frac{\ln(R_2/R_1)}{2\pi L k_w} + \frac{1}{2\pi R_2 L \langle h_B \rangle}} \quad (4)$$

On the other hand, the rate of heat loss,  $\dot{Q}^*$ , when  $R_3 = R^*$  is

$$\dot{Q}^* = \frac{T_A - T_B}{\frac{1}{2\pi R_1 L \langle h_A \rangle} + \frac{\ln(R_2/R_1)}{2\pi L k_w} + \frac{\ln(R^*/R_2)}{2\pi L k_i} + \frac{1}{2\pi R^* L \langle h_B \rangle}} \quad (5)$$

Equating Eqs. (4) and (5) gives

$$\frac{R^*}{R_2} - \frac{\langle h_B \rangle R^*}{k_i} \ln \left( \frac{R^*}{R_2} \right) = 1 \quad (6)$$

$R^*$  can be determined from Eq. (6) for the given values of  $R_2$ ,  $\langle h_B \rangle$ , and  $k_i$ .

**Comment:** For insulating materials, the largest value of the thermal conductivity is in the order of 0.1 W/m.K. On the other hand, the smallest value of  $\langle h_B \rangle$  is

around  $3 \text{ W/m}^2 \cdot \text{K}$ . Therefore, the maximum value of the critical radius is approximately 3.3 cm, and in most practical applications, this will not pose a problem. Therefore, critical radius of insulation is of importance only for small diameter wires or tubes.

**Example 8.8** Steam (fluid A) flows in a pipe of  $R_1 = 30 \text{ cm}$  and  $R_2 = 45 \text{ cm}$ . The pipe is surrounded by fluid B. Calculate the overall heat transfer coefficients and sketch the representative temperature profiles for the following cases:

- a)  $\langle h_A \rangle = 10 \text{ W/m}^2 \cdot \text{K}$ ;  $\langle h_B \rangle = 5000 \text{ W/m}^2 \cdot \text{K}$ ;  $k = 2000 \text{ W/m}^2 \cdot \text{K}$   
 b)  $\langle h_A \rangle = 5000 \text{ W/m}^2 \cdot \text{K}$ ;  $\langle h_B \rangle = 8000 \text{ W/m}^2 \cdot \text{K}$ ;  $k = 0.02 \text{ W/m}^2 \cdot \text{K}$   
 c)  $\langle h_A \rangle = 5000 \text{ W/m}^2 \cdot \text{K}$ ;  $\langle h_B \rangle = 10 \text{ W/m}^2 \cdot \text{K}$ ;  $k = 2000 \text{ W/m}^2 \cdot \text{K}$

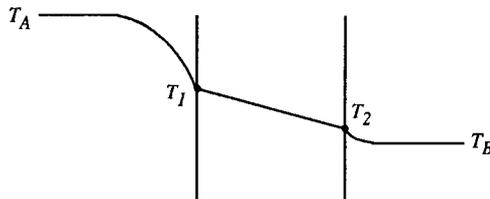
### Solution

a) Note that the dominant resistance to heat transfer is that of fluid A. Therefore, one expects the largest temperature drop in this region. Hence Eqs. (8.2-42) and (8.2-43) give the overall heat transfer coefficients as

$$U_A = \left( \frac{1}{\langle h_A \rangle} \right)^{-1} = \langle h_A \rangle = 10 \text{ W/m}^2 \cdot \text{K}$$

$$U_B = \left( \frac{R_2}{\langle h_A \rangle R_1} \right)^{-1} = \langle h_A \rangle \left( \frac{R_1}{R_2} \right) = \frac{(10)(30)}{45} = 6.67 \text{ W/m}^2 \cdot \text{K}$$

The expected temperature profile for this case is shown below.

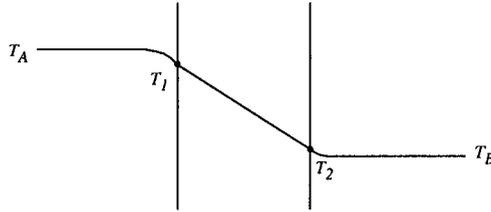


b) In this case the dominant resistance to heat transfer is that of the pipe wall. The overall heat transfer coefficients are

$$U_A = \frac{k}{R_1 \ln(R_2/R_1)} = \frac{0.02}{(0.3) \ln(45/30)} = 0.16 \text{ W/m}^2 \cdot \text{K}$$

$$U_B = \frac{k}{R_2 \ln(R_2/R_1)} = \frac{0.02}{(0.45) \ln(45/30)} = 0.11 \text{ W/m}^2 \cdot \text{K}$$

The expected temperature profile for this case is shown below:

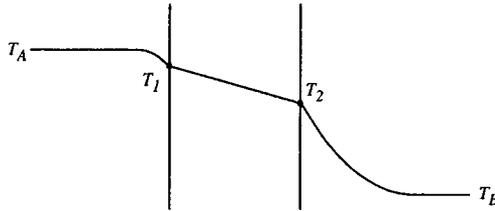


c) The dominant resistance to heat transfer is the resistance of fluid B. Hence, the overall heat transfer coefficients are

$$U_A = \left( \frac{R_1}{\langle h_B \rangle R_2} \right)^{-1} = \langle h_B \rangle \left( \frac{R_2}{R_1} \right) = \frac{(10)(45)}{30} = 15 \text{ W/m}^2 \cdot \text{K}$$

$$U_B = \left( \frac{1}{\langle h_B \rangle} \right)^{-1} = \langle h_B \rangle = 10 \text{ W/m}^2 \cdot \text{K}$$

The expected temperature profile for this case is shown below:



**Comment:** The region with the largest thermal resistance has the largest temperature drop.

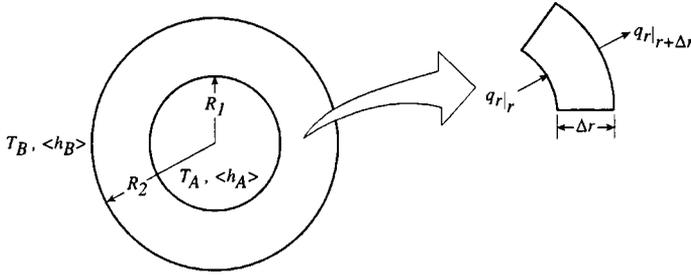
### 8.2.3 Conduction in Spherical Coordinates

Consider one-dimensional transfer of energy in the  $r$ -direction through a hollow sphere of inner and outer radii of  $R_1$  and  $R_2$ , respectively, as shown in Figure 8.19. Since  $T = T(r)$ , Table C.6 in Appendix C indicates that the only non-zero energy flux component is  $e_r$  and it is given by

$$e_r = q_r = -k \frac{dT}{dr} \tag{8.2-44}$$

For a spherical differential volume element of thickness  $\Delta r$  as shown in Fig. 8.19, Eq. (8.2-1) is expressed in the form

$$(Aq_r)|_r - (Aq_r)|_{r+\Delta r} = 0 \tag{8.2-45}$$



**Figure 8.19** Conduction through a hollow sphere.

Dividing Eq. (8.2-45) by  $\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(Aq_r)|_r - (Aq_r)|_{r+\Delta r}}{\Delta r} = 0 \tag{8.2-46}$$

or,

$$\frac{d(Aq_r)}{dr} = 0 \tag{8.2-47}$$

Since flux times area gives the heat transfer rate,  $\dot{Q}$ , it is possible to conclude that

$$Aq_r = \text{constant} = \dot{Q} \tag{8.2-48}$$

The area  $A$  in Eq. (8.2-48) is perpendicular to the direction of energy flux in the  $r$ -direction and it is given by

$$A = 4\pi r^2 \tag{8.2-49}$$

Substitution of Eqs. (8.2-44) and (8.2-49) into Eq. (8.2-48) and integration gives

$$\boxed{\int_0^T k(T) dT = \left(\frac{\dot{Q}}{4\pi}\right) \frac{1}{r} + C} \tag{8.2-50}$$

where  $C$  is an integration constant.

If the surface temperatures are specified, i.e.,

$$\begin{aligned} \text{at } r = R_1 \quad T = T_1 \\ \text{at } r = R_2 \quad T = T_2 \end{aligned} \tag{8.2-51}$$

the heat transfer rate as well as the temperature distribution as a function of position are given in Table 8.5. On the other hand, if one surface is exposed to a constant heat flux while the other one is maintained at a constant temperature, i.e.,

$$\begin{aligned} \text{at } r = R_1 \quad -k \frac{dT}{dr} = q_1 \\ \text{at } r = R_2 \quad T = T_2 \end{aligned} \tag{8.2-52}$$

the resulting heat transfer rate and the temperature distribution as a function of position are given in Table 8.6.

**Table 8.5** Heat transfer rate and temperature distribution for one-dimensional conduction in a hollow sphere for the boundary conditions given by Eq. (8.2-51).

Constants	Heat Transfer Rate	Temperature Distribution
None	$\frac{4\pi \int_{T_2}^{T_1} k(T) dT}{\frac{1}{R_1} - \frac{1}{R_2}} \quad (\text{A})$	$\frac{\int_{T_2}^T k(T) dT}{\int_{T_2}^{T_1} k(T) dT} = \frac{\frac{1}{r} - \frac{1}{R_2}}{\frac{1}{R_1} - \frac{1}{R_2}} \quad (\text{C})$
$k$	$\frac{4\pi k(T_1 - T_2)}{\frac{1}{R_1} - \frac{1}{R_2}} \quad (\text{B})$	$\frac{T - T_2}{T_1 - T_2} = \frac{\frac{1}{r} - \frac{1}{R_2}}{\frac{1}{R_1} - \frac{1}{R_2}} \quad (\text{D})$

**Table 8.6** Heat transfer rate and temperature distribution for one-dimensional conduction in a hollow sphere for the boundary conditions given by Eq. (8.2-52).

Constants	Heat Transfer Rate	Temperature Distribution
None	$4\pi R_1^2 q_1 \quad (\text{A})$	$\int_{T_2}^T k(T) dT = q_1 R_1^2 \left( \frac{1}{r} - \frac{1}{R_2} \right) \quad (\text{C})$
$k$	$4\pi R_1^2 q_1 \quad (\text{B})$	$T - T_2 = \frac{q_1 R_1^2}{k} \left( \frac{1}{r} - \frac{1}{R_2} \right) \quad (\text{D})$

**Example 8.9** A spherical metal ball of radius  $R$  is placed in an infinitely large volume of motionless fluid. The ball is maintained at a temperature of  $T_R$  while the temperature of the fluid far from the ball is  $T_\infty$ .

- a) Determine the rate of heat transferred to the fluid.
- b) Determine the temperature distribution within the fluid.
- c) Determine the Nusselt number.

**Solution**

**Assumptions**

- 1. Steady-state conditions prevail.

2. The heat transfer from the ball to the fluid takes place only by conduction.
3. The thermal conductivity of the fluid is constant.

### Analysis

a) The use of Eq. (B) in Table 8.5 with  $T_1 = T_R$ ,  $T_2 = T_\infty$ ,  $R_1 = R$  and  $R_2 = \infty$  gives the rate of heat transferred from the ball to the fluid as

$$\dot{Q} = \frac{4\pi k (T_R - T_\infty)}{1/R} = 4\pi R k (T_R - T_\infty) \quad (1)$$

b) The temperature distribution can be obtained from Eq. (D) of Table 8.5 in the form

$$\frac{T - T_\infty}{T_R - T_\infty} = \frac{R}{r} \quad (2)$$

c) The amount of heat transferred can also be calculated from Newton's law of cooling, Eq. (3.2-7), as

$$\dot{Q} = 4\pi R^2 \langle h \rangle (T_R - T_\infty) \quad (3)$$

Equating Eqs. (1) and (3) leads to

$$\frac{\langle h \rangle}{k} = \frac{1}{R} = \frac{2}{D} \quad (4)$$

Therefore, the Nusselt number is

$$\text{Nu} = \frac{\langle h \rangle D}{k} = 2 \quad (5)$$

#### 8.2.3.1 Electrical circuit analogy

Equation (B) in Table 8.5 can be rearranged in the form

$$\dot{Q} = \frac{T_1 - T_2}{\frac{\ln(R_2/R_1)}{4\pi k R_1 R_2}} \quad (8.2-53)$$

Comparison of Eq. (8.2-53) with Eq. (8.2-10) indicates that the resistance is given by

$$\boxed{\text{Resistance} = \frac{R_2 - R_1}{4\pi k R_1 R_2}} \quad (8.2-54)$$

In order to express the resistance in the form given by Eq. (8.2-13), let us define a geometric mean area,  $A_{GM}$ , as

$$\begin{aligned} A_{GM} &= \sqrt{A_1 A_2} \\ &= \sqrt{(4\pi R_1^2)(4\pi R_2^2)} = 4\pi R_1 R_2 \end{aligned} \quad (8.2-55)$$

so that Eq. (8.2-54) takes the form

$$\boxed{\text{Resistance} = \frac{R_2 - R_1}{kA_{GM}} = \frac{\text{Thickness}}{(\text{Transport property})(\text{Area})}} \quad (8.2-56)$$

The electrical circuit analog of the spherical wall can be represented as shown in Figure 8.20.

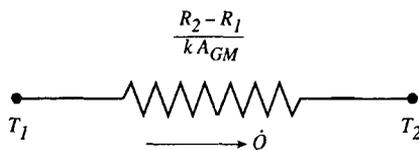


Figure 8.20 Electrical circuit analog of the spherical wall.

### 8.2.3.2 Transfer rate in terms of bulk fluid properties

The use of Eq. (8.2-53) in the calculation of the transfer rate requires surface values  $T_1$  and  $T_2$  to be known or measured. In common practice, the bulk temperatures of the adjoining fluids to the surfaces at  $r = R_1$  and  $r = R_2$ , i.e.,  $T_A$  and  $T_B$ , are known. It is then necessary to relate  $T_1$  and  $T_2$  to  $T_A$  and  $T_B$ .

The procedure for the spherical case is similar to that for the cylindrical case and left as an exercise to the students. If the procedure given in Section 8.2.2.2 is followed, the result is

$$\boxed{\dot{Q} = \frac{T_A - T_B}{\frac{1}{A_1 \langle h_A \rangle} + \frac{R_2 - R_1}{A_{GM} k} + \frac{1}{A_2 \langle h_B \rangle}}} \quad (8.2-57)$$

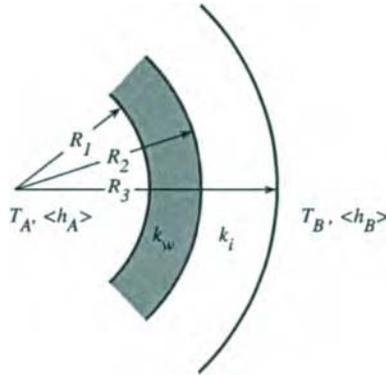
**Example 8.10** Consider a spherical tank with inner and outer radii of  $R_1$  and  $R_2$ , respectively, and investigate how the rate of heat loss varies as a function of insulation thickness.

#### Solution

The solution procedure for this problem is similar to Example 8.7. For the geometry shown in Figure 8.21, the rate of heat loss is given by

$$\dot{Q} = \frac{4\pi(T_A - T_B)}{\frac{1}{R_1^2 \langle h_A \rangle} + \frac{R_2 - R_1}{R_1 R_2 k_w} + \underbrace{\frac{R_3 - R_2}{R_2 R_3 k_i} + \frac{1}{R_3^2 \langle h_B \rangle}}_X} \quad (1)$$

where  $k_w$  and  $k_i$  are the thermal conductivities of the wall and the insulating material, respectively.



**Figure 8.21** Conduction through an insulated hollow sphere.

Differentiation of  $X$  with respect to  $R_3$  gives

$$\frac{dX}{dR_3} = 0 \quad \Rightarrow \quad R_3 = \frac{2k_i}{\langle h_B \rangle} \quad (2)$$

To determine whether this point corresponds to a minimum or a maximum value, it is necessary to calculate the second derivative, i.e.,

$$\left. \frac{d^2X}{dR_3^2} \right|_{R_3=2k_i/\langle h_B \rangle} = \frac{1}{8} \frac{\langle h_B \rangle^3}{k_i^4} > 0 \quad (3)$$

Therefore, the critical thickness of insulation for the spherical geometry is given by

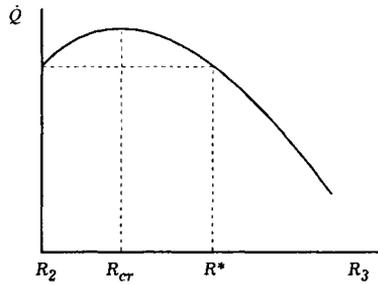
$$R_{cr} = \frac{2k_i}{\langle h_B \rangle} \quad (4)$$

A representative graph showing the variation of heat transfer rate with insulation thickness is given in Figure 8.22.

Another point of interest is to determine the value of  $R^*$ , the point at which the rate of heat loss is equal to that of the bare pipe. Following the procedure given in Example 8.7, the result is

$$\left( \frac{R^*}{R_2} \right)^2 = \frac{\langle h_B \rangle R^*}{k_i} \left( \frac{R^*}{R_2} - 1 \right) + 1 \quad (5)$$

$R^*$  can be determined from Eq. (5) for the given values of  $R_2$ ,  $\langle h_B \rangle$ , and  $k_i$ .



**Figure 8.22** Rate of heat loss as a function of insulation thickness.

**Example 8.11** Consider a hollow steel sphere of inside radius  $R_1 = 10$  cm and outside radius  $R_2 = 20$  cm. The inside surface is maintained at a constant temperature of  $180^\circ\text{C}$  and the outside surface dissipates heat to ambient temperature at  $20^\circ\text{C}$  by convection with an average heat transfer coefficient of  $11 \text{ W/m}^2\cdot\text{K}$ . To reduce the rate of heat loss, it is proposed to cover the outer surface of the sphere by two types of insulating materials  $X$  and  $Y$  in series. Each insulating material has a thickness of 3 cm. The thermal conductivities of the insulating materials  $X$  and  $Y$  are  $0.04$  and  $0.12 \text{ W/m}\cdot\text{K}$ , respectively. One of your friends claims that the order in which the two insulating materials are put around the sphere does not make a difference in the rate of heat loss. As an engineer, do you agree?

### Solution

#### Physical properties

For steel:  $k = 45 \text{ W/m}\cdot\text{K}$

#### Analysis

The rate of heat loss can be determined from Eq. (8.2-57). If the surface is first covered by  $X$  and then  $Y$ , the rate of heat loss is

$$\begin{aligned} \dot{Q} &= \frac{4\pi(180-20)}{\frac{0.1}{(45)(0.1)(0.2)} + \frac{0.03}{(0.04)(0.2)(0.23)} + \frac{0.03}{(0.12)(0.23)(0.26)} + \frac{1}{(0.26)^2(11)}} \\ &= 91.6 \text{ W} \end{aligned}$$

On the other hand, covering the surface first by  $Y$  and then  $X$  gives the rate of heat loss as

$$\begin{aligned} \dot{Q} &= \frac{4\pi(180-20)}{\frac{0.1}{(45)(0.1)(0.2)} + \frac{0.03}{(0.12)(0.2)(0.23)} + \frac{0.03}{(0.04)(0.23)(0.26)} + \frac{1}{(0.26)^2(11)}} \\ &= 103.5 \text{ W} \end{aligned}$$

Therefore, the order of the layers with different thermal conductivities does make a difference.

### 8.2.4 Conduction in a Fin

In the previous sections we have considered one-dimensional conduction examples. The extension of the procedure for these problems to conduction in two- or three-dimensional cases is straightforward. The difficulty with multi-dimensional conduction problems lies in the solution of the resulting partial differential equations. An excellent book by Carslaw and Jaeger (1959) gives the solutions of conduction problems with various boundary conditions.

In this section first the governing equation for temperature distribution will be developed for three-dimensional conduction in a rectangular geometry. Then the use of area averaging<sup>4</sup> will be introduced to simplify the problem.

Fins are extensively used in heat transfer applications to enhance the heat transfer rate by increasing heat transfer area. Let us consider a simple rectangular fin as shown in Figure 8.23. As an engineer we are interested in the rate of heat loss from the surfaces of the fin. This can be calculated if the temperature distribution within the fin is known. The problem will be analyzed with the following assumptions:

1. Steady state conditions prevail.
2. The thermal conductivity of the fin is constant.
3. The average heat transfer coefficient is constant.
4. There is no heat loss from the edges and the tip of the fin.

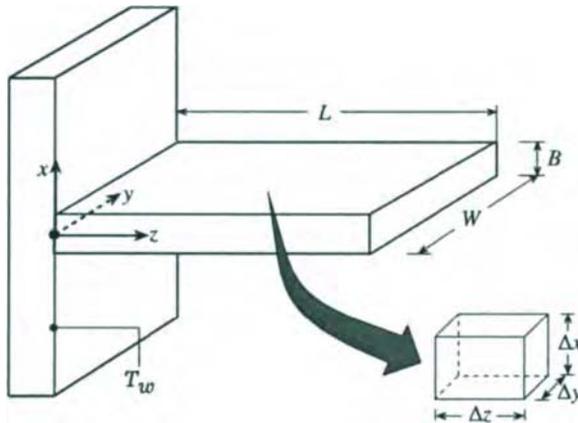


Figure 8.23 Conduction in a rectangular fin.

<sup>4</sup>The first systematic use of the area averaging technique in a textbook can be attributed to Slattery (1972).

For a rectangular volume element of thickness  $\Delta x$ , width  $\Delta y$  and length  $\Delta z$ , as shown in Figure 8.23, Eq. (8.2-1) is expressed as

$$(q_x|_x \Delta y \Delta z + q_y|_y \Delta x \Delta z + q_z|_z \Delta x \Delta y) - (q_x|_{x+\Delta x} \Delta y \Delta z + q_y|_{y+\Delta y} \Delta x \Delta z + q_z|_{z+\Delta z} \Delta x \Delta y) = 0 \quad (8.2-58)$$

Dividing by  $\Delta x \Delta y \Delta z$  and taking the limit as  $\Delta x \rightarrow 0$ ,  $\Delta y \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta x \rightarrow 0} \frac{q_x|_x - q_x|_{x+\Delta x}}{\Delta x} + \lim_{\Delta y \rightarrow 0} \frac{q_y|_y - q_y|_{y+\Delta y}}{\Delta y} + \lim_{\Delta z \rightarrow 0} \frac{q_z|_z - q_z|_{z+\Delta z}}{\Delta z} = 0 \quad (8.2-59)$$

or,

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = 0 \quad (8.2-60)$$

From Table C.4 in Appendix C, the components of the conductive flux are given by

$$q_x = -k \frac{\partial T}{\partial x} \quad (8.2-61)$$

$$q_y = -k \frac{\partial T}{\partial y} \quad (8.2-62)$$

$$q_z = -k \frac{\partial T}{\partial z} \quad (8.2-63)$$

Substitution of Eqs. (8.2-61)-(8.2-63) into Eq. (8.2-60) gives the governing equation for temperature as

$$\boxed{\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = 0} \quad (8.2-64)$$

The boundary conditions associated with Eq. (8.2-64) are

$$\text{at } x = B/2 \quad -k \frac{\partial T}{\partial x} = \langle h \rangle (T - T_\infty) \quad (8.2-65)$$

$$\text{at } x = -B/2 \quad k \frac{\partial T}{\partial x} = \langle h \rangle (T - T_\infty) \quad (8.2-66)$$

$$\text{at } y = 0 \quad \frac{\partial T}{\partial y} = 0 \quad (8.2-67)$$

$$\text{at } y = W \quad \frac{\partial T}{\partial y} = 0 \quad (8.2-68)$$

$$\text{at } z = 0 \quad T = T_w \quad (8.2-69)$$

$$\text{at } z = L \quad \frac{\partial T}{\partial z} = 0 \quad (8.2-70)$$

where  $T_\infty$  is the temperature of the fluid surrounding the fin.

If the measuring instrument, i.e., the temperature probe, is not sensitive enough to detect temperature variations in the  $x$ -direction, then it is necessary to change the scale of the problem to match that of the measuring device. In other words, it is necessary to average the governing equation up to the scale of the temperature measuring probe.

The area-averaged temperature is defined by

$$\langle T \rangle = \frac{\int_0^W \int_{-B/2}^{B/2} T \, dx dy}{\int_0^W \int_{-B/2}^{B/2} dx dy} = \frac{1}{WB} \int_0^W \int_{-B/2}^{B/2} T \, dx dy \quad (8.2-71)$$

Note that although the local temperature,  $T$ , is dependent on  $x$ ,  $y$  and  $z$ , the area-averaged temperature,  $\langle T \rangle$ , depends only on  $z$ .

Area averaging is performed by integrating Eq. (8.2-64) over the cross-sectional area of the fin. The result is

$$\int_0^W \int_{-B/2}^{B/2} \frac{\partial^2 T}{\partial x^2} \, dx dy + \int_0^W \int_{-B/2}^{B/2} \frac{\partial^2 T}{\partial y^2} \, dx dy + \int_0^W \int_{-B/2}^{B/2} \frac{\partial^2 T}{\partial z^2} \, dx dy = 0 \quad (8.2-72)$$

or,

$$\int_0^W \left( \left. \frac{\partial T}{\partial x} \right|_{x=B/2} - \left. \frac{\partial T}{\partial x} \right|_{x=-B/2} \right) dy + \int_{-B/2}^{B/2} \left( \left. \frac{\partial T}{\partial y} \right|_{y=W} - \left. \frac{\partial T}{\partial y} \right|_{y=0} \right) dx + \frac{d^2}{dz^2} \left( \int_0^W \int_{-B/2}^{B/2} T \, dx dy \right) = 0 \quad (8.2-73)$$

The use of the boundary conditions defined by Eqs. (8.2-65)-(8.2-68) together with the definition of the average temperature, Eq. (8.2-71) in Eq. (8.2-73) gives

$$W \left[ -\frac{\langle h \rangle}{k} (T|_{x=B/2} - T_\infty) - \frac{\langle h \rangle}{k} (T|_{x=-B/2} - T_\infty) \right] + WB \frac{d^2 \langle T \rangle}{dz^2} = 0 \quad (8.2-74)$$

Since  $T|_{x=B/2} = T|_{x=-B/2}$  as a result of symmetry, Eq. (8.2-74) takes the form

$$k \frac{d^2 \langle T \rangle}{dz^2} - \frac{2}{B} \langle h \rangle (T|_{x=B/2} - T_\infty) = 0 \quad (8.2-75)$$

Note that Eq. (8.2-75) contains two dependent variables,  $\langle T \rangle$  and  $T|_{x=B/2}$ , which are at two different scales. It is generally assumed, although not expressed explicitly, that

$$\langle T \rangle \approx T|_{x=B/2} \quad (8.2-76)$$

This approximation is valid for  $\text{Bi}_H \ll 1$ . Substitution of Eq. (8.2-76) into Eq. (8.2-75) gives

$$\boxed{k \frac{d^2 \langle T \rangle}{dz^2} = \frac{2}{B} \langle h \rangle (\langle T \rangle - T_\infty)} \quad (8.2-77)$$

Integration of Eqs. (8.2-69) and (8.2-70) over the cross-sectional area of the fin gives the boundary conditions associated with Eq. (8.2-77) as

$$\text{at } z = 0 \quad \langle T \rangle = T_w \tag{8.2-78}$$

$$\text{at } z = L \quad \frac{d\langle T \rangle}{dz} = 0 \tag{8.2-79}$$

It is important to note that Eqs. (8.2-64) and (8.2-77) are at two different scales. Equation (8.2-77) is obtained by averaging Eq. (8.2-64) over the cross-sectional area perpendicular to the direction of energy flux. In this way the boundary condition, i.e., the heat transfer coefficient, is incorporated into the governing equation. Accuracy of the measurements dictates the equation to work with since the scale of the measurements should be compatible with the scale of the equation.

The term  $2/B$  in Eq. (8.2-77) represents the heat transfer area per unit volume of the fin, i.e.,

$$\frac{2}{B} = \frac{2LW}{BLW} = \frac{\text{Heat transfer area}}{\text{Fin volume}} \tag{8.2-80}$$

The physical significance and the order of magnitude<sup>5</sup> of the terms in Eq. (8.2-77) are given in Table 8.7.

**Table 8.7** The physical significance and the order of magnitude of the terms in Eq. (8.2-77).

Term	Physical Significance	Order of Magnitude
$k \frac{d^2\langle T \rangle}{dz^2}$	Rate of conduction	$\frac{k(T_w - T_\infty)}{L^2}$
$\frac{2\langle h \rangle}{B} (\langle T \rangle - T_\infty)$	Rate of heat transfer from the fin to the surroundings	$\frac{2\langle h \rangle(T_w - T_\infty)}{B}$

Therefore, the ratio of the rate of heat transfer from the fin surface to the rate of conduction is given by

$$\frac{\text{Rate of heat transfer}}{\text{Rate of conduction}} = \frac{2\langle h \rangle(T_w - T_\infty)/B}{k(T_w - T_\infty)/L^2} = \frac{2\langle h \rangle L^2}{kB} \tag{8.2-81}$$

<sup>5</sup>The *order of magnitude* or *scale analysis* is a powerful tool for those interested in mathematical modelling. As stated by Astarita (1997), "Very often more than nine-tenths of what one can ever hope to know about a problem can be obtained from this tool, without actually solving the problem; the remaining one-tenth requires painstaking algebra and/or lots of computer time, it adds very little to our understanding of the problem, and if we have not done the first part right, all that the algebra and the computer will produce will be a lot of nonsense. Of course, when nonsense comes out of a computer people have a lot of respect for it, and that is exactly the problem." For more details on the order of magnitude analysis, see Bejan (1984), Whitaker (1976).

Before solving Eq. (8.2-77), it is convenient to express the governing equation and the boundary conditions in dimensionless form. The reason for doing this is the fact that the inventory equations in dimensionless form represent the solution to the entire class of geometrically similar problems when they are applied to a particular geometry.

Introduction of the dimensionless variables

$$\theta = \frac{\langle T \rangle - T_\infty}{T_w - T_\infty} \quad (8.2-82)$$

$$\xi = \frac{z}{L} \quad (8.2-83)$$

$$\Lambda = \sqrt{\frac{2\langle h \rangle L^2}{kB}} \quad (8.2-84)$$

reduces Eqs. (8.2-77)-(8.2-79) to

$$\frac{d^2\theta}{d\xi^2} = \Lambda^2\theta \quad (8.2-85)$$

$$\text{at } \xi = 0 \quad \theta = 1 \quad (8.2-86)$$

$$\text{at } \xi = 1 \quad \frac{d\theta}{d\xi} = 0 \quad (8.2-87)$$

The solution of Eq. (8.2-85) is

$$\theta = C_1 \sinh(\Lambda\xi) + C_2 \cosh(\Lambda\xi) \quad (8.2-88)$$

where  $C_1$  and  $C_2$  are constants. Application of the boundary conditions, Eqs. (8.2-86) and (8.2-87), gives the solution as

$$\theta = \frac{\cosh \Lambda \cosh(\Lambda\xi) - \sinh \Lambda \sinh(\Lambda\xi)}{\cosh \Lambda} \quad (8.2-89)$$

The use of the identity

$$\cosh(x - y) = \cosh x \cosh y - \sinh x \sinh y \quad (8.2-90)$$

reduces the solution to the form

$$\theta = \frac{\cosh[\Lambda(1 - \xi)]}{\cosh \Lambda} \quad (8.2-91)$$

### 8.2.4.1 Macroscopic equation

Integration of the governing differential equation, Eq. (8.2-77), over the volume of the system gives the macroscopic energy balance, i.e.,

$$\int_0^L \int_0^W \int_{-B/2}^{B/2} k \frac{d^2 \langle T \rangle}{dz^2} dx dy dz = \int_0^L \int_0^W \int_{-B/2}^{B/2} \frac{2}{B} \langle h \rangle (\langle T \rangle - T_\infty) dx dy dz \quad (8.2-92)$$

Evaluation of the integrations yields

$$\underbrace{BW \left( -k \frac{d \langle T \rangle}{dz} \Big|_{z=0} \right)}_{\text{Rate of energy entering into the fin through the surface at } z=0} = \underbrace{2W \langle h \rangle \int_0^L (\langle T \rangle - T_\infty) dz}_{\text{Rate of energy loss from the top and bottom surfaces of the fin to the surroundings}} \quad (8.2-93)$$

Note that Eq. (8.2-93) is simply the macroscopic inventory rate equation for thermal energy by considering the fin as a system. The use of Eq. (8.2-91) in Eq. (8.2-93) gives the rate of heat loss from the fin as

$$\boxed{\dot{Q}_{loss} = \frac{BWk(T_w - T_\infty)\Lambda \tanh \Lambda}{L}} \quad (8.2-94)$$

### 8.2.4.2 Fin efficiency

The *fin efficiency*,  $\eta$ , is defined as the ratio of the apparent rate of heat dissipation of a fin to the ideal rate of heat dissipation if the entire fin surface were at  $T_w$ , i.e.,

$$\eta = \frac{2W \langle h \rangle \int_0^L (\langle T \rangle - T_\infty) dz}{2W \langle h \rangle (T_w - T_\infty)L} = \frac{\int_0^L (\langle T \rangle - T_\infty) dz}{(T_w - T_\infty)L} \quad (8.2-95)$$

In terms of the dimensionless quantities, Eq. (8.2-95) becomes

$$\eta = \int_0^1 \theta d\xi \quad (8.2-96)$$

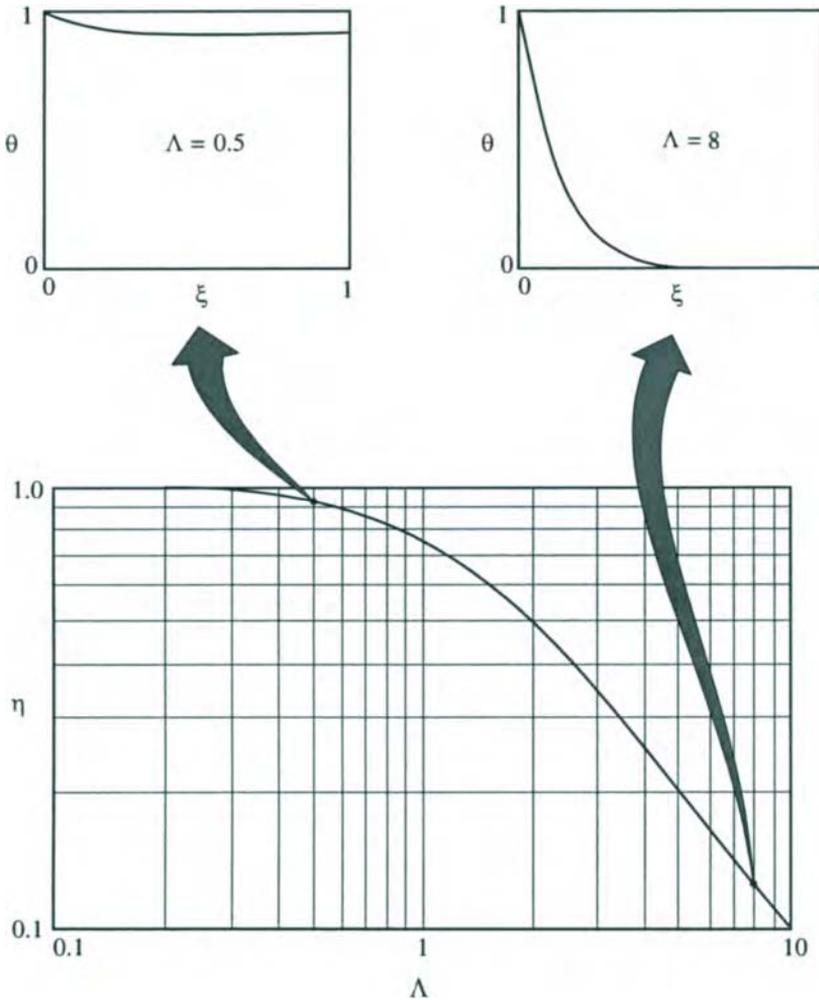
Substitution of Eq. (8.2-91) into Eq. (8.2-96) gives the fin efficiency as

$$\boxed{\eta = \frac{\tanh \Lambda}{\Lambda}} \quad (8.2-97)$$

The variation of the fin efficiency as a function of  $\Lambda$  is shown in Figure 8.24. When  $\Lambda \rightarrow 0$ , this means that the rate of conduction is much larger than the rate of heat dissipation. The Taylor series expansion of  $\eta$  in terms of  $\Lambda$  gives

$$\eta = 1 - \frac{1}{3} \Lambda^2 + \frac{2}{15} \Lambda^4 - \frac{17}{315} \Lambda^6 + \dots \quad (8.2-98)$$

Therefore,  $\eta$  approaches unity as  $\Lambda \rightarrow 0$ , indicating that the entire fin surface is at the wall temperature.



**Figure 8.24** Variation of the fin efficiency,  $\eta$ , as a function of  $\Lambda$ .

On the other hand, large values of  $\Lambda$  corresponds to cases in which the heat transfer rate by conduction is very slow and the rate of heat transfer from the fin surface is very rapid. Under these conditions the fin efficiency becomes

$$\eta = \frac{1}{\Lambda} \tag{8.2-99}$$

Equation (8.2-99) indicates that  $\eta$  approaches zero as  $\Lambda \rightarrow \infty$ .

Since the fin efficiency is inversely proportional to  $\Lambda$ , it can be improved either by increasing  $k$  and  $B$ , or by decreasing  $\langle h \rangle$  and  $L$ . If the average heat transfer coefficient,  $\langle h \rangle$ , is increased due to an increase in the air velocity past the fin, the fin efficiency decreases. This means that the length of the fin,  $L$ , can be smaller for the larger  $\langle h \rangle$  if the fin efficiency remains constant. In other words, fins are not necessary at high speeds of fluid velocity.

### 8.2.4.3 Comment

In general, the governing differential equations represent the variation of the dependent variables, such as temperature and concentration, as a function of position and time. On the other hand, the transfer coefficients, which represent the interaction of the system with the surroundings, appear in the boundary conditions. If the transfer coefficients appear in the governing equations rather than the boundary conditions, this implies that these equations are obtained as a result of the averaging process.

## 8.3 ENERGY TRANSPORT WITH CONVECTION

Heat transfer by convection involves both the equation of motion and the equation of energy. Since we restrict the analysis to cases in which neither momentum nor energy is generated, this obviously limits the problems we might encounter.

Consider Couette flow of a Newtonian fluid between two large parallel plates under steady conditions as shown in Figure 8.25. Note that this geometry not only considers flow between parallel plates but also tangential flow between concentric cylinders. The surfaces at  $x = 0$  and  $x = B$  are maintained at  $T_0$  and  $T_1$ , respectively, with  $T_0 > T_1$ . It is required to determine the temperature distribution within the fluid.

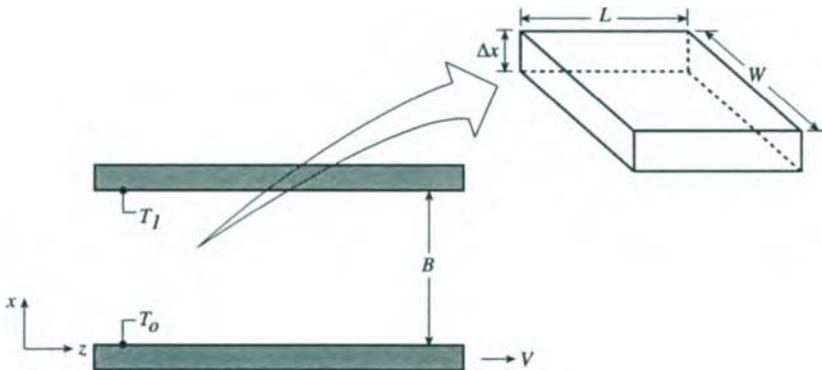


Figure 8.25 Couette flow between parallel plates.

The velocity distribution for this problem is given by Eq. (8.1-12) as

$$\frac{v_z}{V} = 1 - \frac{x}{B} \quad (8.3-1)$$

On the other hand, the boundary conditions for the temperature, i.e.,

$$\text{at } x = 0 \quad T = T_o \quad (8.3-2)$$

$$\text{at } x = B \quad T = T_1 \quad (8.3-3)$$

suggest that  $T = T(x)$ . Therefore, Table C.4 in Appendix C indicates that the only non-zero energy flux component is  $e_x$  and it is given by

$$e_x = q_x = -k \frac{dT}{dx} \quad (8.3-4)$$

For a rectangular volume element of thickness  $\Delta x$ , as shown in Figure 8.25, Eq. (8.2-1) is expressed as

$$q_x|_x WL - q_x|_{x+\Delta x} WL = 0 \quad (8.3-5)$$

Dividing each term by  $WL \Delta x$  and taking the limit as  $\Delta x \rightarrow 0$  gives

$$\lim_{\Delta x \rightarrow 0} \frac{q_x|_x - q_x|_{x+\Delta x}}{\Delta x} = 0 \quad (8.3-6)$$

or,

$$\frac{dq_x}{dx} = 0 \quad (8.3-7)$$

Substitution of Eq. (8.3-4) into Eq. (8.3-7) gives the governing equation for temperature in the form

$$\frac{d^2T}{dx^2} = 0 \quad (8.3-8)$$

The solution of Eq. (8.3-8) is

$$T = C_1 + C_2 x \quad (8.3-9)$$

The use of boundary conditions defined by Eqs. (8.3-2) and (8.3-3) gives the linear temperature distribution as

$$\boxed{\frac{T - T_o}{T_1 - T_o} = \frac{x}{B}} \quad (8.3-10)$$

## 8.4 MASS TRANSPORT WITHOUT CONVECTION

The inventory rate equation for transfer of species  $\mathcal{A}$  at the microscopic level is called the *equation of continuity for species  $\mathcal{A}$* . Under steady conditions without generation, the conservation statement for the mass of species  $\mathcal{A}$  is given by

$$(\text{Rate of mass of } \mathcal{A} \text{ in}) - (\text{Rate of mass of } \mathcal{A} \text{ out}) = 0 \quad (8.4-1)$$

The rate of mass of  $\mathcal{A}$  entering and leaving the system is determined from the mass (or, molar) flux. As stated in Chapter 2, the total flux is the sum of the molecular and convective fluxes. For a one-dimensional transfer of species  $\mathcal{A}$  in the  $z$ -direction in rectangular coordinates, the total molar flux is expressed as

$$N_{A_z} = \underbrace{-cD_{AB} \frac{dx_A}{dz}}_{\text{Molecular flux}} + \underbrace{c_A v_z^*}_{\text{Convective flux}} \quad (8.4-2)$$

where  $v_z^*$  is the molar average velocity defined by Eq. (2.3-2). For a binary system composed of species  $\mathcal{A}$  and  $\mathcal{B}$ , the molar average velocity is given by

$$v_z^* = \frac{c_A v_{A_z} + c_B v_{B_z}}{c_A + c_B} = \frac{N_{A_z} + N_{B_z}}{c} \quad (8.4-3)$$

As we did for heat transfer, we will first consider the case of mass transfer without convection. For the transport of heat without convection, we focused our attention on conduction in solids and stationary liquids simply because energy is transferred by collisions of adjacent molecules and the migration of free electrons. In the case of mass transport, however, since species have individual velocities<sup>6</sup>, the neglect of the convection term is not straightforward. It is customary in the literature to neglect the convective flux in comparison with the molecular flux when mass transfer takes place in solids and stationary liquids. The reason for this can be explained as follows. Substitution of Eq. (8.4-3) into Eq. (8.4-2) gives

$$N_{A_z} = -cD_{AB} \frac{dx_A}{dz} + x_A(N_{A_z} + N_{B_z}) \quad (8.4-4)$$

Since  $x_A$  is usually very small in solids and liquids, the convective term is considered negligible. It should be kept in mind, however, that if  $x_A$  is small, this does not imply that its gradient, i.e.,  $dx_A/dz$ , is also small.

Another point of interest is the equimolar counterdiffusion in gases. The term “*equimolar counterdiffusion*” implies that for every mole of species  $\mathcal{A}$  diffusing in the positive  $z$ -direction, one mole of species  $\mathcal{B}$  diffuses back in the negative  $z$ -direction, i.e.,

$$N_{A_z} = -N_{B_z} \quad \Rightarrow \quad c_A v_{A_z} = -c_B v_{B_z} \quad (8.4-5)$$

Under these circumstances the molar average velocity, Eq. (8.4-3), becomes

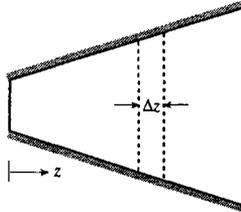
$$v_z^* = \frac{N_{A_z} + (-N_{A_z})}{c} = 0 \quad (8.4-6)$$

and the convective flux automatically drops out in Eq. (8.4-2).

<sup>6</sup>Transport of mass by diffusion as a result of random molecular motion is called a Brownian motion.

### 8.4.1 Diffusion in Rectangular Coordinates

Consider the transfer of species  $\mathcal{A}$  by diffusion through a slightly tapered slab as shown in Figure 8.26.



**Figure 8.26** Diffusion through a slightly tapered conical duct.

If the taper angle is small, mass transport can be considered one-dimensional in the  $z$ -direction. Since  $x_A = x_A(z)$ , Table C.7 in Appendix C indicates that the only non-zero molar flux component is  $N_{A_z}$  and it is given by

$$N_{A_z} = J_{A_z}^* = -c \mathcal{D}_{AB} \frac{dx_A}{dz} \quad (8.4-7)$$

Note that the negative sign in Eq. (8.4-7) implies that positive  $z$ -direction is in the direction of decreasing concentration. If the answer turns out to be negative, this implies that the flux is in the negative  $z$ -direction.

Over a differential volume element of thickness  $\Delta z$ , as shown in Figure 8.26, Eq. (8.4-1) is written as

$$(AN_{A_z})|_z - (AN_{A_z})|_{z+\Delta z} = 0 \quad (8.4-8)$$

Dividing Eq. (8.4-8) by  $\Delta z$  and taking the limit as  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{(AN_{A_z})|_z - (AN_{A_z})|_{z+\Delta z}}{\Delta z} = 0 \quad (8.4-9)$$

or,

$$\frac{d(AN_{A_z})}{dz} = 0 \quad (8.4-10)$$

Since flux times area gives the molar transfer rate of species  $\mathcal{A}$ ,  $\dot{n}_A$ , it is possible to conclude that

$$AN_{A_z} = \text{constant} = \dot{n}_A \quad (8.4-11)$$

in which the area  $A$  is perpendicular to the direction of mass flux.

Substitution of Eq. (8.4-7) into Eq. (8.4-11) and integration gives

$$c \int_0^{x_A} \mathcal{D}_{AB}(x_A) dx_A = -\dot{n}_A \int_0^z \frac{dz}{A(z)} + K \quad (8.4-12)$$

where  $K$  is an integration constant. The determination of  $\dot{n}_A$  and  $K$  requires two boundary conditions. Depending on the type of the boundary conditions used, the molar transfer rate of species  $A$  as well as the concentration distribution of species  $A$  as a function of position are determined from Eq. (8.4-12).

If the surface concentrations are specified, i.e.,

$$\begin{aligned} \text{at } z = 0 & \quad x_A = x_{A_0} \\ \text{at } z = L & \quad x_A = x_{A_L} \end{aligned} \quad (8.4-13)$$

the molar transfer rate and the concentration distribution of species  $A$  are given in Table 8.8.

**Table 8.8** Rate of transfer and concentration distribution for one-dimensional diffusion in rectangular coordinates for the boundary conditions given by Eq. (8.4-13).

Constants	Molar Transfer Rate	Concentration Distribution
None	(A) $\frac{c \int_{x_{A_L}}^{x_{A_0}} \mathcal{D}_{AB} dx_A}{\int_0^L \frac{dz}{A(z)}}$	(E) $\frac{\int_{x_A}^{x_{A_0}} \mathcal{D}_{AB} dx_A}{\int_{x_{A_L}}^{x_{A_0}} \mathcal{D}_{AB} dx_A} = \frac{\int_0^z \frac{dz}{A(z)}}{\int_0^L \frac{dz}{A(z)}}$
$\mathcal{D}_{AB}$	(B) $\frac{c \mathcal{D}_{AB} (x_{A_0} - x_{A_L})}{\int_0^L \frac{dz}{A(z)}}$	(F) $\frac{x_{A_0} - x_A}{x_{A_0} - x_{A_L}} = \frac{\int_0^z \frac{dz}{A(z)}}{\int_0^L \frac{dz}{A(z)}}$
$A$	(C) $\frac{A c \int_{x_{A_L}}^{x_{A_0}} \mathcal{D}_{AB} dx_A}{L}$	(G) $\frac{\int_{x_A}^{x_{A_0}} \mathcal{D}_{AB} dx_A}{\int_{x_{A_L}}^{x_{A_0}} \mathcal{D}_{AB} dx_A} = \frac{z}{L}$
$\frac{\mathcal{D}_{AB}}{A}$	(D) $\frac{c \mathcal{D}_{AB} (x_{A_0} - x_{A_L}) A}{L}$	(H) $\frac{x_{A_0} - x_A}{x_{A_0} - x_{A_L}} = \frac{z}{L}$

**Example 8.12** Two large tanks are connected by a truncated conical duct as shown in Figure 8.27. The diameter at  $z = 0$  is 6 mm and the diameter at  $z = 0.2$  m is 10 mm. Gas compositions in the tanks are given in terms of mole percentages. The pressure and temperature throughout the system are 1 atm and 25 °C, respectively, and  $\mathcal{D}_{AB} = 3 \times 10^{-5} \text{ m}^2/\text{s}$ .

- a) Determine the initial molar flow rate of species *A* between the vessels.  
 b) What would be the initial molar flow rate of species *A* if the conical duct were replaced with a circular tube of 8 mm diameter?

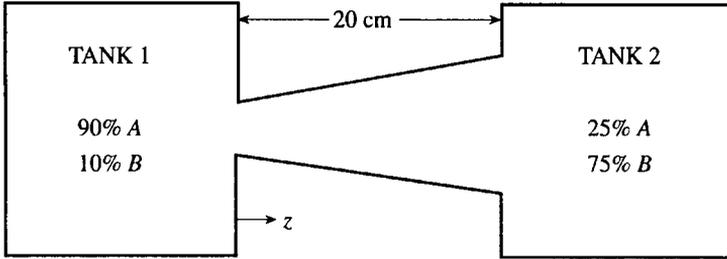


Figure 8.27 Diffusion through a conical duct.

**Solution**

Since the total pressure remains constant, the total number of moles in the conical duct does not change. This implies that equimolar counterdiffusion takes place within the conical duct and the molar average velocity is zero. Equation (B) in Table 8.8 gives the molar flow rate of species *A* as

$$\dot{n}_A = \frac{cD_{AB}(x_{A_o} - x_{A_L})}{\int_0^{0.2} \frac{dz}{A(z)}} \tag{1}$$

The variation of the diameter as a function of position is represented by

$$D(z) = 0.006 + 0.02z \tag{2}$$

so that the area is

$$A(z) = \frac{\pi}{4} (0.006 + 0.02z)^2 \tag{3}$$

Substitution of Eq. (3) into Eq. (1) and integration gives

$$\dot{n}_A = \frac{cD_{AB}(x_{A_o} - x_{A_L})}{4244.1} \tag{4}$$

The total molar concentration is

$$\begin{aligned} c &= \frac{P}{RT} \\ &= \frac{101.325 \times 10^3}{(8.314 \times 10^3)(25 + 273)} = 0.041 \text{ kmol/m}^3 \end{aligned} \tag{5}$$

Therefore, the initial molar flow rate of species  $A$  is

$$\dot{n}_A = \frac{(41)(3 \times 10^{-5})(0.9 - 0.25)}{4244.1} = 1.88 \times 10^{-7} \text{ mol/s} \quad (6)$$

b) From Eq. (D) in Table 8.8

$$\begin{aligned} \dot{n}_A &= \frac{c D_{AB}(x_{A_o} - x_{A_L})A}{L} \\ &= \frac{(41)(3 \times 10^{-5})(0.9 - 0.25) [\pi(0.008)^2/4]}{0.2} = 2.01 \times 10^{-7} \text{ mol/s} \end{aligned} \quad (7)$$

#### 8.4.1.1 Electrical circuit analogy

The molar transfer rate of species  $A$  is given by Eq. (D) in Table 8.8 as

$$\dot{n}_A = \frac{c_{A_o} - c_{A_L}}{\frac{L}{D_{AB}A}} \quad (8.4-14)$$

Comparison of Eq. (8.4-14) with Eq. (8.2-10) indicates that

$$\text{Driving force} = c_{A_o} - c_{A_L} \quad (8.4-15)$$

$\text{Resistance} = \frac{L}{D_{AB}A} = \frac{\text{Thickness}}{(\text{Transport property})(\text{Area})} \quad (8.4-16)$
--

#### 8.4.1.2 Transfer rate in terms of bulk fluid properties

Since it is much easier to measure the bulk concentrations of the adjacent solutions to the surfaces at  $z = 0$  and  $z = L$ , it is necessary to relate the surface concentrations,  $x_{A_o}$  and  $x_{A_L}$ , to the bulk concentrations.

For energy transfer, the assumption of thermal equilibrium at a solid-fluid boundary leads to the equality of temperatures and this condition is generally stated as, "temperature is continuous at a solid-fluid boundary." In the case of mass transfer, the condition of phase equilibrium for a nonreacting multicomponent system at a solid-fluid boundary implies the equality of chemical potentials or partial molar Gibbs free energies. Therefore, concentrations at a solid-fluid boundary are not necessarily equal to each other with a resulting discontinuity in the concentration distribution. For example, consider a homogeneous membrane which is chemically different from the solution it is separating. In that case, the solute may be more (or, less) soluble in the membrane than in the bulk solution. A typical distribution of concentration is shown in Figure 8.28. Under these conditions, a thermodynamic property  $H$ , called the *partition coefficient*, is introduced

which relates the concentration of species in the membrane at equilibrium to the concentration in bulk solution. For the problem depicted in Figure 8.28, the partition coefficients can be defined as

$$H^- = \frac{c_{A_o}}{c_{A_i}^-} \quad (8.4-17)$$

$$H^+ = \frac{c_{A_L}}{c_{A_i}^+} \quad (8.4-18)$$

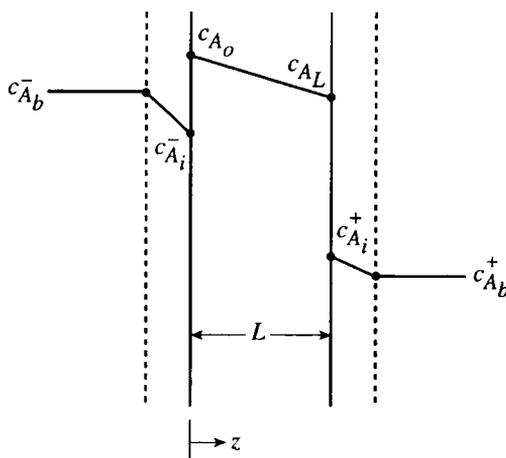


Figure 8.28 Concentration distribution across a membrane.

The molar rate of transfer of species across the membrane under steady conditions can be expressed as

$$\dot{n}_A = A k_c^- (c_{A_b}^- - c_{A_i}^-) = A k_c^+ (c_{A_i}^+ - c_{A_b}^+) \quad (8.4-19)$$

On the other hand, the use of Eqs. (8.4-17) and (8.4-18) in Eq. (8.4-14) leads to

$$\dot{n}_A = \frac{A \mathcal{D}_{AB} (H^- c_{A_i}^- - H^+ c_{A_i}^+)}{L} \quad (8.4-20)$$

Equations (8.4-19)-(8.4-20) can be rearranged in the form

$$c_{A_b}^- - c_{A_i}^- = \dot{n}_A \left( \frac{1}{A k_c^-} \right) \quad \parallel \times H^- \quad (8.4-21)$$

$$H^- c_{A_i}^- - H^+ c_{A_i}^+ = \dot{n}_A \left( \frac{L}{A \mathcal{D}_{AB}} \right) \quad (8.4-22)$$

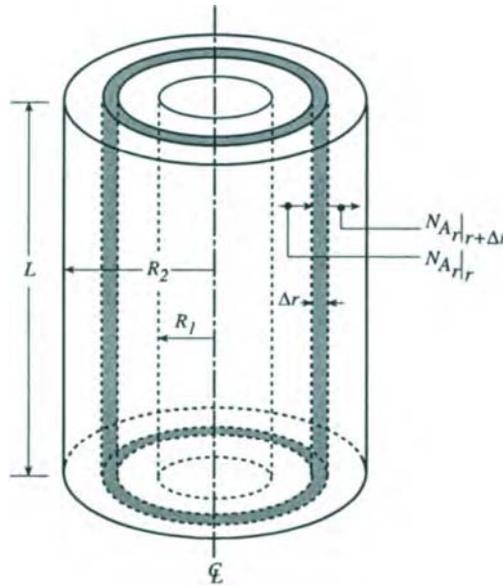
$$c_{A_i}^+ - c_{A_b}^+ = \dot{n}_A \left( \frac{1}{A k_c^+} \right) \quad \parallel \times H^+ \quad (8.4-23)$$

Multiplication of Eqs. (8.4-21) and (8.4-23) by  $H^-$  and  $H^+$ , respectively, and the addition of these equations with Eq. (8.4-22) gives

$$\dot{n}_A = \frac{c_{A_b}^- - \left(\frac{H^+}{H^-}\right) c_{A_b}^+}{\frac{1}{A k_c^-} + \frac{L}{A \mathcal{D}_{AB} H^-} + \left(\frac{H^+}{H^-}\right) \left(\frac{1}{A k_c^+}\right)} \quad (8.4-24)$$

### 8.4.2 Diffusion in Cylindrical Coordinates

Consider one-dimensional diffusion of species  $A$  in the radial direction through a hollow circular pipe with inner and outer radii of  $R_1$  and  $R_2$ , respectively, as shown in Figure 8.29.



**Figure 8.29** Diffusion through a hollow cylinder.

Since  $x_A = x_A(r)$ , Table C.8 in Appendix C indicates that the only non-zero molar flux component is  $N_{A,r}$  and it is given by

$$N_{A,r} = J_{A,r}^* = -c \mathcal{D}_{AB} \frac{dx_A}{dr} \quad (8.4-25)$$

For a cylindrical differential volume element of thickness  $\Delta r$ , as shown in Figure 8.29, Equation (8.4-1) is expressed in the form

$$(AN_{A,r})|_r - (AN_{A,r})|_{r+\Delta r} = 0 \quad (8.4-26)$$

Dividing Eq. (8.4-26) by  $\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(AN_{A_r})|_r - (AN_{A_r})|_{r+\Delta r}}{\Delta r} = 0 \quad (8.4-27)$$

or,

$$\frac{d(AN_{A_r})}{dr} = 0 \quad (8.4-28)$$

Since flux times area gives the molar transfer rate of species  $A$ ,  $\dot{n}_A$ , it is possible to conclude that

$$AN_{A_r} = \text{constant} = \dot{n}_A \quad (8.4-29)$$

Note that the area  $A$  in Eq. (8.4-29) is perpendicular to the direction of mass flux, and is given by

$$A = 2\pi rL \quad (8.4-30)$$

Substitution of Eqs. (8.4-25) and (8.4-30) into Eq. (8.4-29) and integration gives

$$\boxed{c \int_0^{x_A} \mathcal{D}_{AB}(x_A) dx_A = - \left( \frac{\dot{n}_A}{2\pi L} \right) \ln r + K} \quad (8.4-31)$$

where  $K$  is an integration constant.

If the surface concentrations are specified, i.e.,

$$\begin{aligned} \text{at } r = R_1 \quad x_A &= x_{A_1} \\ \text{at } r = R_2 \quad x_A &= x_{A_2} \end{aligned} \quad (8.4-32)$$

the molar transfer rate and the concentration distribution of species  $A$  are given in Table 8.9.

**Table 8.9** Rate of transfer and concentration distribution for one-dimensional diffusion in a hollow cylinder for the boundary conditions given by Eq. (8.4-32).

Constant	Molar Transfer Rate	Concentration Distribution
None	$\frac{2\pi Lc \int_{x_{A_1}}^{x_{A_2}} \mathcal{D}_{AB} dx_A}{\ln \left( \frac{R_1}{R_2} \right)}$ (A)	$\frac{\int_{x_A}^{x_{A_2}} \mathcal{D}_{AB} dx_A}{\int_{x_{A_1}}^{x_{A_2}} \mathcal{D}_{AB} dx_A} = \frac{\ln \left( \frac{r}{R_2} \right)}{\ln \left( \frac{R_1}{R_2} \right)}$ (C)
$\mathcal{D}_{AB}$	$\frac{2\pi Lc \mathcal{D}_{AB}(x_{A_2} - x_{A_1})}{\ln \left( \frac{R_1}{R_2} \right)}$ (B)	$\frac{x_{A_2} - x_A}{x_{A_2} - x_{A_1}} = \frac{\ln \left( \frac{r}{R_2} \right)}{\ln \left( \frac{R_1}{R_2} \right)}$ (D)

### 8.4.3 Diffusion in Spherical Coordinates

Consider one-dimensional diffusion of species  $A$  in the radial direction through a hollow sphere with inner and outer radii of  $R_1$  and  $R_2$ , respectively, as shown in Figure 8.30.

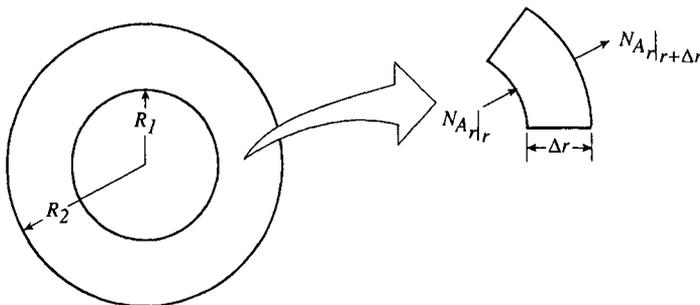


Figure 8.30 Diffusion through a hollow sphere.

Since  $x_A = x_A(r)$ , Table C.9 in Appendix C indicates that the only non-zero molar flux component is  $N_{A,r}$  and it is given by

$$N_{A,r} = -c \mathcal{D}_{AB} \frac{dx_A}{dr} \quad (8.4-33)$$

For a spherical differential volume element of thickness  $\Delta r$ , as shown in Figure 8.30, Eq. (8.4-1) is expressed in the form

$$(AN_{A,r})|_r - (AN_{A,r})|_{r+\Delta r} = 0 \quad (8.4-34)$$

Dividing Eq. (8.4-34) by  $\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(AN_{A,r})|_r - (AN_{A,r})|_{r+\Delta r}}{\Delta r} = 0 \quad (8.4-35)$$

or,

$$\frac{d(AN_{A,r})}{dr} = 0 \quad (8.4-36)$$

Since flux times area gives the molar transfer rate of species  $A$ ,  $\dot{n}_A$ , it is possible to conclude that

$$AN_{A,r} = \text{constant} = \dot{n}_A \quad (8.4-37)$$

Note that the area  $A$  in Eq. (8.4-37) is perpendicular to the direction of mass flux, and is given by

$$A = 4\pi r^2 \quad (8.4-38)$$

Substitution of Eqs. (8.4-33) and (8.4-38) into Eq. (8.4-37) and integration gives

$$c \int_0^{x_A} \mathcal{D}_{AB}(x_A) dx_A = \left( \frac{\dot{n}_A}{4\pi} \right) \frac{1}{r} + K \quad (8.4-39)$$

where  $K$  is an integration constant.

If the surface concentrations are specified, i.e.,

$$\begin{aligned} \text{at } r = R_1 \quad x_A &= x_{A_1} \\ \text{at } r = R_2 \quad x_A &= x_{A_2} \end{aligned} \tag{8.4-40}$$

the molar transfer rate and the concentration distribution of species  $A$  are given in Table 8.10.

**Table 8.10** Rate of transfer and concentration distribution for one-dimensional diffusion in a hollow sphere for the boundary conditions given by Eq. (8.4-40).

Constant	Molar Transfer Rate	Concentration Distribution
None	$\frac{4\pi c \int_{x_{A_2}}^{x_{A_1}} \mathcal{D}_{AB} dx_A}{\frac{1}{R_1} - \frac{1}{R_2}} \tag{A}$	$\frac{\int_{x_{A_2}}^{x_A} \mathcal{D}_{AB} dx_A}{\int_{x_{A_2}}^{x_{A_1}} \mathcal{D}_{AB} dx_A} = \frac{\frac{1}{r} - \frac{1}{R_2}}{\frac{1}{R_1} - \frac{1}{R_2}} \tag{C}$
$\mathcal{D}_{AB}$	$\frac{4\pi c \mathcal{D}_{AB}(x_{A_1} - x_{A_2})}{\frac{1}{R_1} - \frac{1}{R_2}} \tag{B}$	$\frac{x_A - x_{A_2}}{x_{A_1} - x_{A_2}} = \frac{\frac{1}{r} - \frac{1}{R_2}}{\frac{1}{R_1} - \frac{1}{R_2}} \tag{D}$

**Example 8.13** Consider the transfer of species  $A$  from a spherical drop or a bubble of radius  $R$  to a stationary fluid.

- a) Determine the molar rate of species  $A$  transferred to the fluid.
- b) Determine the concentration distribution of species  $A$  within the fluid.
- c) Determine the Sherwood number.

**Solution**

**Assumptions**

- 1. Steady-state conditions prevail.
- 2. The concentration at the surface of the sphere is constant at  $c_{A_w}$ .
- 3. The concentration of species  $A$  far from the sphere is  $c_{A_\infty}$ .

**Analysis**

a) The use of Eq. (B) in Table 8.10 with  $c_{A_1} = c_{A_w}$ ,  $c_{A_2} = c_{A_\infty}$ ,  $R_1 = R$  and  $R_2 = \infty$  gives the molar rate of transfer of species  $\mathcal{A}$  to the fluid as

$$\dot{n}_A = \frac{4\pi D_{AB}(c_{A_w} - c_{A_\infty})}{\frac{1}{R}} = 4\pi D_{AB}R(c_{A_w} - c_{A_\infty}) \quad (1)$$

b) The concentration distribution is obtained from Eq. (D) of Table 8.10 in the form

$$\frac{c_A - c_{A_\infty}}{c_{A_w} - c_{A_\infty}} = \frac{R}{r} \quad (2)$$

c) The molar transfer rate can also be calculated from Eq. (3.3-7) as

$$\dot{n}_A = 4\pi R^2 \langle k_c \rangle (c_{A_w} - c_{A_\infty}) \quad (3)$$

Equating Eqs. (1) and (3) leads to

$$\frac{\langle k_c \rangle}{D_{AB}} = \frac{1}{R} = \frac{2}{D} \quad (4)$$

Therefore, the Sherwood number is

$$\text{Sh} = \frac{\langle k_c \rangle D}{D_{AB}} = 2 \quad (5)$$

**8.4.4 Diffusion and Reaction in a Catalyst Pore**

At first, it may seem strange to a student to have an example on a reaction in a catalyst pore in a chapter which deals with “steady-state microscopic balances **without generation.**” In general, reactions can be classified as heterogeneous and homogeneous reactions. A *heterogeneous reaction* occurs on the surface and is usually a catalytic reaction. A *homogeneous reaction*, on the other hand, occurs throughout a given phase. In Chapter 5, the rate of generation of species  $i$  per unit volume as a result of a chemical reaction,  $\mathfrak{R}_i$ , was given by Eq. (5.3-26) in the form

$$\mathfrak{R}_i = \alpha_i r \quad (8.4-41)$$

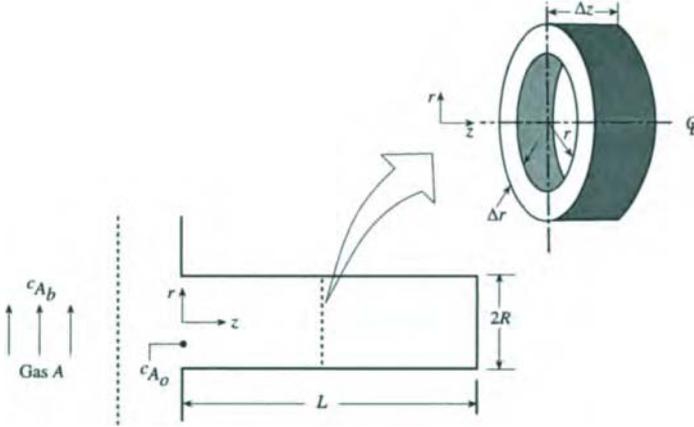
in which the term  $r$  represents a homogeneous reaction rate. Therefore, a homogeneous reaction rate appears in the inventory of chemical species, whereas a heterogeneous reaction rate appears in the boundary conditions.

Consider an idealized single cylindrical pore of radius  $R$  and length  $L$  in a catalyst particle as shown in Figure 8.31. The bulk gas stream has a species  $\mathcal{A}$  concentration of  $c_{A_b}$ . Species  $\mathcal{A}$  diffuses through the gas film and its concentration

at the pore mouth, i.e.,  $z = 0$ , is  $c_{A_0}$ . As the species  $A$  diffuses into the catalyst pore, it undergoes a first-order irreversible reaction



on the interior surface of the catalyst.



**Figure 8.31** Diffusion and reaction in a cylindrical pore.

The problem will be analyzed with the following assumptions:

1. Steady-state conditions prevail.
2. The system is isothermal.
3. The diffusion coefficient is constant.

For a cylindrical differential volume element of thickness  $\Delta r$  and length  $\Delta z$ , as shown in Figure 8.31, Eq. (8.4-1) is expressed as

$$(N_{A_r}|_r 2\pi r \Delta z + N_{A_z}|_z 2\pi r \Delta r) - [N_{A_r}|_{r+\Delta r} 2\pi(r + \Delta r) \Delta z + N_{A_z}|_{z+\Delta z} 2\pi r \Delta r] = 0 \quad (8.4-42)$$

Dividing Eq. (8.4-42) by  $2\pi \Delta r \Delta z$  and taking the limit as  $\Delta r \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\frac{1}{r} \lim_{\Delta r \rightarrow 0} \frac{(rN_{A_r})|_r - (rN_{A_r})|_{r+\Delta r}}{\Delta r} + \lim_{\Delta z \rightarrow 0} \frac{N_{A_z}|_z - N_{A_z}|_{z+\Delta z}}{\Delta z} = 0 \quad (8.4-43)$$

or,

$$\frac{1}{r} \frac{\partial}{\partial r} (rN_{A_r}) + \frac{\partial N_{A_z}}{\partial z} = 0 \quad (8.4-44)$$

Since the temperature is constant and there is no volume change due to reaction, the pressure and hence the total molar concentration,  $c$ , remains constant. Under these conditions, from Table C.8 in Appendix C, the components of the molar flux become<sup>7</sup>

$$N_{A_r} = -D_{AB} \frac{\partial c_A}{\partial r} \quad (8.4-45)$$

$$N_{A_z} = -D_{AB} \frac{\partial c_A}{\partial z} \quad (8.4-46)$$

Substitution of Eqs. (8.4-45) and (8.4-46) into Eq. (8.4-44) gives the governing equation for the concentration of species  $A$  as

$$\boxed{\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right) + \frac{\partial^2 c_A}{\partial z^2} = 0} \quad (8.4-47)$$

The boundary conditions associated with Eq. (8.4-47) are

$$\text{at } r = 0 \quad \frac{\partial c_A}{\partial r} = 0 \quad (8.4-48)$$

$$\text{at } r = R \quad -D_{AB} \frac{\partial c_A}{\partial r} = k^s c_A \quad (8.4-49)$$

$$\text{at } z = 0 \quad c_A = c_{A_0} \quad (8.4-50)$$

$$\text{at } z = L \quad \frac{\partial c_A}{\partial z} = 0 \quad (8.4-51)$$

The term  $k^s$  in Eq. (8.4-49) is the first-order surface reaction rate constant. In writing Eq. (8.4-51) it is implicitly assumed that no reaction takes place on the surface at  $z = L$ . Since there is no mass transfer through this surface,  $\partial c_A / \partial z = 0$ .

As we did in Section 8.2.4, this complicated problem will be solved by making use of the area averaging technique. The area-averaged concentration for species  $A$  is defined by

$$\langle c_A \rangle = \frac{\int_0^{2\pi} \int_0^R c_A r \, dr d\theta}{\int_0^{2\pi} \int_0^R r \, dr d\theta} = \frac{1}{\pi R^2} \int_0^{2\pi} \int_0^R c_A r \, dr d\theta \quad (8.4-52)$$

Although the local concentration,  $c_A$ , is dependent on  $r$  and  $z$ , the area-averaged concentration,  $\langle c_A \rangle$ , depends only on  $z$ .

Area averaging is performed by integrating Eq. (8.4-47) over the cross-sectional area of the pore. The result is

$$\int_0^{2\pi} \int_0^R \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right) r \, dr d\theta + \int_0^{2\pi} \int_0^R \frac{\partial^2 c_A}{\partial z^2} r \, dr d\theta = 0 \quad (8.4-53)$$

<sup>7</sup>From the stoichiometry of the reaction, the molar average velocity is zero.

Since the limits of the integration are constant, the order of differentiation and integration in the second term of Eq. (8.4-53) can be interchanged to get

$$\int_0^{2\pi} \int_0^R \frac{\partial^2 c_A}{\partial z^2} r \, dr d\theta = \frac{d^2}{dz^2} \left( \int_0^{2\pi} \int_0^R c_A r \, dr d\theta \right) = \pi R^2 \frac{d^2 \langle c_A \rangle}{dz^2} \quad (8.4-54)$$

Substitution of Eq. (8.4-54) into Eq. (8.4-53) yields

$$2\pi R \left. \frac{\partial c_A}{\partial r} \right|_{r=R} + \pi R^2 \frac{d^2 \langle c_A \rangle}{dz^2} = 0 \quad (8.4-55)$$

The use of the boundary condition given by Eq. (8.4-49) leads to

$$\mathcal{D}_{AB} \frac{d^2 \langle c_A \rangle}{dz^2} = \frac{2}{R} k^s c_A|_{r=R} \quad (8.4-56)$$

Note that Eq. (8.4-56) contains two dependent variables,  $\langle c_A \rangle$  and  $c_A|_{r=R}$ , which are at two different scales. It is generally assumed, although not expressed explicitly, that

$$c_A|_{r=R} \simeq \langle c_A \rangle \quad (8.4-57)$$

This approximation is valid for  $\text{Bi}_M \ll 1$ . Substitution of Eq. (8.4-57) into Eq. (8.4-56) gives

$$\boxed{\mathcal{D}_{AB} \frac{d^2 \langle c_A \rangle}{dz^2} = \frac{2}{R} k^s \langle c_A \rangle} \quad (8.4-58)$$

Integration of Eqs. (8.4-50) and (8.4-51) over the cross-sectional area of the pore gives the boundary conditions associated with Eq. (8.4-58) as

$$\text{at } z = 0 \quad \langle c_A \rangle = c_{A_0} \quad (8.4-59)$$

$$\text{at } z = L \quad \frac{d \langle c_A \rangle}{dz} = 0 \quad (8.4-60)$$

Equations (8.4-47) and (8.4-58) are at two different scales. Equation (8.4-58) is obtained by averaging Eq. (8.4-47) over the cross-sectional area perpendicular to the direction of mass flux. As a result, the boundary condition, i.e., the heterogeneous reaction rate expression, appears in the conservation statement.

Note that the term  $2/R$  in Eq. (8.4-58) is the catalyst surface area per unit volume, i.e.,

$$\frac{2}{R} = \frac{2\pi RL}{\pi R^2 L} = a_v = \frac{\text{Catalyst surface area}}{\text{Pore volume}} \quad (8.4-61)$$

Since heterogeneous reaction rate expression has the units of moles/(area)(time), multiplication of this term by  $a_v$  converts the units to moles/(volume)(time).

The physical significance and the order of magnitude of the terms in Eq. (8.4-58) are given in Table 8.11.

**Table 8.11** The physical significance and the order of magnitude of the terms in Eq. (8.4-58).

Term	Physical Significance	Order of Magnitude
$\mathcal{D}_{AB} \frac{d^2 \langle c_A \rangle}{dz^2}$	Rate of diffusion	$\mathcal{D}_{AB} \frac{c_{A_0}}{L^2}$
$\frac{2 k^s \langle c_A \rangle}{R}$	Rate of reaction	$\frac{2 k^s c_{A_0}}{R}$

Therefore, the ratio of the rate of reaction to the rate of diffusion is given by

$$\frac{\text{Rate of reaction}}{\text{Rate of diffusion}} = \frac{2 k^s c_{A_0} / R}{\mathcal{D}_{AB} c_{A_0} / L^2} = \frac{2 k^s L^2}{R \mathcal{D}_{AB}} \quad (8.4-62)$$

In the literature, this ratio is often referred to as the *Thiele modulus* or the *Damköhler number*<sup>8</sup> and expressed as

$$\Lambda = \sqrt{\frac{2 k^s L^2}{R \mathcal{D}_{AB}}} \quad (8.4-63)$$

Before solving Eq. (8.4-58), it is convenient to express the governing equation and the boundary conditions in dimensionless form. Introduction of the dimensionless quantities

$$\theta = \frac{\langle c_A \rangle}{c_{A_0}} \quad (8.4-64)$$

$$\xi = \frac{z}{L} \quad (8.4-65)$$

reduces Eqs. (8.4-58)-(8.4-60) to

$$\frac{d^2 \theta}{d\xi^2} = \Lambda^2 \theta \quad (8.4-66)$$

$$\text{at } \xi = 0 \quad \theta = 1 \quad (8.4-67)$$

$$\text{at } \xi = 1 \quad \frac{d\theta}{d\xi} = 0 \quad (8.4-68)$$

Note that these equations are exactly equal to the equations developed for the fin problem in Section 8.2.4. Therefore, the solution is given by Eq. (8.2-91), i.e.,

$$\theta = \frac{\cosh[\Lambda(1 - \xi)]}{\cosh \Lambda} \quad (8.4-69)$$

<sup>8</sup> While the Thiele modulus is preferred in the analysis of mass transport in a porous medium, the Damköhler number is used for packed bed analysis.

### 8.4.4.1 Macroscopic equation

Integration of the microscopic level equations over the volume of the system gives the equations at the macroscopic level. Integration of Eq. (8.4-58) over the volume of the system gives

$$\int_0^L \int_0^{2\pi} \int_0^R \mathcal{D}_{AB} \frac{d^2 \langle c_A \rangle}{dz^2} r \, dr d\theta dz = \int_0^L \int_0^{2\pi} \int_0^R \frac{2}{R} k^s \langle c_A \rangle r \, dr d\theta dz \quad (8.4-70)$$

Carrying out the integrations yields

$$\underbrace{\pi R^2 \left( -\mathcal{D}_{AB} \frac{d \langle c_A \rangle}{dz} \Big|_{z=0} \right)}_{\text{Rate of moles of species } \mathcal{A} \text{ entering into the pore through the surface at } z=0} = \underbrace{2\pi R k^s \int_0^L \langle c_A \rangle dz}_{\text{Rate of conversion of species } \mathcal{A} \text{ to species } \mathcal{B} \text{ at the catalyst surface}} \quad (8.4-71)$$

Note that Eq. (8.4-71) is simply the macroscopic inventory rate equation for the conservation of species  $\mathcal{A}$  by considering the catalyst pore as a system. The use of Eq. (8.4-69) in Eq. (8.4-71) gives the molar rate of conversion of species  $\mathcal{A}$ ,  $\dot{n}_A$ , as

$$\boxed{\dot{n}_A = \frac{\pi R^2 \mathcal{D}_{AB} c_{A_0} \Lambda \tanh \Lambda}{L}} \quad (8.4-72)$$

### 8.4.4.2 Effectiveness factor

The effectiveness factor,  $\eta$ , is defined as the ratio of the apparent rate of conversion to the rate if the entire internal surface were exposed to the concentration  $c_{A_0}$ , i.e.,

$$\eta = \frac{2\pi R k^s \int_0^L \langle c_A \rangle dz}{2\pi R k^s c_{A_0} L} = \frac{\int_0^L \langle c_A \rangle dz}{c_{A_0} L} \quad (8.4-73)$$

In terms of the dimensionless quantities, Eq. (8.4-73) becomes

$$\eta = \int_0^1 \theta \, d\xi \quad (8.4-74)$$

Substitution of Eq. (8.4-69) into Eq. (8.4-74) gives the effectiveness factor as

$$\boxed{\eta = \frac{\tanh \Lambda}{\Lambda}} \quad (8.4-75)$$

Note that the effectiveness factor for a first-order irreversible reaction is exactly identical with the fin efficiency. Therefore, Figure 8.24, which shows the variation of  $\eta$  as a function of  $\Lambda$ , is also valid for this case.

When  $\Lambda \rightarrow 0$ , this means that the rate of diffusion is much larger than the rate of reaction. The Taylor series expansion of  $\eta$  in terms of  $\Lambda$  gives

$$\eta = 1 - \frac{1}{3}\Lambda^2 + \frac{2}{15}\Lambda^4 - \frac{17}{315}\Lambda^6 + \dots \quad (8.4-76)$$

Therefore,  $\eta$  approaches unity as  $\Lambda \rightarrow 0$ , indicating that the entire surface is exposed to a reactant. On the other hand, large values of  $\Lambda$  corresponds to cases in which diffusion rate is very slow and the surface reaction is very rapid. Under these conditions the effectiveness factor becomes

$$\eta = \frac{1}{\Lambda} \quad (8.4-77)$$

As  $\Lambda \rightarrow \infty$ ,  $\eta$  approaches zero. This implies that a good part of the catalyst surface is starved for a reactant and hence not effective.

## 8.5 MASS TRANSPORT WITH CONVECTION

In the case of mass transfer, each species involved in the transfer has its own individual velocity. For a single phase system composed of the binary species  $\mathcal{A}$  and  $\mathcal{B}$ , the characteristic velocity for the mixture can be defined by several ways as stated in Section 2.3. If the mass transfer takes place in the  $z$ -direction, the three characteristic velocities are given in Table 8.12.

**Table 8.12** Characteristic velocities in the  $z$ -direction for a binary system.

Velocity	Definition
Mass average	$v_z = \frac{\rho_A v_{A_z} + \rho_B v_{B_z}}{\rho_A + \rho_B} = \frac{\mathcal{W}_{A_z} + \mathcal{W}_{B_z}}{\rho}$ (A)
Molar average	$v_z^* = \frac{c_A v_{A_z} + c_B v_{B_z}}{c_A + c_B} = \frac{N_{A_z} + N_{B_z}}{c}$ (B)
Volume average	$v_z^\square = c_A \bar{V}_A v_{A_z} + c_B \bar{V}_B v_{B_z} = \bar{V}_A N_{A_z} + \bar{V}_B N_{B_z}$ (C)

Hence, the total mass or molar flux of species  $\mathcal{A}$  can be expressed as

$$\mathcal{W}_{A_z} = \underbrace{-\rho \mathcal{D}_{AB} \frac{d\omega_A}{dz}}_{\text{Molecular flux}} + \underbrace{\rho_A v_z}_{\text{Convective flux}} \quad (8.5-1)$$

$$N_{A_z} = \underbrace{-c \mathcal{D}_{AB} \frac{dx_A}{dz}}_{\text{Molecular flux}} + \underbrace{c_A v_z^*}_{\text{Convective flux}} \quad (8.5-2)$$

$$N_{A_z} = \underbrace{-D_{AB} \frac{dc_A}{dz}}_{\text{Molecular flux}} + \underbrace{c_A v_z}_{\text{Convective flux}} \quad (8.5-3)$$

The tricky part of the mass transfer problems is that there is no need to have a bulk motion of the mixture as a result of external means, such as pressure drop, to have a non-zero convective flux term in Eqs. (8.5-1)-(8.5-3). Even in the case of the diffusion of species  $\mathcal{A}$  through a stagnant film of  $\mathcal{B}$ , non-zero convective term arises as can be seen from the following examples.

It should also be noted that if one of the characteristic velocities is zero, this does not necessarily imply that the other characteristic velocities are also zero. For example, in Section 8.4, it was shown that the molar average velocity is zero for an equimolar counterdiffusion since  $N_{A_z} = -N_{B_z}$ . The mass average velocity for this case is given by

$$v_z = \frac{W_{A_z} + W_{B_z}}{\rho} \quad (8.5-4)$$

The mass and molar fluxes are related by

$$N_{i_z} = \frac{W_{i_z}}{\mathcal{M}_i} \quad (8.5-5)$$

where  $\mathcal{M}_i$  is the molecular weight of species  $i$ . The use of Eq. (8.5-5) in Eq. (8.5-4) gives

$$v_z = \frac{\mathcal{M}_A N_{A_z} + \mathcal{M}_B N_{B_z}}{\rho} = \frac{N_{A_z}(\mathcal{M}_A - \mathcal{M}_B)}{\rho} \quad (8.5-6)$$

which is non-zero unless  $\mathcal{M}_A = \mathcal{M}_B$ .

## 8.5.1 Diffusion Through a Stagnant Gas

### 8.5.1.1 Evaporation from a tapered tank

Consider a pure liquid  $\mathcal{A}$  in an open cylindrical tank with a slightly tapered top as shown in Figure 8.32. The apparatus is arranged in such a manner that the liquid-gas interface remains fixed in space as the evaporation takes place. As an engineer, we are interested in the rate of evaporation of  $\mathcal{A}$  from the liquid surface into a mixture of  $\mathcal{A}$  and  $\mathcal{B}$ . For this purpose, it is necessary to determine the concentration distribution of  $\mathcal{A}$  in the gas phase. The problem will be analyzed with the following assumptions:

1. Steady-state conditions prevail.
2. Species  $\mathcal{A}$  and  $\mathcal{B}$  form an ideal gas mixture.
3. Species  $\mathcal{B}$  has a negligible solubility in liquid  $\mathcal{A}$ .

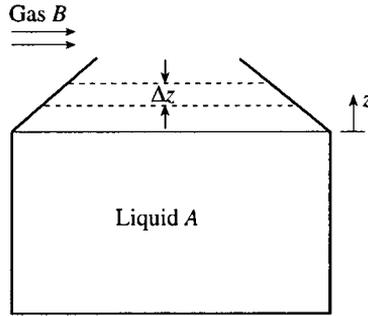


Figure 8.32 Evaporation from a tapered tank.

4. The entire system is maintained at a constant temperature and pressure, i.e., the total molar concentration in the gas phase,  $c = P/RT$ , is constant.
5. There is no chemical reaction between species  $\mathcal{A}$  and  $\mathcal{B}$ .

If the taper angle is small, mass transport can be considered one-dimensional in the  $z$ -direction and the conservation statement for species  $\mathcal{A}$ , Eq. (8.4-1), can be written over a differential volume element of thickness  $\Delta z$  as

$$(AN_{A_z})|_z - (AN_{A_z})|_{z+\Delta z} = 0 \quad (8.5-7)$$

Dividing Eq. (8.5-7) by  $\Delta z$  and letting  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{(AN_{A_z})|_z - (AN_{A_z})|_{z+\Delta z}}{\Delta z} = 0 \quad (8.5-8)$$

or,

$$\frac{d(AN_{A_z})}{dz} = 0 \quad (8.5-9)$$

Equation (8.5-9) indicates that

$$AN_{A_z} = \dot{n}_A = \text{constant} \quad (8.5-10)$$

In a similar way, the rate equation for the conservation of species  $\mathcal{B}$  leads to

$$AN_{B_z} = \text{constant} \quad (8.5-11)$$

Since species  $\mathcal{B}$  is insoluble in liquid  $\mathcal{A}$ , i.e.,  $N_{B_z}|_{z=0} = 0$ , this implies that

$$N_{B_z} = 0 \quad \text{for} \quad 0 \leq z \leq L \quad (8.5-12)$$

From Table 8.12, the total molar flux of species  $\mathcal{A}$  is given by

$$N_{A_z} = -cD_{AB} \frac{dx_A}{dz} + c_A v_z^* \quad (8.5-13)$$

in which the molar average velocity is given by

$$v_z^* = \frac{N_{Az} + N_{Bz}}{c} = \frac{N_{Az}}{c} \quad (8.5-14)$$

which indicates non-zero convective flux. The use of Eq. (8.5-14) in Eq. (8.5-13) results in

$$N_{Az} = -\frac{cD_{AB}}{1-x_A} \frac{dx_A}{dz} \quad (8.5-15)$$

Substitution of (8.5-15) into Eq. (8.5-10) and rearrangement gives

$$\dot{n}_A \int_0^L \frac{dz}{A(z)} = -cD_{AB} \int_{x_{A_0}}^{x_{A_L}} \frac{dx_A}{1-x_A} \quad (8.5-16)$$

or,

$$\dot{n}_A = \frac{cD_{AB}}{\int_0^L \frac{dz}{A(z)}} \ln \left( \frac{1-x_{A_L}}{1-x_{A_0}} \right) \quad (8.5-17)$$

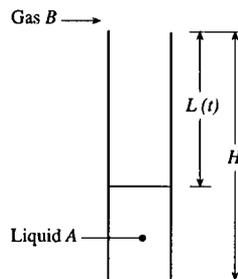
Since  $\dot{n}_A$  is constant, Eq. (8.5-17) holds for  $0 \leq z \leq L$ .

Note that  $x_{A_0}$ , i.e., the value of  $x_A$  at  $z = 0$ , is the mole fraction of species  $A$  in the gas mixture that is in equilibrium with the pure liquid  $A$  at the existing temperature and pressure. The use of Dalton's and Raoult's laws at the gas-liquid interface indicates that

$$x_{A_0} = \frac{P_A^{sat}}{P} \quad (8.5-18)$$

where  $P$  is the total pressure.

**Example 8.14** *One way of measuring the diffusion coefficients of vapors is to place a small amount of liquid in a vertical capillary, generally known as the Stefan diffusion tube, and to blow a gas stream of known composition across the top as shown in Figure 8.33. Show how one can estimate the diffusion coefficient by observing the decrease in the liquid-gas interface as a function of time.*



**Figure 8.33** The Stefan diffusion tube.

**Solution****Assumptions**

1. *Pseudo-steady-state behavior.*
2. *The system is isothermal.*
3. *The total pressure remains constant.*
4. *The mole fraction of species A at the top of the tube is zero.*
5. *No turbulence is observed at the top of the tube.*

**Analysis**

*System: Liquid in the tube*

*The inventory rate equation for mass of A gives*

$$- \text{Rate of moles of A out} = \text{Rate of accumulation of moles of A} \quad (1)$$

or,

$$-\dot{n}_A = \frac{d}{dt} \left[ (H - L)A \frac{\rho_A^L}{\mathcal{M}_A} \right] \quad (2)$$

where  $\rho_A^L$  is the density of species A in the liquid phase and A is the cross-sectional area of the tube.

The rate of evaporation from the liquid surface,  $\dot{n}_A$ , can be determined from Eq. (8.5-17). For  $A = \text{constant}$  and  $x_{A_L} = 0$ , Eq. (8.5-17) reduces to

$$\dot{n}_A = - \frac{AcD_{AB}}{L} \ln(1 - x_{A_o}) \quad (3)$$

It should be kept in mind that Eq. (8.5-17) was developed for a steady-state case. For the unsteady problem at hand, the pseudo-steady-state assumption implies that Eq. (3) holds at any given instant, i.e.,

$$\dot{n}_A(t) = - \frac{AcD_{AB}}{L(t)} \ln(1 - x_{A_o}) \quad (4)$$

Substitution of Eq. (4) into Eq. (2) gives

$$-cD_{AB} \ln(1 - x_{A_o}) \int_0^t dt = \frac{\rho_A^L}{\mathcal{M}_A} \int_{L_o}^L L dL \quad (5)$$

or,

$$L^2 = - \left[ \frac{2\mathcal{M}_A c D_{AB} \ln(1 - x_{A_o})}{\rho_A^L} \right] t + L_o^2 \quad (6)$$

Therefore, the diffusion coefficient is determined from the slope of the  $L^2$  versus  $t$  plot. Alternatively, rearrangement of Eq. (6) yields

$$\frac{t}{L - L_o} = - \left[ \frac{\rho_A^L}{2 \mathcal{M}_{AC} \mathcal{D}_{AB} \ln(1 - x_{A_o})} \right] (L - L_o) + \frac{\rho_A^L L_o}{\mathcal{M}_{AC} \mathcal{D}_{AB} \ln(1 - x_{A_o})} \quad (7)$$

In this case, the diffusion coefficient is determined from the slope of the  $t/(L - L_o)$  versus  $(L - L_o)$  plot. What is the advantage of using Eq. (7) over Eq. (6)?

**Example 8.15** To decrease the evaporation loss from open storage tanks, it is recommended to use a tapered top as shown in Figure 8.34. Calculate the rate of ethanol loss from the storage tank under steady conditions at 25 °C.

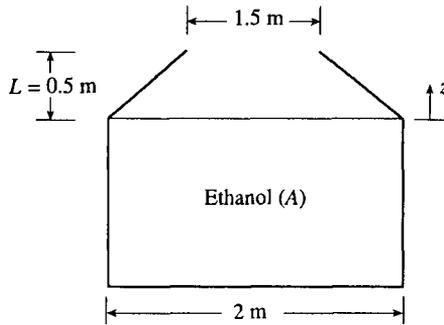


Figure 8.34 Evaporation from a tapered tank.

### Solution

#### Physical properties

Diffusion coefficient of ethanol (A) in air (B) at 25 °C (298 K) :

$$\begin{aligned} (\mathcal{D}_{AB})_{298} &= (\mathcal{D}_{AB})_{313} \left( \frac{298}{313} \right)^{3/2} \\ &= (1.45 \times 10^{-5}) \left( \frac{298}{313} \right)^{3/2} = 1.35 \times 10^{-5} \text{ m}^2/\text{s} \end{aligned}$$

$$P_A^{sat} = 58.6 \text{ mmHg}$$

#### Analysis

In order to determine the molar flow rate of species A from Eq. (8.5-17), it is first necessary to express the variation of the cross-sectional area in the direction of  $z$ . The variation of the diameter as a function of  $z$  is

$$D(z) = D_o - \left( \frac{D_o - D_L}{L} \right) z \quad (1)$$

where  $D_o$  and  $D_L$  are the tank diameters at  $z=0$  and  $z=L$ , respectively. Therefore, the variation of the cross-sectional area is

$$\begin{aligned} A(z) &= \frac{\pi D^2(z)}{4} \\ &= \frac{\pi}{4} \left[ D_o - \left( \frac{D_o - D_L}{L} \right) z \right]^2 \end{aligned} \quad (2)$$

Substitution of Eq. (2) into Eq. (8.5-17) and integration gives the molar rate of evaporation as

$$\dot{n}_A = - \frac{\pi c \mathcal{D}_{AB} (D_o - D_L) \ln(1 - x_{A_o})}{4L \left( \frac{1}{D_L} - \frac{1}{D_o} \right)} \quad (3)$$

The numerical values are

$$D_o = 2 \text{ m}$$

$$D_L = 1.5 \text{ m}$$

$$L = 0.5 \text{ m}$$

$$x_{A_o} = \frac{P_A^{sat}}{P} = \frac{58.6}{760} = 0.077$$

$$c = \frac{P}{\mathcal{R}T} = \frac{1}{(0.08205)(25 + 273)} = 41 \times 10^{-3} \text{ kmol/m}^3 = 41 \text{ mol/m}^3$$

Substitution of these values into Eq. (3) gives

$$\dot{n}_A = - \frac{\pi(41)(1.35 \times 10^{-5})(2 - 1.5) \ln(1 - 0.077)}{(4)(0.5) \left( \frac{1}{1.5} - \frac{1}{2} \right)} \simeq 2.1 \times 10^{-4} \text{ mol/s}$$

**Comment:** When  $D_L \rightarrow D_o$ , application of L'Hopital's rule gives

$$\lim_{D_L \rightarrow D_o} \frac{D_o - D_L}{\frac{1}{D_L} - \frac{1}{D_o}} = \lim_{D_L \rightarrow D_o} \frac{-1}{-\frac{1}{D_L^2}} = D_o^2$$

and Eq. (3) reduces to

$$\dot{n}_A = - \frac{(\pi D_o^2/4)c \mathcal{D}_{AB}}{L} \ln(1 - x_{A_o})$$

which is Eq. (4) of Example 8.14.

## 8.5.1.2 Evaporation of a spherical drop

A liquid ( $\mathcal{A}$ ) droplet of radius  $R$  is suspended in a stagnant gas  $\mathcal{B}$  as shown in Figure 8.35. We want to determine the rate of evaporation under steady conditions.

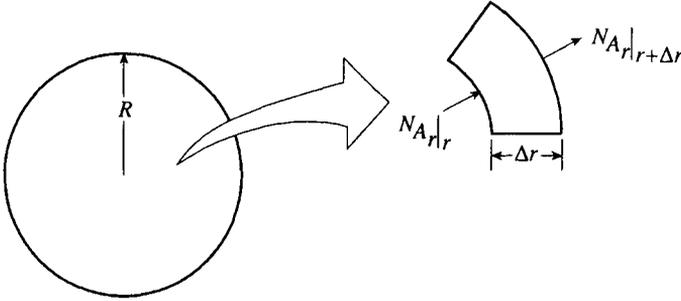


Figure 8.35 Mass transfer from a spherical drop.

Over a differential volume element of thickness  $\Delta r$ , as shown in Figure 8.35, the conservation statement for species  $\mathcal{A}$ , Eq. (8.4-1), is written as

$$(AN_{A_r})|_r - (AN_{A_r})|_{r+\Delta r} = 0 \quad (8.5-19)$$

Dividing Eq. (8.5-19) by  $\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(AN_{A_r})|_r - (AN_{A_r})|_{r+\Delta r}}{\Delta r} = 0 \quad (8.5-20)$$

or,

$$\frac{d(AN_{A_r})}{dr} = 0 \quad (8.5-21)$$

Since flux times area gives the molar transfer rate of species  $\mathcal{A}$ ,  $\dot{n}_A$ , it is possible to conclude that

$$AN_{A_r} = \text{constant} = \dot{n}_A \quad (8.5-22)$$

Note that the area  $A$  in Eq. (8.5-22) is perpendicular to the direction of mass flux and is given by

$$A = 4\pi r^2 \quad (8.5-23)$$

Since the temperature and the total pressure remain constant, the total molar concentration,  $c$ , in the gas phase is constant. From Table C.9 in Appendix C, the total molar flux of species  $\mathcal{A}$  in the  $r$ -direction is given by

$$N_{A_r} = -\mathcal{D}_{AB} \frac{dc_A}{dr} + c_A v_r^* \quad (8.5-24)$$

Since species  $\mathcal{B}$  is stagnant, the molar average velocity is expressed as

$$v_r^* = \frac{N_{A_r} + N_{B_r}}{c} = \frac{N_{A_r}}{c} \quad (8.5-25)$$

which indicates non-zero convective flux. Using Eq. (8.5-25) in Eq. (8.5-24) results in

$$N_{A,r} = -\frac{c\mathcal{D}_{AB}}{c-c_A} \frac{dc_A}{dr} \quad (8.5-26)$$

Substitution of Eq. (8.5-26) into Eq. (8.5-22) and rearrangement gives

$$-4\pi c\mathcal{D}_{AB} \int_{c_A^*}^0 \frac{dc_A}{c-c_A} = \dot{n}_A \int_R^\infty \frac{dr}{r^2} \quad (8.5-27)$$

where  $c_A^*$  is the saturation concentration of species  $A$  in  $B$  at  $r = R$  in the gas phase. Carrying out the integrations in Eq. (8.5-27) yields

$$\boxed{\dot{n}_A = 4\pi c\mathcal{D}_{AB}R \ln\left(\frac{c}{c-c_A^*}\right)} \quad (8.5-28)$$

**Example 8.16** *A benzene droplet with a diameter of 8 mm is suspended by a wire in a laboratory. The temperature and pressure are maintained constant at 25 °C and 1 atm, respectively. Estimate the diffusion coefficient of benzene in air if the variation of the droplet diameter as a function of time is recorded as follows:*

$t$ (min)	$D$ (mm)
5	7.3
10	6.5
15	5.5
20	4.4
25	2.9

### Solution

#### Physical properties

$$\text{For benzene (A)} : \begin{cases} \rho_A = 879 \text{ kg/m}^3 \\ \mathcal{M}_A = 78 \\ P_A^{\text{sat}} = 94.5 \text{ mmHg} \end{cases}$$

#### Assumptions

1. *Pseudo-steady-state behavior.*
2. *Air is insoluble in the droplet.*

**Analysis**

*System: Benzene droplet*

*The inventory rate equation for mass of A gives*

$$- \text{Rate of moles of A out} = \text{Rate of accumulation of moles of A} \quad (1)$$

or,

$$\begin{aligned} -\dot{n}_A &= \frac{d}{dt} \left[ \frac{4}{3} \pi R^3 \left( \frac{\rho_A^L}{\mathcal{M}_A} \right) \right] \\ &= \frac{4 \pi \rho_A^L}{\mathcal{M}_A} R^2 \frac{dR}{dt} \end{aligned} \quad (2)$$

where  $\rho_A^L$  is the density of species A in the liquid phase.

The rate of evaporation from the droplet surface,  $\dot{n}_A$ , can be determined from Eq. (8.5-28). However, remember that Eq. (8.5-28) was developed for a steady-state case. For the unsteady problem at hand, the pseudo-steady-state assumption implies that Eq. (8.5-28) holds at any given instant, i.e.,

$$\dot{n}_A(t) = 4 \pi c \mathcal{D}_{AB} R(t) \ln \left( \frac{c}{c - c_A^*} \right) \quad (3)$$

Substitution of Eq. (3) into Eq. (2) and rearrangement gives

$$- \frac{\rho_A^L}{\mathcal{M}_A} \int_{R_o}^R R dR = c \mathcal{D}_{AB} \ln \left( \frac{c}{c - c_A^*} \right) \int_0^t dt \quad (4)$$

where  $R_o$  is the initial radius of the liquid droplet. Carrying out the integrations in Eq. (4) yields

$$R^2 = R_o^2 - \left[ \frac{2c \mathcal{D}_{AB} \mathcal{M}_A}{\rho_A^L} \ln \left( \frac{c}{c - c_A^*} \right) \right] t \quad (5)$$

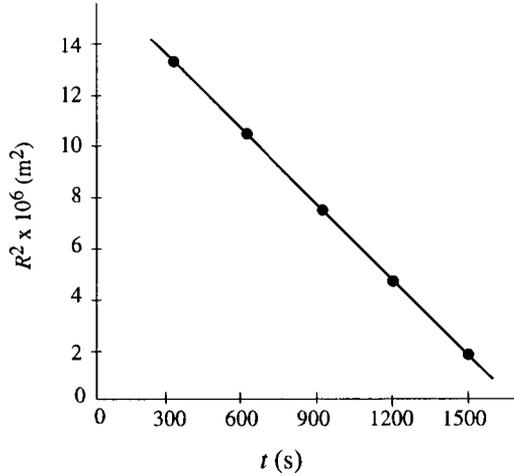
Since

$$c = \frac{P}{\mathcal{R}T} \quad \text{and} \quad c_A^* = \frac{P_A^{sat}}{\mathcal{R}T} \quad (6)$$

Eq. (5) takes the form

$$R^2 = R_o^2 - \left[ \frac{2c \mathcal{D}_{AB} \mathcal{M}_A}{\rho_A^L} \ln \left( \frac{P}{P - P_A^{sat}} \right) \right] t \quad (7)$$

The plot of  $R^2$  versus  $t$  is shown below.



The slope of the straight line is  $-9.387 \times 10^{-9} \text{ m}^2/\text{s}$ . Hence,

$$\frac{2cD_{AB}M_A}{\rho_A L} \ln\left(\frac{P}{P - P_A^{sat}}\right) = 9.387 \times 10^{-9} \quad (8)$$

The total molar concentration is

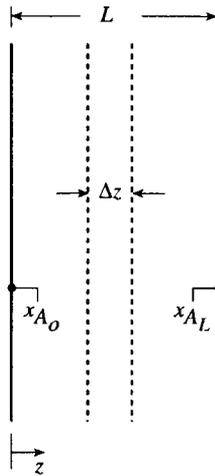
$$c = \frac{P}{RT} = \frac{1}{(0.08205)(25 + 273)} = 0.041 \text{ kmol/m}^3 \quad (9)$$

Substitution of the values into Eq. (8) gives the diffusion coefficient as

$$\begin{aligned} D_{AB} &= 9.387 \times 10^{-9} \left[ \frac{879}{2(0.041)(78) \ln\left(\frac{760}{760 - 94.5}\right)} \right] \\ &= 9.72 \times 10^{-6} \text{ m}^2/\text{s} \end{aligned}$$

### 8.5.2 Diffusion Through a Stagnant Liquid

Consider a one-dimensional diffusion of liquid  $\mathcal{A}$  through a stagnant film of liquid  $\mathcal{B}$  with a thickness  $L$  as shown in Figure 8.36. The mole fractions of  $\mathcal{A}$  at  $z = 0$  and  $z = L$  are known. As an engineer, we are interested in the number of moles of species  $\mathcal{A}$  transferring through the film of  $\mathcal{B}$  under steady conditions.



**Figure 8.36** Diffusion of liquid  $\mathcal{A}$  through a stagnant liquid film  $\mathcal{B}$ .

Over a differential volume of thickness  $\Delta z$ , the conservation statement for species  $\mathcal{A}$ , Eq. (8.4-1), is written as

$$N_{A_z}|_z A - N_{A_z}|_{z+\Delta z} A = 0 \quad (8.5-29)$$

Dividing Eq. (8.5-29) by  $A \Delta z$  and letting  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{N_{A_z}|_z - N_{A_z}|_{z+\Delta z}}{\Delta z} = 0 \quad (8.5-30)$$

or,

$$\frac{dN_{A_z}}{dz} = 0 \quad \Rightarrow \quad N_{A_z} = \text{constant} \quad (8.5-31)$$

To proceed further, it is necessary to express the total molar flux of species  $\mathcal{A}$ , i.e.,  $N_{A_z}$ , either by Eq. (8.5-2) or by Eq. (8.5-3).

### 8.5.2.1 Analysis based on the molar average velocity

From Eq. (8.5-2), the total molar flux of species  $\mathcal{A}$  is given as

$$N_{A_z} = -c D_{AB} \frac{dx_A}{dz} + c_A v_z^* \quad (8.5-32)$$

It is important to note in this problem that the total molar concentration,  $c$ , is not constant but dependent on the mole fractions of species  $\mathcal{A}$  and  $\mathcal{B}$ . Since species  $\mathcal{B}$  is stagnant, the expression for the molar average velocity becomes

$$v_z^* = \frac{N_{A_z} + N_{B_z}}{c} = \frac{N_{A_z}}{c} \quad (8.5-33)$$

Substitution of Eq. (8.5-33) into Eq. (8.5-32) gives the molar flux of species  $A$  as

$$N_{A_z} = -\frac{c\mathcal{D}_{AB}}{1-x_A} \frac{dx_A}{dz} \quad (8.5-34)$$

Since the total molar concentration,  $c$ , is not constant, it is necessary to express  $c$  in terms of mole fractions. Assuming ideal solution behavior, i.e., the partial molar volume is equal to the molar volume of the pure substance, the total molar concentration is expressed in the form

$$c = \frac{1}{\tilde{V}_{mix}} = \frac{1}{x_A\tilde{V}_A + x_B\tilde{V}_B} \quad (8.5-35)$$

Substitution of  $x_B = 1 - x_A$  yields

$$c = \frac{1}{\tilde{V}_B + (\tilde{V}_A - \tilde{V}_B)x_A} \quad (8.5-36)$$

Combining Eqs. (8.5-34) and (8.5-36) and rearrangement gives

$$N_{A_z} \int_0^L dz = -\mathcal{D}_{AB} \int_{x_{A_o}}^{x_{A_L}} \frac{dx_A}{[\tilde{V}_B + (\tilde{V}_A - \tilde{V}_B)x_A](1-x_A)} \quad (8.5-37)$$

Integration of Eq. (8.5-37) results in

$$\begin{aligned} N_{A_z} &= \frac{\mathcal{D}_{AB}}{L\tilde{V}_A} \left\{ \ln \left( \frac{1-x_{A_L}}{1-x_{A_o}} \right) - \ln \left[ \frac{\tilde{V}_B + (\tilde{V}_A - \tilde{V}_B)x_{A_L}}{\tilde{V}_B + (\tilde{V}_A - \tilde{V}_B)x_{A_o}} \right] \right\} \\ &= \frac{\mathcal{D}_{AB}}{L\tilde{V}_A} \ln \left( \frac{c_{B_L}}{c_{B_o}} \right) \end{aligned} \quad (8.5-38)$$

### 8.5.2.2 Analysis based on the volume average velocity

The use of Eq. (8.5-3) gives the total molar flux of species  $A$  as

$$N_{A_z} = -c\mathcal{D}_{AB} \frac{dx_A}{dz} + c_A v_z^\blacksquare \quad (8.5-39)$$

From Eq. (C) in Table 8.12, the volume average velocity is expressed as

$$\begin{aligned} v_z^\blacksquare &= \bar{V}_A N_{A_z} + \bar{V}_B N_{B_z} \\ &= \bar{V}_A N_{A_z} = \tilde{V}_A N_{A_z} \end{aligned} \quad (8.5-40)$$

Using Eq. (8.5-40) in Eq. (8.5-39) yields

$$N_{A_z} = -\frac{\mathcal{D}_{AB}}{1-\tilde{V}_A c_A} \frac{dc_A}{dz} \quad (8.5-41)$$

Rearrangement of Eq. (8.5-41) results in

$$N_{A_z} \int_0^L dz = -D_{AB} \int_{c_{A_0}}^{c_{A_L}} \frac{dc_A}{1 - \tilde{V}_A c_A} \quad (8.5-42)$$

Integration of Eq. (8.5-42) leads to

$$N_{A_z} = \frac{D_{AB}}{L \tilde{V}_A} \ln \left( \frac{1 - \tilde{V}_A c_{A_L}}{1 - \tilde{V}_A c_{A_0}} \right) \quad (8.5-43)$$

The use of the identity from Eq. (8.5-35), i.e.,

$$1 - \tilde{V}_A c_A = \tilde{V}_B c_B \quad (8.5-44)$$

simplifies Eq. (8.5-43) to

$$N_{A_z} = \frac{D_{AB}}{L \tilde{V}_A} \ln \left( \frac{c_{B_L}}{c_{B_0}} \right) \quad (8.5-45)$$

which is identical with Eq. (8.5-38).

**Example 8.17** *Cyclohexane (A) is diffusing through a 1.5 mm thick stagnant benzene (B) film at 25°C. If  $x_{A_0} = 0.15$  and  $x_{A_L} = 0.05$ , determine the molar flux of cyclohexane under steady conditions.*

### Solution

#### Physical properties

$$\text{For cyclohexane (A)} : \begin{cases} \rho_A = 0.779 \text{ g/cm}^3 \\ \mathcal{M}_A = 84 \end{cases}$$

$$\text{For benzene (B)} : \begin{cases} \rho_B = 0.879 \text{ g/cm}^3 \\ \mathcal{M}_B = 78 \end{cases}$$

### Analysis

The molar volumes of species A and B are

$$\begin{aligned} \tilde{V}_A &= \frac{\mathcal{M}_A}{\rho_A} \\ &= \frac{84}{0.779} = 107.8 \text{ cm}^3/\text{mol} \end{aligned}$$

$$\begin{aligned} \tilde{V}_B &= \frac{\mathcal{M}_B}{\rho_B} \\ &= \frac{78}{0.879} = 88.7 \text{ cm}^3/\text{mol} \end{aligned}$$

The values of the total molar concentration at  $z = 0$  and  $z = L$  are calculated from Eq. (8.5-36) as

$$\begin{aligned} c_o &= \frac{1}{\tilde{V}_B + (\tilde{V}_A - \tilde{V}_B) x_{A_o}} \\ &= \frac{1}{88.7 + (107.8 - 88.7)(0.15)} = 10.9 \times 10^{-3} \text{ mol/cm}^3 \end{aligned}$$

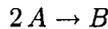
$$\begin{aligned} c_L &= \frac{1}{\tilde{V}_B + (\tilde{V}_A - \tilde{V}_B) x_{A_L}} \\ &= \frac{1}{88.7 + (107.8 - 88.7)(0.05)} = 11.2 \times 10^{-3} \text{ mol/cm}^3 \end{aligned}$$

Therefore, the use of Eq. (8.5-38) gives the molar flux of cyclohexane through benzene layer as

$$\begin{aligned} N_{A_z} &= \frac{D_{AB}}{L \tilde{V}_A} \ln \left( \frac{c_{B_L}}{c_{B_o}} \right) \\ &= \frac{2.09 \times 10^{-5}}{(0.15)(107.8)} \ln \left[ \frac{(11.2 \times 10^{-3})(1 - 0.05)}{(10.9 \times 10^{-3})(1 - 0.15)} \right] = 1.8 \times 10^{-7} \text{ mol/cm}^2 \cdot \text{s} \end{aligned}$$

### 8.5.3 Diffusion With Heterogeneous Chemical Reaction

An ideal gas  $A$  diffuses at steady-state in the positive  $z$ -direction through a flat gas film of thickness  $\delta$  as shown in Figure 8.37. At  $z = \delta$  there is a solid catalytic surface at which  $A$  undergoes a first-order heterogeneous dimerization reaction



As an engineer, we are interested in the determination of the molar flux of species  $A$  in the gas film under steady conditions. The gas composition at  $z = 0$ , i.e.,  $x_{A_o}$ , is known.

The conservation statement for species  $A$ , Eq. (8.4-1), can be written over a differential volume element of thickness  $\Delta z$  as

$$N_{A_z}|_z A - N_{A_z}|_{z+\Delta z} A = 0 \quad (8.5-46)$$

Dividing Eq. (8.5-46) by  $A \Delta z$  and letting  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{N_{A_z}|_z - N_{A_z}|_{z+\Delta z}}{\Delta z} = 0 \quad (8.5-47)$$

or,

$$\frac{dN_{A_z}}{dz} = 0 \quad \Rightarrow \quad N_{A_z} = \text{constant} \quad (8.5-48)$$

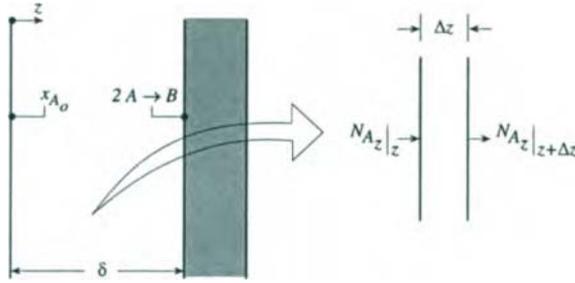


Figure 8.37 Heterogeneous reaction on a catalyst surface.

The total molar flux can be calculated from Eq. (8.5-2) as

$$N_{A_z} = -cD_{AB} \frac{dx_A}{dz} + c_A v_z^* \quad (8.5-49)$$

in which the molar average velocity is given by

$$v_z^* = \frac{N_{A_z} + N_{B_z}}{c} \quad (8.5-50)$$

The stoichiometry of the chemical reaction implies that for every 2 moles of  $A$  diffusing in the positive  $z$ -direction, 1 mole of  $B$  diffuses back in the negative  $z$ -direction. Therefore, the relationship between the fluxes can be expressed as

$$\frac{1}{2} N_{A_z} = -N_{B_z} \quad (8.5-51)$$

The use of Eq. (8.5-51) in Eq. (8.5-50) gives

$$v_z^* = \frac{0.5 N_{A_z}}{c} \quad (8.5-52)$$

Substitution of Eq. (8.5-52) into Eq. (8.5-49) gives

$$N_{A_z} = -\frac{cD_{AB}}{1 - 0.5x_A} \frac{dx_A}{dz} \quad (8.5-53)$$

Since  $N_{A_z}$  is constant, Eq. (8.5-53) can be rearranged as

$$N_{A_z} \int_0^\delta dz = -cD_{AB} \int_{x_{A_0}}^{x_{A_\delta}} \frac{dx_A}{1 - 0.5x_A} \quad (8.5-54)$$

or,

$$N_{A_z} = \frac{2cD_{AB}}{\delta} \ln \left( \frac{1 - 0.5x_{A_\delta}}{1 - 0.5x_{A_0}} \right) \quad (8.5-55)$$

Note that although  $x_{A_0}$  is a known quantity, the mole fraction of species  $\mathcal{A}$  in the gas phase at the catalytic surface,  $x_{A_\delta}$ , is unknown and must be determined from the boundary condition. For heterogeneous reactions, the rate of reaction is empirically specified as

$$\text{at } z = \delta \quad N_{A_z} = k^s c_A = k^s c x_A \quad (8.5-56)$$

where  $k^s$  is the surface reaction rate constant. Therefore,  $x_{A_\delta}$  is expressed from Eq. (8.5-56) as

$$x_{A_\delta} = \frac{N_{A_z}}{c k^s} \quad (8.5-57)$$

Substitution of Eq. (8.5-57) into Eq. (8.5-55) results in

$$\boxed{N_{A_z} = \frac{2cD_{AB}}{\delta} \ln \left[ \frac{1 - 0.5(N_{A_z}/ck^s)}{1 - 0.5x_{A_0}} \right]} \quad (8.5-58)$$

which is a transcendental equation in  $N_{A_z}$ . It is interesting to investigate two limiting cases of Eq. (8.5-58).

**Case (i)  $k^s$  is large**

Since  $\ln(1-x) \simeq -x$  for small values of  $x$ , then

$$\ln [1 - 0.5(N_{A_z}/ck^s)] \simeq -0.5(N_{A_z}/ck^s) \quad (8.5-59)$$

so that Eq. (8.5-58) reduces to

$$N_{A_z} = \frac{2cD_{AB}}{\delta} \left( \frac{\Lambda^2}{\Lambda^2 + 1} \right) \ln \left( \frac{1}{1 - 0.5x_{A_0}} \right) \quad (8.5-60)$$

in which  $\Lambda$  represents the ratio of the rate of heterogeneous reaction to the rate of diffusion and it is given by

$$\Lambda = \sqrt{\frac{k^s \delta}{D_{AB}}} \quad (8.5-61)$$

**Case (ii)  $k^s = \infty$**

This condition implies instantaneous reaction and Eq. (8.5-58) takes the form

$$N_{A_z} = \frac{2cD_{AB}}{\delta} \ln \left( \frac{1}{1 - 0.5x_{A_0}} \right) \quad (8.5-62)$$

When  $k^s = \infty$ , once species  $\mathcal{A}$  reaches the catalytic surface, it is immediately converted to species  $\mathcal{B}$  so that  $x_{A_\delta} = 0$ . Note that Eq. (8.5-62) can also be obtained from Eq. (8.5-55) by letting  $x_{A_\delta} = 0$ .

## 8.5.3.1 Comment

The molar average velocity is given by Eq. (8.5-52) and since both  $N_{A_z}$  and  $c$  are constants,  $v_z^*$  remain constant for  $0 \leq z \leq \delta$ . On the other hand, from Eq. (8.5-6) the mass average velocity is

$$v_z = \frac{\mathcal{M}_A N_{A_z} + \mathcal{M}_B N_{B_z}}{\rho} \quad (8.5-63)$$

Expressing  $N_{B_z}$  in terms of  $N_{A_z}$  by using Eq. (8.5-51) reduces Eq. (8.5-63) to

$$v_z = \frac{N_{A_z}(\mathcal{M}_A - 0.5\mathcal{M}_B)}{\rho} \quad (8.5-64)$$

As a result of the dimerization reaction  $\mathcal{M}_A = 0.5\mathcal{M}_B$  and we get

$$v_z = 0 \quad (8.5-65)$$

In this specific example, therefore, the mass average velocity can be determined on the basis of a solution to a diffusion problem rather than a conservation of momentum.

## NOTATION

$A$	area, $\text{m}^2$
$a_v$	catalyst surface area per unit volume, $1/\text{m}$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ}/\text{kg}\cdot\text{K}$
$c$	total concentration, $\text{kmol}/\text{m}^3$
$c_i$	concentration of species $i$ , $\text{kmol}/\text{m}^3$
$D$	diameter, $\text{m}$
$\mathcal{D}_{AB}$	diffusion coefficient for system $A$ - $B$ , $\text{m}^2/\text{s}$
$e$	total energy flux, $\text{W}/\text{m}^2$
$F_D$	drag force, $\text{N}$
$H$	enthalpy, $\text{J}$ ; partition coefficient
$h$	heat transfer coefficient, $\text{W}/\text{m}^2\cdot\text{K}$
$J^*$	molecular molar flux, $\text{kmol}/\text{m}^2\cdot\text{s}$
$k$	thermal conductivity, $\text{W}/\text{m}\cdot\text{K}$
$k^s$	surface reaction rate constant
$L$	length, $\text{m}$
$\dot{m}$	mass flow rate, $\text{kg}/\text{s}$
$\mathcal{M}$	molecular weight, $\text{kg}/\text{kmol}$
$N$	total molar flux, $\text{kmol}/\text{m}^2\cdot\text{s}$
$\dot{n}$	total molar flow rate, $\text{kmol}/\text{s}$
$\dot{n}_i$	molar flow rate of species $i$ , $\text{kmol}/\text{s}$

$P$	pressure, Pa
$\dot{Q}$	heat transfer rate, W
$Q$	volumetric flow rate, m <sup>3</sup> /s
$q$	heat flux, W/m <sup>2</sup>
$R$	radius, m; resistance, K/W
$\mathcal{R}$	gas constant, J/mol.K
$T$	temperature, °C or K
$t$	time, s
$U$	overall heat transfer coefficient, W/m <sup>2</sup> .K
$V$	velocity of the plate in Couette flow, m/s; volume, m <sup>3</sup>
$v$	mass average velocity, m/s
$v^*$	molar average velocity, m/s
$v^{\blacksquare}$	volume average velocity, m/s
$W$	width, m
$\mathcal{W}$	total mass flux, kg/m <sup>2</sup> .s
$x_i$	mole fraction of species $i$
$\Delta$	difference
$\eta$	fin efficiency; effectiveness factor
$\lambda$	latent heat of vaporization, J
$\mu$	viscosity, kg/m.s
$\nu$	kinematic viscosity, m <sup>2</sup> /s
$\pi$	total momentum flux, N/m <sup>2</sup>
$\rho$	density, kg/m <sup>3</sup>
$\tau_{ij}$	shear stress (flux of $j$ – momentum in the $i$ – direction), N/m <sup>2</sup>
$\omega$	mass fraction

**Overlines**

$\sim$	per mole
$\hat{\phantom{a}}$	per unit mass
$\text{—}$	partial molar

**Bracket**

$\langle a \rangle$	average value of $a$
---------------------	----------------------

**Superscript**

$_{sat}$	saturation
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**Subscripts**

$A, B$	species in binary systems
$ch$	characteristic
$GM$	geometric mean
$i$	species in multicomponent systems
$in$	inlet
$LM$	log-mean
$mix$	mixture

<i>out</i>	out
<i>w</i>	wall or surface
$\infty$	free stream

**Dimensionless Numbers**

$Bi_H$	Biot number for heat transfer
$Bi_M$	Biot number for mass transfer
$Nu$	Nusselt number
$Pr$	Prandtl number
$Re$	Reynolds number
$Sc$	Schmidt number
$Sh$	Sherwood number

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## PROBLEMS

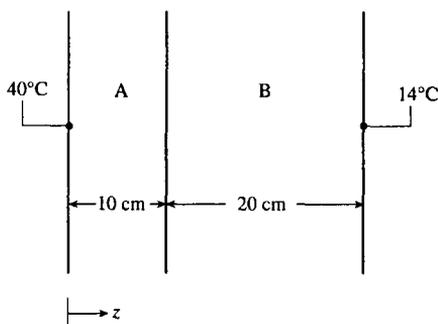
8.1 When the ratio of the radius of the inner pipe to that of the outer pipe is close to unity, a concentric annulus may be considered to be a thin plate slit and its curvature can be neglected. Use this approximation and show that Eqs. (8.1-12) and (8.1-15) can be modified as

$$\frac{v_z}{V} = 1 - \frac{1}{1 - \kappa} \left( \frac{r}{R} - 1 \right)$$

$$Q = \frac{\pi R^2 V (1 - \kappa^2)}{2}$$

to determine the velocity distribution and volumetric flow rate for Couette flow in a concentric annulus with inner and outer radii of  $\kappa R$  and  $R$ , respectively.

8.2 The composite wall shown below consists of materials A and B with thermal conductivities  $k_A = 10 \text{ W/m.K}$  and  $k_B = 0.8 \text{ W/m.K}$ . If the surface area of the wall is  $5 \text{ m}^2$ , determine the interface temperature between A and B.



(Answer: 39 °C)

**8.3** A spherical tank containing liquid nitrogen at 1 atm pressure is insulated with a material having a thermal conductivity of  $1.73 \times 10^{-3}$  W/m.K. The inside diameter of the tank is 60 cm, and the insulation thickness is 2.5 cm. Estimate the kilograms of nitrogen vaporized per day if the outside surface of the insulation is at 21 °C. The normal boiling point of nitrogen is  $-196$  °C and its latent heat of vaporization is 200 kJ/kg.

(Answer: 7.95 kg/day)

**8.4** For a rectangular fin of Section 8.2.4 the parameters are given as:  $T_\infty = 175$  °C,  $T_w = 260$  °C,  $k = 105$  W/m.K,  $L = 4$  cm,  $W = 30$  cm,  $B = 5$  mm.

a) Calculate the average heat transfer coefficient and the rate of heat loss through the fin surface for  $\Lambda = 0.3, 0.6, 0.8, 1.0, 3.0, 6.0$ , and 8.0.

b) One of your friends claims that as the fin efficiency increases, the process becomes more reversible. Do you agree?

**8.5** Show that the mass average velocity for the Stefan diffusion tube experiment, Example 8.16, is given by

$$v_z = \frac{\mathcal{M}_A D_{AB}}{\mathcal{M} L} \ln \left( \frac{1}{1 - x_{A_o}} \right)$$

where  $\mathcal{M}$  is the molecular weight of the mixture. Note that this result leads to the following interesting conclusions:

i) The mass average velocity is determined on the basis of a solution to a diffusion problem rather than a conservation of momentum.

ii) No-slip boundary condition at the wall of the tube is violated.

For a more thorough analysis of the Stefan diffusion tube problem, see Whitaker (1991).

**8.6** Repeat the analysis given in Section 8.4.4 for a zero-order reaction in the following way:

a) Show that the concentration distribution is given by

$$\theta = 1 + \Lambda^2 \left( \frac{\xi^2}{2} - \xi \right) \quad (1)$$

where

$$\theta = \frac{\langle c_A \rangle}{c_{A_o}} \quad (2)$$

$$\xi = \frac{z}{L} \quad (3)$$

$$\Lambda = \sqrt{\frac{2 k^s L^2}{R D_{AB} c_{A_o}}} \quad (4)$$

b) Plot  $\theta$  versus  $\xi$  for  $\Lambda = 1, \sqrt{2}$ , and  $\sqrt{3}$ . Show why the solution given by Eq. (1) is valid only for  $\Lambda \leq \sqrt{2}$ .

c) For  $\Lambda > \sqrt{2}$ , only a fraction  $\phi$  ( $0 < \phi < 1$ ) of the surface is available for the chemical reaction. Under these circumstances show that the concentration distribution is given by

$$\theta = 1 + \Lambda^2 \left( \frac{\xi^2}{2} - \phi \xi \right) \quad 0 \leq \xi \leq \phi \quad (5)$$

**8.7** Consider a spherical catalyst particle of radius  $R$  over which a first-order heterogeneous reaction



takes place. The concentration of species  $\mathcal{A}$  at a distance far away from the catalyst particle is  $c_{A\infty}$ .

a) Show that the concentration distribution is

$$\frac{c_A}{c_{A\infty}} = 1 - \left( \frac{\Lambda^2}{1 + \Lambda^2} \right) \frac{R}{r}$$

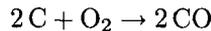
where  $\Lambda$  is defined by

$$\Lambda = \sqrt{\frac{k^s R}{D_{AB}}}$$

b) Show that the molar rate of consumption of species  $\mathcal{A}$ ,  $\dot{n}_A$ , is given by

$$\dot{n}_A = 4\pi D_{AB} \left( \frac{\Lambda^2}{1 + \Lambda^2} \right) c_{A\infty} R$$

**8.8** Consider a spherical carbon particle of initial radius  $R_o$  surrounded by an atmosphere of oxygen. A very rapid heterogeneous reaction



takes place on the surface of the carbon particle. Show that the time it takes for the carbon particle to disappear completely is

$$t = \frac{1}{48 \ln 2} \frac{R_o^2 \rho_C}{c D_{O_2-CO}}$$

where  $\rho_C$  is the density of carbon.

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# Chapter 9

## Steady-State Microscopic Balances With Generation

This chapter is the continuation of Chapter 8 with the addition of the generation term in the inventory rate equation. The breakdown of the chapter is the same as Chapter 8. Once the governing equations for the velocity, temperature or concentration are developed, the physical significance of the terms appearing in these equations are explained and the solutions are given in detail. Obtaining the macroscopic level design equations by integrating the microscopic level equations over the volume of the system is also presented.

### 9.1 MOMENTUM TRANSPORT

For steady transfer of momentum, the inventory rate equation takes the form

$$\left( \begin{array}{c} \text{Rate of} \\ \text{momentum in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{momentum out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{momentum generation} \end{array} \right) = 0 \quad (9.1-1)$$

In Section 5.1 it was shown that momentum is generated as a result of forces acting on a system, i.e., gravitational and pressure forces. Therefore, Eq. (9.1-1) may also be expressed as

$$\left( \begin{array}{c} \text{Rate of} \\ \text{momentum in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{momentum out} \end{array} \right) + \left( \begin{array}{c} \text{Forces acting} \\ \text{on a system} \end{array} \right) = 0 \quad (9.1-2)$$

As in Chapter 8, our analysis will again be restricted to cases in which the following assumptions hold:

1. Incompressible Newtonian fluid.
2. One-dimensional, fully developed laminar flow,
3. Constant physical properties.

### 9.1.1 Flow Between Parallel Plates

Consider the flow of a Newtonian fluid between two parallel plates under steady conditions as shown in Figure 9.1. The pressure gradient is imposed in the  $z$ -direction while both plates are held stationary.

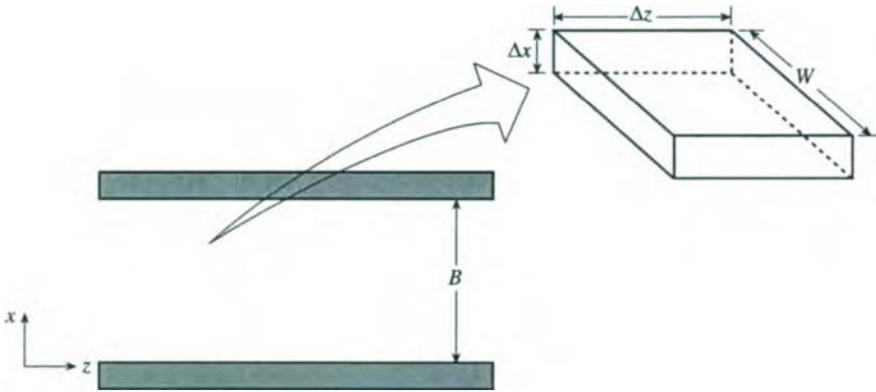


Figure 9.1 Flow between two parallel plates.

Velocity components are simplified according to Figure 8.2. Since  $v_z = v_z(x)$  and  $v_x = v_y = 0$ , Table C.1 in Appendix C indicates that the only non-zero shear-stress component is  $\tau_{xz}$ . Hence, the components of the total momentum flux are given by

$$\pi_{xz} = \tau_{xz} + (\rho v_z) v_x = \tau_{xz} = -\mu \frac{dv_z}{dx} \quad (9.1-3)$$

$$\pi_{yz} = \tau_{yz} + (\rho v_z) v_y = 0 \quad (9.1-4)$$

$$\pi_{zz} = \tau_{zz} + (\rho v_z) v_z = \rho v_z^2 \quad (9.1-5)$$

The pressure, on the other hand, may depend on both  $x$  and  $z$ . Therefore, it is necessary to write the  $x$ - and  $z$ -components of the equation of motion.

#### $x$ -component of the equation of motion

For a rectangular differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , as shown in Figure 9.1, Eq. (9.1-2) is expressed as

$$(P|_x - P|_{x+\Delta x}) W \Delta z + \rho g W \Delta x \Delta z = 0 \quad (9.1-6)$$

Dividing Eq. (9.1-6) by  $W \Delta x \Delta z$  and taking the limit as  $\Delta x \rightarrow 0$  gives

$$\lim_{\Delta x \rightarrow 0} \frac{P|_x - P|_{x+\Delta x}}{\Delta x} + \rho g = 0 \quad (9.1-7)$$

or,

$$\frac{\partial P}{\partial x} = \rho g \quad (9.1-8)$$

Note that Eq. (9.1-8) indicates the hydrostatic pressure distribution in the  $x$ -direction.

### $z$ -component of the equation of motion

Over the differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , Eq. (9.1-2) takes the form

$$\begin{aligned} (\pi_{zz}|_z W \Delta x + \pi_{xz}|_x W \Delta z) - (\pi_{zz}|_{z+\Delta z} W \Delta x + \pi_{xz}|_{x+\Delta x} W \Delta z) \\ + (P|_z - P|_{z+\Delta z}) W \Delta x = 0 \end{aligned} \quad (9.1-9)$$

Dividing Eq. (9.1-9) by  $\Delta x \Delta z W$  and taking the limit as  $\Delta x \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\begin{aligned} \lim_{\Delta z \rightarrow 0} \frac{\pi_{zz}|_z - \pi_{zz}|_{z+\Delta z}}{\Delta z} + \lim_{\Delta x \rightarrow 0} \frac{\pi_{xz}|_x - \pi_{xz}|_{x+\Delta x}}{\Delta x} \\ + \lim_{\Delta z \rightarrow 0} \frac{P|_z - P|_{z+\Delta z}}{\Delta z} = 0 \end{aligned} \quad (9.1-10)$$

or,

$$\frac{\partial \pi_{zz}}{\partial z} + \frac{d\pi_{xz}}{dx} + \frac{\partial P}{\partial z} = 0 \quad (9.1-11)$$

Substitution of Eqs. (9.1-3) and (9.1-5) into Eq. (9.1-11) and noting that  $\partial v_z / \partial z = 0$  yields

$$\underbrace{\mu \frac{d^2 v_z}{dx^2}}_{f(x)} = \underbrace{\frac{\partial P}{\partial z}}_{f(x,z)} \quad (9.1-12)$$

Since the dependence of  $P$  on  $x$  is not known, integration of Eq. (9.1-12) with respect to  $x$  is not possible at the moment. To circumvent this problem, the effects of the static pressure and the gravitational force are combined in a single term called the *modified pressure*,  $\mathcal{P}$ . According to Eq. (5.1-16), the modified pressure for this problem is defined as

$$\mathcal{P} = P - \rho g x \quad (9.1-13)$$

so that

$$\frac{\partial \mathcal{P}}{\partial x} = \frac{\partial P}{\partial x} - \rho g \quad (9.1-14)$$

and

$$\frac{\partial \mathcal{P}}{\partial z} = \frac{\partial P}{\partial z} \quad (9.1-15)$$

Combination of Eqs. (9.1-8) and (9.1-14) yields

$$\frac{\partial \mathcal{P}}{\partial x} = 0 \quad (9.1-16)$$

which implies that  $\mathcal{P} = \mathcal{P}(z)$  only. Therefore, the use of Eq. (9.1-15) in Eq. (9.1-12) gives

$$\underbrace{\mu \frac{d^2 v_z}{dx^2}}_{f(x)} = \underbrace{\frac{d\mathcal{P}}{dz}}_{f(z)} \quad (9.1-17)$$

Note that while the right-side of Eq. (9.1-17) is a function of  $z$  only, the left-side is dependent only on  $x$ . This is possible if and only if both sides of Eq. (9.1-17) are equal to a constant, say  $\lambda$ . Hence,

$$\frac{d\mathcal{P}}{dz} = \lambda \quad \Rightarrow \quad \lambda = -\frac{\mathcal{P}_o - \mathcal{P}_L}{L} \quad (9.1-18)$$

where  $\mathcal{P}_o$  and  $\mathcal{P}_L$  are the values of  $\mathcal{P}$  at  $z = 0$  and  $z = L$ , respectively. Substitution of Eq. (9.1-18) into Eq. (9.1-17) gives the governing equation for velocity in the form

$$\boxed{-\mu \frac{d^2 v_z}{dx^2} = \frac{\mathcal{P}_o - \mathcal{P}_L}{L}} \quad (9.1-19)$$

Integration of Eq. (9.1-19) twice results in

$$v_z = -\frac{\mathcal{P}_o - \mathcal{P}_L}{2\mu L} x^2 + C_1 x + C_2 \quad (9.1-20)$$

where  $C_1$  and  $C_2$  are integration constants.

The use of the boundary conditions

$$\text{at } x = 0 \quad v_z = 0 \quad (9.1-21)$$

$$\text{at } x = B \quad v_z = 0 \quad (9.1-22)$$

gives the velocity distribution as

$$\boxed{v_z = \frac{(\mathcal{P}_o - \mathcal{P}_L) B^2}{2\mu L} \left[ \frac{x}{B} - \left( \frac{x}{B} \right)^2 \right]} \quad (9.1-23)$$

The use of the velocity distribution, Eq. (9.1-23), in Eq. (9.1-3) gives the shear stress distribution as

$$\boxed{\tau_{xz} = \frac{(\mathcal{P}_o - \mathcal{P}_L) B}{2L} \left[ 2 \left( \frac{x}{B} \right) - 1 \right]} \quad (9.1-24)$$

The volumetric flow rate can be determined by integrating the velocity distribution over the cross-sectional area, i.e.,

$$Q = \int_0^W \int_0^B v_z dx dy \tag{9.1-25}$$

Substitution of Eq. (9.1-23) into Eq. (9.1-25) gives the volumetric flow rate in the form

$$Q = \frac{(\mathcal{P}_o - \mathcal{P}_L) W B^3}{12 \mu L} \tag{9.1-26}$$

Dividing the volumetric flow rate by the flow area gives the average velocity as

$$\langle v_z \rangle = \frac{Q}{WB} = \frac{(\mathcal{P}_o - \mathcal{P}_L) B^2}{12 \mu L} \tag{9.1-27}$$

### 9.1.1.1 Macroscopic balance

Integration of the governing differential equation, Eq. (9.1-19), over the volume of the system gives the macroscopic momentum balance as

$$-\int_0^L \int_0^W \int_0^B \mu \frac{d^2 v_z}{dx^2} dx dy dz = \int_0^L \int_0^W \int_0^B \frac{\mathcal{P}_o - \mathcal{P}_L}{L} dx dy dz \tag{9.1-28}$$

or

$$\underbrace{(\tau_{xz}|_{x=B} - \tau_{xz}|_{x=0}) LW}_{\text{Drag force}} = \underbrace{(\mathcal{P}_o - \mathcal{P}_L) WB}_{\text{Pressure and gravitational forces}} \tag{9.1-29}$$

Note that Eq. (9.1-29) is nothing more than Newton's second law of motion. The interaction of the system, i.e., the fluid between the parallel plates, with the surroundings is the drag force,  $F_D$ , on the plates and is given by

$$F_D = (\mathcal{P}_o - \mathcal{P}_L) WB \tag{9.1-30}$$

On the other hand, the friction factor is the dimensionless interaction of the system with the surroundings and is defined by Eq. (3.1-7), i.e.,

$$F_D = A_{ch} K_{ch} \langle f \rangle \tag{9.1-31}$$

or,

$$(\mathcal{P}_o - \mathcal{P}_L) WB = (2WL) \left( \frac{1}{2} \rho \langle v_z \rangle^2 \right) \langle f \rangle \tag{9.1-32}$$

Simplification of Eq. (9.1-32) gives

$$\langle f \rangle = \frac{(\mathcal{P}_o - \mathcal{P}_L) B}{\rho L \langle v_z \rangle^2} \tag{9.1-33}$$

Elimination of  $(\mathcal{P}_o - \mathcal{P}_L)$  between Eqs. (9.1-27) and (9.1-33) leads to

$$\langle f \rangle = 12 \left( \frac{\mu}{B \langle v_z \rangle \rho} \right) \quad (9.1-34)$$

For flow in non-circular ducts, the Reynolds number based on the hydraulic equivalent diameter was defined in Chapter 4 by Eq. (4.5-37). Since  $D_h = 2B$ , the Reynolds number is

$$\text{Re}_h = \frac{2B \langle v_z \rangle \rho}{\mu} \quad (9.1-35)$$

Therefore, Eq. (9.1-34) takes the final form as

$$\langle f \rangle = \frac{24}{\text{Re}_h} \quad (9.1-36)$$

### 9.1.2 Falling Film on a Vertical Plate

Consider a film of liquid falling down a vertical plate under the action of gravity as shown in Figure 9.2. Since the liquid is in contact with air, it is necessary to consider both phases. Let superscripts  $L$  and  $A$  represent the liquid and the air, respectively.

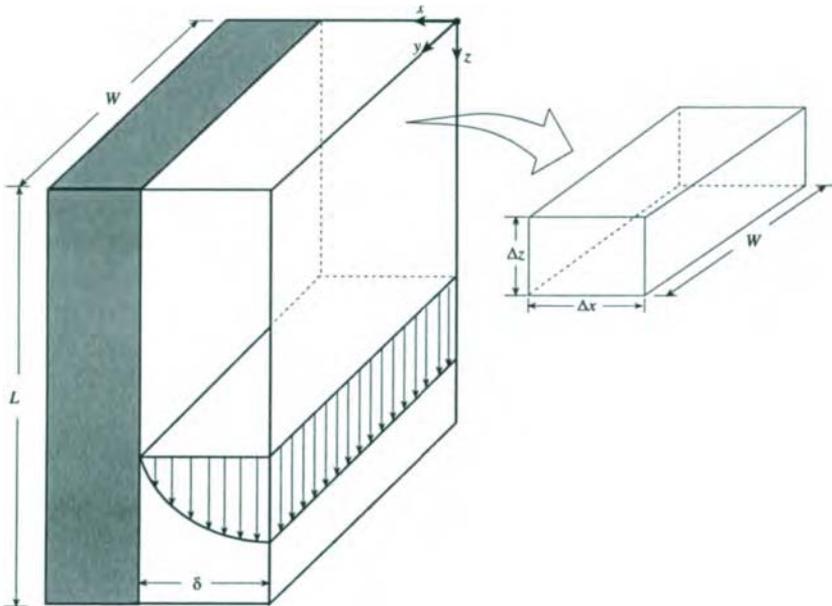


Figure 9.2 Falling film on a vertical plate.

For the liquid phase the velocity components are simplified according to Figure 8.2. Since  $v_z = v_z(x)$  and  $v_x = v_y = 0$ , Table C.1 in Appendix C indicates that the only non-zero shear-stress component is  $\tau_{xz}$ . Hence, the components of the total momentum flux are given by

$$\pi_{xz}^L = \tau_{xz}^L + (\rho^L v_z^L) v_x^L = \tau_{xz}^L = -\mu^L \frac{dv_z^L}{dx} \quad (9.1-37)$$

$$\pi_{yz}^L = \tau_{yz}^L + (\rho^L v_z^L) v_y^L = 0 \quad (9.1-38)$$

$$\pi_{zz}^L = \tau_{zz}^L + (\rho^L v_z^L) v_z^L = \rho^L (v_z^L)^2 \quad (9.1-39)$$

The pressure, on the other hand, depends only on  $z$ . Therefore, only the  $z$ -component of the equation of motion should be considered.

For a rectangular differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , as shown in Figure 9.2, Eq. (9.1-2) is expressed as

$$\begin{aligned} & (\pi_{zz}^L|_z W \Delta x + \pi_{xz}^L|_x W \Delta z) - (\pi_{zz}^L|_{z+\Delta z} W \Delta x + \pi_{xz}^L|_{x+\Delta x} W \Delta z) \\ & + (P^L|_z - P^L|_{z+\Delta z}) W \Delta x + \rho^L g W \Delta x \Delta z = 0 \end{aligned} \quad (9.1-40)$$

Dividing each term by  $W \Delta x \Delta z$  and taking the limit as  $\Delta x \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\begin{aligned} \lim_{\Delta z \rightarrow 0} \frac{\pi_{zz}^L|_z - \pi_{zz}^L|_{z+\Delta z}}{\Delta z} + \lim_{\Delta x \rightarrow 0} \frac{\pi_{xz}^L|_x - \pi_{xz}^L|_{x+\Delta x}}{\Delta x} \\ + \lim_{\Delta z \rightarrow 0} \frac{P^L|_z - P^L|_{z+\Delta z}}{\Delta z} + \rho^L g = 0 \end{aligned} \quad (9.1-41)$$

or,

$$\frac{\partial \pi_{zz}^L}{\partial z} + \frac{d\pi_{xz}^L}{dx} + \frac{\partial P^L}{\partial z} - \rho^L g = 0 \quad (9.1-42)$$

Substitution of Eqs. (9.1-37) and (9.1-39) into Eq. (9.1-42) and noting that  $\partial v_z^L / \partial z = 0$  yields

$$-\mu^L \frac{d^2 v_z^L}{dx^2} = -\frac{dP^L}{dz} + \rho^L g \quad (9.1-43)$$

Now, it is necessary to write down the  $z$ -component of the equation of motion for the stagnant air. Over a differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , Eq. (9.1-2) is written as

$$(P^A|_z - P^A|_{z+\Delta z}) W \Delta x + \rho^A g W \Delta x \Delta z = 0 \quad (9.1-44)$$

Dividing each term by  $W \Delta x \Delta z$  and taking the limit as  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{P^A|_z - P^A|_{z+\Delta z}}{\Delta z} + \rho^A g = 0 \quad (9.1-45)$$

or,

$$\frac{dP^A}{dz} = \rho^A g \quad (9.1-46)$$

At the liquid-air interface, the jump momentum balance<sup>1</sup> indicates that the normal and tangential components of the total stress tensor are equal to each other, i.e.,

$$\text{at } x = 0 \quad P^L = P^A \quad \text{for all } z \quad (9.1-47)$$

$$\text{at } x = 0 \quad \tau_{xz}^L = \tau_{xz}^A \quad \text{for all } z \quad (9.1-48)$$

Since both  $P^L$  and  $P^A$  depend only on  $z$ , then

$$\frac{dP^L}{dz} = \frac{dP^A}{dz} \quad (9.1-49)$$

From Eqs. (9.1-46) and (9.1-49) one can conclude that

$$\frac{dP^L}{dz} = \rho^A g \quad (9.1-50)$$

Substitution of Eq. (9.1-50) into Eq. (9.1-43) gives

$$-\mu^L \frac{d^2 v_z^L}{dx^2} = (\rho^L - \rho^A) g \quad (9.1-51)$$

Since  $\rho^L \gg \rho^A$ , then  $\rho^L - \rho^A \approx \rho^L$  and Eq. (9.1-51) takes the form

$$-\mu^L \frac{d^2 v_z^L}{dx^2} = \rho^L g \quad (9.1-52)$$

This analysis shows the reason why the pressure term does not appear in the equation of motion when a fluid flows under the action of gravity. This point is usually overlooked in the literature by simply stating that “free surface  $\Rightarrow$  no pressure gradient.”

For simplicity, superscripts in Eq. (9.1-52) will be dropped for the rest of the analysis with the understanding that properties are those of the liquid. Therefore, the governing equation takes the form

$$\boxed{-\mu \frac{d^2 v_z}{dx^2} = \rho g} \quad (9.1-53)$$

Integration of Eq. (9.1-53) twice leads to

$$v_z = -\frac{\rho g}{2\mu} x^2 + C_1 x + C_2 \quad (9.1-54)$$

The boundary conditions are

$$\text{at } x = 0 \quad \frac{dv_z}{dx} = 0 \quad (9.1-55)$$

$$\text{at } x = \delta \quad v_z = 0 \quad (9.1-56)$$

<sup>1</sup>For a thorough discussion on jump balances, see Slattery (1999).

Note that Eq. (9.1-55) is a consequence of the jump condition given by Eq. (9.1-48). Application of the boundary conditions results in

$$\boxed{v_z = \frac{\rho g \delta^2}{2\mu} \left[ 1 - \left( \frac{x}{\delta} \right)^2 \right]} \quad (9.1-57)$$

The maximum velocity takes place at the liquid-air interface, i.e., at  $x = 0$ , as

$$v_{\max} = \frac{\rho g \delta^2}{2\mu} \quad (9.1-58)$$

The use of the velocity distribution, Eq. (9.1-57), in Eq. (9.1-37) gives the shear stress distribution as

$$\boxed{\tau_{xz} = \rho g x} \quad (9.1-59)$$

Integration of the velocity profile across the flow area gives the volumetric flow rate, i.e.,

$$Q = \int_0^W \int_0^\delta v_z \, dx dy \quad (9.1-60)$$

Substitution of Eq. (9.1-57) into Eq. (9.1-60) yields

$$\boxed{Q = \frac{\rho g \delta^3 W}{3\mu}} \quad (9.1-61)$$

Dividing the volumetric flow rate by the flow area gives the average velocity as

$$\boxed{\langle v_z \rangle = \frac{Q}{W\delta} = \frac{\rho g \delta^2}{3\mu}} \quad (9.1-62)$$

### 9.1.2.1 Macroscopic balance

Integration of the governing equation, Eq. (9.1-53), over the volume of the system gives the macroscopic equation as

$$-\int_0^L \int_0^W \int_0^\delta \mu \frac{d^2 v_z}{dx^2} \, dx dy dz = \int_0^L \int_0^W \int_0^\delta \rho g \, dx dy dz \quad (9.1-63)$$

or,

$$\underbrace{\tau_{xz}|_{x=\delta} WL}_{\text{Drag force}} = \underbrace{\rho g \delta WL}_{\text{Mass of the liquid}} \quad (9.1-64)$$

### 9.1.3 Flow in a Circular Tube

Consider the flow of a Newtonian fluid in a vertical circular pipe under steady conditions as shown in Figure 9.3. The pressure gradient is imposed in the  $z$ -direction.

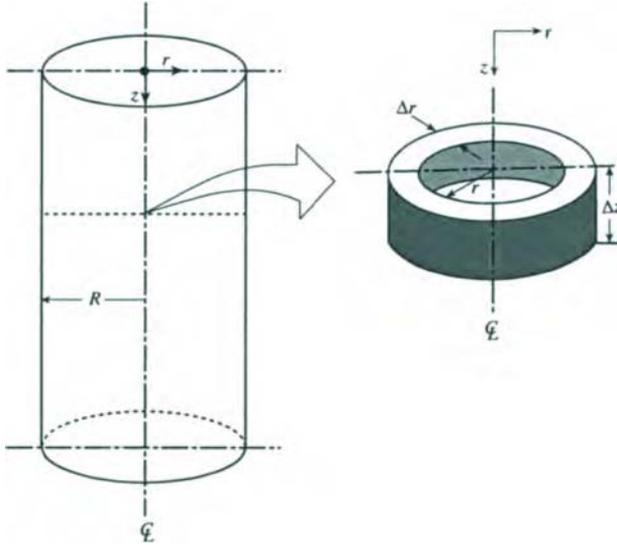


Figure 9.3 Flow in a circular pipe.

Simplification of the velocity components according to Figure 8.4 shows that  $v_z = v_z(r)$  and  $v_r = v_\theta = 0$ . Therefore, from Table C.2 in Appendix C, the only non-zero shear stress component is  $\tau_{rz}$  and the components of the total momentum flux are given by

$$\pi_{rz} = \tau_{rz} + (\rho v_z) v_r = \tau_{rz} = -\mu \frac{dv_z}{dr} \quad (9.1-65)$$

$$\pi_{\theta z} = \tau_{\theta z} + (\rho v_z) v_\theta \quad (9.1-66)$$

$$\pi_{zz} = \tau_{zz} + (\rho v_z) v_z \quad (9.1-67)$$

The pressure in the pipe depends on  $z$ . Therefore, it is necessary to consider only the  $z$ -component of the equation of motion.

For a cylindrical differential volume element of thickness  $\Delta r$  and length  $\Delta z$ , as shown in Figure 9.3, Eq. (9.1-2) is expressed as

$$(\pi_{zz}|_z 2\pi r \Delta r + \pi_{rz}|_r 2\pi r \Delta z) - [\pi_{zz}|_{z+\Delta z} 2\pi r \Delta r + \pi_{rz}|_{r+\Delta r} 2\pi(r+\Delta r)\Delta z] + (P|_z - P|_{z+\Delta z})2\pi r \Delta r + \rho g 2\pi r \Delta r \Delta z = 0 \quad (9.1-68)$$

Dividing Eq. (9.1-68) by  $2\pi\Delta r\Delta z$  and taking the limit as  $\Delta r \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} r \left( \frac{\pi_{zz}|_z - \pi_{zz}|_{z+\Delta z}}{\Delta z} \right) + \lim_{\Delta r \rightarrow 0} \frac{(r\pi_{rz})|_r - (r\pi_{rz})|_{r+\Delta r}}{\Delta r} + \lim_{\Delta z \rightarrow 0} r \left( \frac{P|_z - P|_{z+\Delta z}}{\Delta z} \right) + r\rho g = 0 \quad (9.1-69)$$

or,

$$\frac{\partial \pi_{zz}}{\partial z} + \frac{1}{r} \frac{d(r\pi_{rz})}{dr} = -\frac{dP}{dz} + \rho g \quad (9.1-70)$$

Substitution of Eqs. (9.1-65) and (9.1-67) into Eq. (9.1-70) and noting that  $\partial v_z / \partial z = 0$  gives

$$-\frac{\mu}{r} \frac{d}{dr} \left[ r \left( \frac{dv_z}{dr} \right) \right] = -\frac{dP}{dz} + \rho g \quad (9.1-71)$$

The modified pressure is defined by

$$\mathcal{P} = P - \rho g z \quad (9.1-72)$$

so that

$$\frac{d\mathcal{P}}{dz} = \frac{dP}{dz} - \rho g \quad (9.1-73)$$

Substitution of Eq. (9.1-73) into Eq. (9.1-71) yields

$$\underbrace{\frac{\mu}{r} \frac{d}{dr} \left[ r \left( \frac{dv_z}{dr} \right) \right]}_{f(r)} = \underbrace{\frac{d\mathcal{P}}{dz}}_{f(z)} \quad (9.1-74)$$

Note that while the right-side of Eq. (9.1-74) is a function of  $z$  only, the left-side is dependent only on  $r$ . This is possible if and only if both sides of Eq. (9.1-74) are equal to a constant, say  $\lambda$ . Hence,

$$\frac{d\mathcal{P}}{dz} = \lambda \quad \Rightarrow \quad \lambda = -\frac{\mathcal{P}_o - \mathcal{P}_L}{L} \quad (9.1-75)$$

where  $\mathcal{P}_o$  and  $\mathcal{P}_L$  are the values of  $\mathcal{P}$  at  $z = 0$  and  $z = L$ , respectively. Substitution of Eq. (9.1-75) into Eq. (9.1-74) gives the governing equation for velocity as

$$\boxed{-\frac{\mu}{r} \frac{d}{dr} \left[ r \left( \frac{dv_z}{dr} \right) \right] = \frac{\mathcal{P}_o - \mathcal{P}_L}{L}} \quad (9.1-76)$$

Integration of Eq. (9.1-76) twice leads to

$$v_z = -\frac{(\mathcal{P}_o - \mathcal{P}_L)}{4\mu L} r^2 + C_1 \ln r + C_2 \quad (9.1-77)$$

where  $C_1$  and  $C_2$  are integration constants.

The center of the tube, i.e.,  $r = 0$ , is included in the flow domain. However, the presence of the term  $\ln r$  makes  $v_z \rightarrow -\infty$  as  $r \rightarrow 0$ . Therefore, a physically possible solution exists only if  $C_1 = 0$ . This condition is usually expressed as “ $v_z$  is finite at  $r = 0$ .” Alternatively, the use of the symmetry condition, i.e.,  $dv_z/dr = 0$  at  $r = 0$ , also leads to  $C_1 = 0$ . The constant  $C_2$  can be evaluated by using the no-slip boundary condition on the surface of the tube, i.e.,

$$\text{at } r = R \quad v_z = 0 \quad (9.1-78)$$

so that the velocity distribution becomes

$$v_z = \frac{(\mathcal{P}_o - \mathcal{P}_L) R^2}{4\mu L} \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \quad (9.1-79)$$

The maximum velocity takes place at the center of the tube, i.e.,

$$v_{\max} = \frac{(\mathcal{P}_o - \mathcal{P}_L) R^2}{4\mu L} \quad (9.1-80)$$

The use of Eq. (9.1-79) in Eq. (9.1-65) gives the shear stress distribution as

$$\tau_{rz} = \frac{(\mathcal{P}_o - \mathcal{P}_L) r}{2L} \quad (9.1-81)$$

The volumetric flow rate can be determined by integrating the velocity distribution over the cross-sectional area, i.e.,

$$Q = \int_0^{2\pi} \int_0^R v_z r \, dr d\theta \quad (9.1-82)$$

Substitution of Eq. (9.1-79) into Eq. (9.1-82) and integration gives

$$Q = \frac{\pi (\mathcal{P}_o - \mathcal{P}_L) R^4}{8\mu L} \quad (9.1-83)$$

which is known as the *Hagen-Poiseuille law*. Dividing the volumetric flow rate by the flow area gives the average velocity as

$$\langle v_z \rangle = \frac{Q}{\pi R^2} = \frac{(\mathcal{P}_o - \mathcal{P}_L) R^2}{8\mu L} \quad (9.1-84)$$

### 9.1.3.1 Macroscopic balance

Integration of the governing differential equation, Eq. (9.1-76), over the volume of the system gives

$$\begin{aligned}
 - \int_0^L \int_0^{2\pi} \int_0^R \frac{\mu}{r} \frac{d}{dr} \left[ r \left( \frac{dv_z}{dr} \right) \right] r \, dr d\theta dz \\
 = \int_0^L \int_0^{2\pi} \int_0^R \frac{(\mathcal{P}_o - \mathcal{P}_L)}{L} r \, dr d\theta dz \quad (9.1-85)
 \end{aligned}$$

or,

$$\underbrace{\tau_{rz}|_{r=R} 2\pi RL}_{\text{Drag force}} = \underbrace{\pi R^2 (\mathcal{P}_o - \mathcal{P}_L)}_{\text{Pressure and gravitational forces}} \quad (9.1-86)$$

The interaction of the system, i.e., the fluid in the tube, with the surroundings manifests itself as the drag force,  $F_D$ , on the wall and is given by

$$\boxed{F_D = \pi R^2 (\mathcal{P}_o - \mathcal{P}_L)} \quad (9.1-87)$$

On the other hand, the dimensionless interaction of the system with the surroundings, i.e., the friction factor, is given by Eq. (3.1-7), i.e.,

$$F_D = A_{ch} K_{ch} \langle f \rangle \quad (9.1-88)$$

or,

$$\pi R^2 (\mathcal{P}_o - \mathcal{P}_L) = (2\pi RL) \left( \frac{1}{2} \rho \langle v_z \rangle^2 \right) \langle f \rangle \quad (9.1-89)$$

Expressing the average velocity in terms of the volumetric flow rate by using Eq. (9.1-84) reduces Eq. (9.1-89) to

$$\langle f \rangle = \frac{\pi^2 D^5 (\mathcal{P}_o - \mathcal{P}_L)}{32 \rho L Q^2} \quad (9.1-90)$$

which is nothing more than Eq. (4.5-76).

Elimination of  $(\mathcal{P}_o - \mathcal{P}_L)$  between Eqs. (9.1-84) and (9.1-89) leads to

$$\boxed{\langle f \rangle = 16 \left( \frac{\mu}{D \langle v_z \rangle \rho} \right) = \frac{16}{\text{Re}}} \quad (9.1-91)$$

## 9.1.4 Axial Flow in an Annulus

Consider the flow of a Newtonian fluid in a vertical concentric annulus under steady conditions as shown in Figure 9.4. A constant pressure gradient is imposed in the positive  $z$ -direction while the inner rod is stationary.

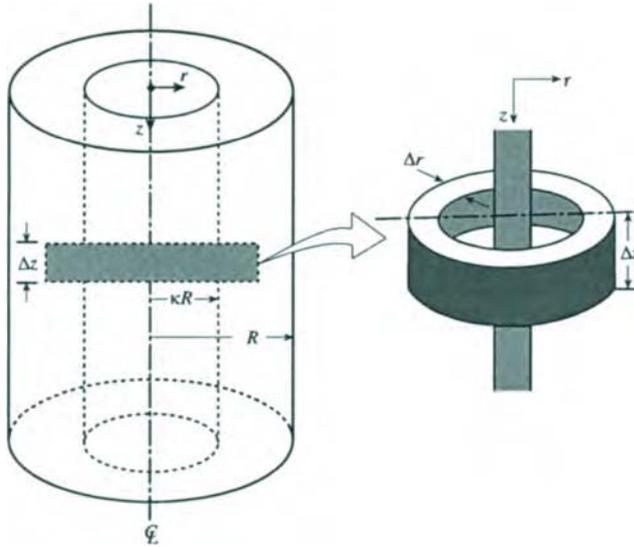


Figure 9.4 Flow in a concentric annulus.

The development of the velocity distribution follows the same lines for flow in a circular tube with the result

$$\boxed{-\frac{\mu}{r} \frac{d}{dr} \left[ r \left( \frac{dv_z}{dr} \right) \right] = \frac{\mathcal{P}_o - \mathcal{P}_L}{L}} \quad (9.1-92)$$

Integration of Eq. (9.1-92) leads to

$$v_z = -\frac{(\mathcal{P}_o - \mathcal{P}_L)}{4\mu L} r^2 + C_1 \ln r + C_2 \quad (9.1-93)$$

In this case, however,  $r = 0$  is not within the flow field. The use of the boundary conditions

$$\text{at } r = R \quad v_z = 0 \quad (9.1-94)$$

$$\text{at } r = \kappa R \quad v_z = 0 \quad (9.1-95)$$

gives the velocity distribution as

$$\boxed{v_z = \frac{(\mathcal{P}_o - \mathcal{P}_L) R^2}{4\mu L} \left[ 1 - \left( \frac{r}{R} \right)^2 - \left( \frac{1 - \kappa^2}{\ln \kappa} \right) \ln \left( \frac{r}{R} \right) \right]} \quad (9.1-96)$$

The use of Eq. (9.1-96) in Eq. (9.1-65) gives the shear stress distribution as

$$\boxed{\tau_{rz} = \frac{(\mathcal{P}_o - \mathcal{P}_L) R}{2L} \left[ \frac{r}{R} + \frac{1 - \kappa^2}{2 \ln \kappa} \left( \frac{R}{r} \right) \right]} \quad (9.1-97)$$

The volumetric flow rate can be determined by integrating the velocity distribution over the annular cross-sectional area, i.e.,

$$Q = \int_0^{2\pi} \int_{\kappa R}^R v_z r \, dr d\theta \tag{9.1-98}$$

Substitution of Eq. (9.1-96) into Eq. (9.1-98) and integration gives

$$Q = \frac{\pi (\mathcal{P}_o - \mathcal{P}_L) R^4}{8 \mu L} \left[ 1 - \kappa^4 + \frac{(1 - \kappa^2)^2}{\ln \kappa} \right] \tag{9.1-99}$$

Dividing the volumetric flow rate by the flow area gives the average velocity as

$$\langle v_z \rangle = \frac{Q}{\pi R^2 (1 - \kappa^2)} = \frac{(\mathcal{P}_o - \mathcal{P}_L) R^2}{8 \mu L} \left( 1 + \kappa^2 + \frac{1 - \kappa^2}{\ln \kappa} \right) \tag{9.1-100}$$

### 9.1.4.1 Macroscopic balance

Integration of the governing differential equation, Eq. (9.1-92), over the volume of the system gives

$$-\int_0^L \int_0^{2\pi} \int_{\kappa R}^R \frac{\mu}{r} \frac{d}{dr} \left[ r \left( \frac{dv_z}{dr} \right) \right] r \, dr d\theta dz = \int_0^L \int_0^{2\pi} \int_{\kappa R}^R \frac{(\mathcal{P}_o - \mathcal{P}_L)}{L} r \, dr d\theta dz \tag{9.1-101}$$

or,

$$\underbrace{\tau_{rz}|_{r=R} 2\pi RL - \tau_{rz}|_{r=\kappa R} 2\pi \kappa RL}_{\text{Drag force}} = \underbrace{\pi R^2 (1 - \kappa^2) (\mathcal{P}_o - \mathcal{P}_L)}_{\text{Pressure and gravitational forces}} \tag{9.1-102}$$

Note that Eq. (9.1-102) is nothing more than Newton's second law of motion. The interaction of the system, i.e., the fluid in the concentric annulus, with the surroundings is the drag force,  $F_D$ , on the walls and is given by

$$F_D = \pi R^2 (1 - \kappa^2) (\mathcal{P}_o - \mathcal{P}_L) \tag{9.1-103}$$

On the other hand, the friction factor is defined by Eq. (3.1-7) as

$$F_D = A_{ch} K_{ch}(f) \tag{9.1-104}$$

or,

$$\pi R^2 (1 - \kappa^2) (\mathcal{P}_o - \mathcal{P}_L) = [2\pi R(1 + \kappa)L] \left( \frac{1}{2} \rho \langle v_z \rangle^2 \right) \langle f \rangle \tag{9.1-105}$$

Elimination of  $(\mathcal{P}_o - \mathcal{P}_L)$  between Eqs. (9.1-100) and (9.1-105) gives

$$\langle f \rangle = \frac{8\mu}{R\langle v_z \rangle \rho} \left( \frac{1 - \kappa}{1 + \kappa^2 + \frac{1 - \kappa^2}{\ln \kappa}} \right) \quad (9.1-106)$$

Since  $D_h = 2R(1 - \kappa)$ , the Reynolds number based on the hydraulic equivalent diameter is

$$Re_h = \frac{2R(1 - \kappa)\langle v_z \rangle \rho}{\mu} \quad (9.1-107)$$

so that Eq. (9.1-106) becomes

$$\boxed{\langle f \rangle = \frac{16}{Re_h} \left[ \frac{(1 - \kappa)^2}{1 + \kappa^2 + \frac{1 - \kappa^2}{\ln \kappa}} \right]} \quad (9.1-108)$$

#### 9.1.4.2 Investigation of the limiting cases

##### ■ Case (i) $\kappa \rightarrow 1$

When the ratio of the radius of the inner pipe to that of the outer pipe is close to unity, i.e.,  $\kappa \rightarrow 1$ , a concentric annulus may be considered to be a thin-plane slit and its curvature can be neglected. Approximation of a concentric annulus as a parallel plate requires the width,  $W$ , and the length,  $L$ , of the plate to be defined as

$$W = \pi R(1 + \kappa) \quad (9.1-109)$$

$$B = R(1 - \kappa) \quad (9.1-110)$$

Therefore, the product  $WB^3$  is equal to

$$WB^3 = \pi R^4(1 - \kappa^2)(1 - \kappa)^2 \implies \pi R^4 = \frac{WB^3}{(1 - \kappa^2)(1 - \kappa)^2} \quad (9.1-111)$$

so that Eq. (9.1-99) becomes

$$Q = \frac{(\mathcal{P}_o - \mathcal{P}_L) WB^3}{8\mu L} \lim_{\kappa \rightarrow 1} \left[ \frac{1 + \kappa^2}{(1 - \kappa)^2} + \frac{1 + \kappa}{(1 - \kappa) \ln \kappa} \right] \quad (9.1-112)$$

Substitution of  $\psi = 1 - \kappa$  into Eq. (9.1-112) gives

$$Q = \frac{(\mathcal{P}_o - \mathcal{P}_L) WB^3}{8\mu L} \lim_{\psi \rightarrow 0} \left[ \frac{\psi^2 - 2\psi + 2}{\psi^2} + \frac{2 - \psi}{\psi \ln(1 - \psi)} \right] \quad (9.1-113)$$

The Taylor series expansion of the term  $\ln(1 - \psi)$  is

$$\ln(1 - \psi) = -\psi - \frac{1}{2}\psi^2 - \frac{1}{3}\psi^3 - \dots \quad (9.1-114)$$

Using Eq. (9.1-114) in Eq. (9.1-113) and carrying out the divisions yields

$$Q = \frac{(\mathcal{P}_o - \mathcal{P}_L) WB^3}{8\mu L} \lim_{\psi \rightarrow 0} \left[ 1 - \frac{2}{\psi} + \frac{2}{\psi^2} + \left( -\frac{2}{\psi^2} + \frac{2}{\psi} - \frac{1}{3} - \frac{\psi}{2} + \dots \right) \right] \quad (9.1-115)$$

or,

$$\begin{aligned} Q &= \frac{(\mathcal{P}_o - \mathcal{P}_L) WB^3}{8\mu L} \lim_{\psi \rightarrow 0} \left( \frac{2}{3} - \frac{\psi}{2} + \dots \right) \\ &= \frac{(\mathcal{P}_o - \mathcal{P}_L) WB^3}{12\mu L} \end{aligned} \quad (9.1-116)$$

Note that Eq. (9.1-116) is equivalent to Eq. (9.1-26).

#### ■ Case (ii) $\kappa \rightarrow 0$

When the ratio of the radius of the inner pipe to that of the outer pipe is close to zero, i.e.,  $\kappa \rightarrow 0$ , a concentric annulus may be considered to be a circular pipe of radius  $R$ . In this case Eq. (9.1-99) becomes

$$Q = \frac{\pi(\mathcal{P}_o - \mathcal{P}_L) R^4}{8\mu L} \lim_{\kappa \rightarrow 0} \left[ 1 - \kappa^4 + \frac{(1 - \kappa^2)^2}{\ln \kappa} \right] \quad (9.1-117)$$

Since  $\ln 0 = -\infty$ , Eq. (9.1-117) reduces to

$$Q = \frac{\pi(\mathcal{P}_o - \mathcal{P}_L) R^4}{8\mu L} \quad (9.1-118)$$

which is identical with Eq. (9.1-83).

### 9.1.5 Physical Significance of the Reynolds Number

The physical significance attributed to the Reynolds number for both laminar and turbulent flows is that it is the ratio of the inertial forces to the viscous forces. However, examination of the governing equations for fully developed laminar flow: (i) between parallel plates, Eq. (9.1-19), (ii) in a circular pipe, Eq. (9.1-76), and (iii) in a concentric annulus, Eq. (9.1-92), indicates that the only forces present are the pressure and the viscous forces. Inertial forces do not exist in these problems. Since both pressure and viscous forces are kept in the governing equation for velocity, they must, more or less, have the same order of magnitude. Therefore, the ratio of pressure to viscous forces, which is a dimensionless number, has an order of magnitude of unity.

On the other hand, the use of  $\frac{1}{2}(\rho\langle v_z \rangle^2)$  term instead of pressure is not appropriate since this term comes from the Bernoulli equation, which is developed for no-friction (or, reversible) flows.

Therefore, in the case of a fully developed laminar flow, attributing a physical significance to the Reynolds number is not correct. For a more thorough discussion on the subject, see Bejan (1984).

## 9.2 ENERGY TRANSPORT WITHOUT CONVECTION

For steady transport of energy, the inventory rate equation takes the form

$$\left( \begin{array}{c} \text{Rate of} \\ \text{energy in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{energy out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{energy generation} \end{array} \right) = 0 \quad (9.2-1)$$

As stated in Section 5.2, generation of energy may occur as a result of chemical and nuclear reactions, absorption radiation, presence of magnetic fields, and viscous dissipation. It is of industrial importance to know the temperature distribution resulting from the internal generation of energy because exceeding of the maximum allowable temperature may lead to deterioration of the material of construction.

### 9.2.1 Conduction in Rectangular Coordinates

Consider one-dimensional transfer of energy in the  $z$ -direction through a plane wall of thickness  $L$  and surface area  $A$  as shown in Figure 9.5. Let  $\mathfrak{R}$  be the rate of energy generation per unit volume within the wall. In general,  $\mathfrak{R}$  may depend on  $z$ .

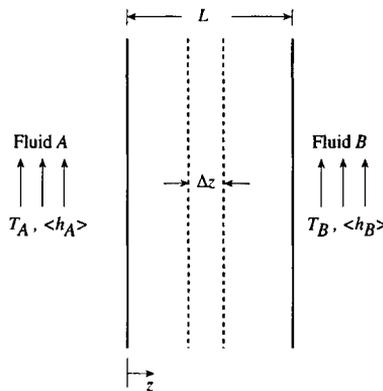


Figure 9.5 Conduction through a plane wall with generation.

Since  $T = T(z)$ , Table C.4 in Appendix C indicates that the only non-zero energy flux component is  $e_z$  and it is given by

$$e_z = q_z = -k \frac{dT}{dz} \quad (9.2-2)$$

For a rectangular volume element of thickness  $\Delta z$  as shown in Figure 9.5, Eq. (9.2-1) is expressed as

$$q_z|_z A - q_z|_{z+\Delta z} A + \mathfrak{R} A \Delta z = 0 \quad (9.2-3)$$

Dividing each term by  $A \Delta z$  and taking the limit as  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{q_z|_z - q_z|_{z+\Delta z}}{\Delta z} + \mathfrak{R} = 0 \quad (9.2-4)$$

or

$$\frac{dq_z}{dz} = \mathfrak{R} \quad (9.2-5)$$

Substitution of Eq. (9.2-2) into Eq. (9.2-5) gives the governing equation for temperature as

$$\boxed{-\frac{d}{dz} \left( k \frac{dT}{dz} \right) = \mathfrak{R}} \quad (9.2-6)$$

Integration of Eq. (9.2-6) gives

$$k \frac{dT}{dz} = - \int_0^z \mathfrak{R}(u) du + C_1 \quad (9.2-7)$$

where  $u$  is a dummy variable of integration and  $C_1$  is an integration constant. Integration of Eq. (9.2-7) once more leads to

$$\boxed{\int_0^T k(T) dT = - \int_0^z \left[ \int_0^z \mathfrak{R}(u) du \right] dz + C_1 z + C_2} \quad (9.2-8)$$

Evaluation of the constants  $C_1$  and  $C_2$  requires the boundary conditions to be specified. The solution of Eq. (9.2-8) will be presented for two types of boundary conditions, namely, Type I and Type II. In the case of Type I boundary condition, the temperatures at both surfaces are specified. On the other hand, Type II boundary condition implies that while the temperature is specified at one of the surfaces, the other surface is subjected to a constant wall heat flux.

### Type I boundary condition

The solution of Eq. (9.2-8) subject to the boundary conditions

$$\begin{aligned} \text{at } z = 0 & \quad T = T_o \\ \text{at } z = L & \quad T = T_L \end{aligned} \quad (9.2-9)$$

is given by

$$\int_{T_o}^T k(T) dT = - \int_0^z \left[ \int_0^z \mathfrak{R}(u) du \right] dz + \left\{ \int_{T_o}^{T_L} k(T) dT + \int_0^L \left[ \int_0^z \mathfrak{R}(u) du \right] dz \right\} \frac{z}{L} \quad (9.2-10)$$

Note that when  $\mathfrak{R} = 0$ , Eq. (9.2-10) reduces to Eq. (G) in Table 8.1. Equation (9.2-10) may be further simplified depending on whether the thermal conductivity and/or energy generation per unit volume are constant.

■ **Case (i)  $k = \text{constant}$**

In this case Eq. (9.2-10) reduces to

$$k(T - T_o) = - \int_0^z \left[ \int_0^z \mathfrak{R}(u) du \right] dz + \left\{ k(T_L - T_o) + \int_0^L \left[ \int_0^z \mathfrak{R}(u) du \right] dz \right\} \frac{z}{L} \quad (9.2-11)$$

When  $\mathfrak{R} = 0$ , Eq. (9.2-11) reduces to Eq. (H) in Table 8.1.

■ **Case (ii)  $k = \text{constant}$ ;  $\mathfrak{R} = \text{constant}$**

In this case Eq. (9.2-10) simplifies to

$$T = T_o + \frac{\mathfrak{R} L^2}{2k} \left[ \frac{z}{L} - \left( \frac{z}{L} \right)^2 \right] - (T_o - T_L) \frac{z}{L} \quad (9.2-12)$$

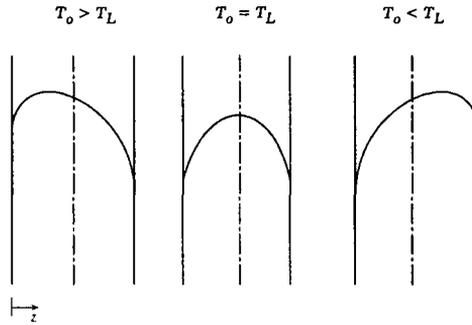
The location of the maximum temperature can be obtained from  $dT/dz = 0$  as

$$\left( \frac{z}{L} \right)_{T=T_{\max}} = \frac{1}{2} - \frac{k}{\mathfrak{R} L^2} (T_o - T_L) \quad (9.2-13)$$

Substitution of Eq. (9.2-13) into Eq. (9.2-12) gives the value of the maximum temperature as

$$T_{\max} = \frac{T_o + T_L}{2} + \frac{\mathfrak{R} L^2}{8k} + \frac{k(T_o - T_L)^2}{2\mathfrak{R} L^2} \quad (9.2-14)$$

The representative temperature profiles depending on the values of  $T_o$  and  $T_L$  are shown in Figure 9.6.



**Figure 9.6** Representative temperature distributions in a rectangular wall with constant generation.

**Type II boundary condition**

The solution of Eq. (9.2-8) subject to the boundary conditions

$$\begin{aligned} \text{at } z = 0 \quad & -k \frac{dT}{dz} = q_o \\ \text{at } z = L \quad & T = T_L \end{aligned} \tag{9.2-15}$$

is given by

$$\int_{T_L}^T k(T) dT = \int_z^L \left[ \int_0^z \mathfrak{R}(u) du \right] dz + q_o L \left( 1 - \frac{z}{L} \right) \tag{9.2-16}$$

Note that when  $\mathfrak{R} = 0$ , Eq. (9.2-16) reduces to Eq. (G) in Table 8.2. Further simplification of Eq. (9.2-16) depending on whether  $k$  and/or  $\mathfrak{R}$  are constant are given below.

■ **Case (i)  $k = \text{constant}$**

In this case Eq. (9.2-16) reduces to

$$k(T - T_L) = \int_z^L \left[ \int_0^z \mathfrak{R}(u) du \right] dz + q_o L \left( 1 - \frac{z}{L} \right) \tag{9.2-17}$$

When  $\mathfrak{R} = 0$ , Eq. (9.2-17) reduces to Eq. (H) in Table 8.2.

■ **Case (ii)  $k = \text{constant}; \mathfrak{R} = \text{constant}$**

In this case Eq. (9.2-16) reduces to

$$T = T_L + \frac{\mathfrak{R} L^2}{2k} \left[ 1 - \left( \frac{z}{L} \right)^2 \right] + \frac{q_o L}{k} \left( 1 - \frac{z}{L} \right) \tag{9.2-18}$$

### 9.2.1.1 Macroscopic equation

The integration of the governing equation, Eq. (9.2-6) over the volume of the system gives

$$-\int_0^L \int_0^W \int_0^H \frac{d}{dz} \left( k \frac{dT}{dz} \right) dx dy dz = \int_0^L \int_0^W \int_0^H \mathfrak{R} dx dy dz \quad (9.2-19)$$

Integration of Eq. (9.2-19) yields

$$\underbrace{WH \left[ \left( -k \frac{dT}{dz} \right)_{z=L} + \left( k \frac{dT}{dz} \right)_{z=0} \right]}_{\text{Net rate of energy out}} = \underbrace{WH \int_0^L \mathfrak{R} dz}_{\text{Rate of energy generation}} \quad (9.2-20)$$

Equation (9.2-20) is simply the macroscopic energy balance under steady conditions by considering the plane wall as a system. Note that energy must leave the system from at least one of the surfaces to maintain steady conditions. The “net rate of energy out” in Eq. (9.2-20) implies the rate of energy leaving the system in excess of the rate of energy entering into it.

It is also possible to make use of Newton’s law of cooling to express the rate of heat loss from the system. If the heat is lost from both surfaces to the surroundings, Eq. (9.2-20) can be written as

$$\langle h_A \rangle (T_o - T_A) + \langle h_B \rangle (T_L - T_B) = \int_0^L \mathfrak{R} dz \quad (9.2-21)$$

where  $T_o$  and  $T_L$  are the surface temperatures at  $z = 0$  and  $z = L$ , respectively.

**Example 9.1** *Energy generation rate as a result of an exothermic reaction is  $1 \times 10^4 \text{ W/m}^3$  in a 50 cm thick wall of thermal conductivity  $20 \text{ W/m.K}$ . The left-face of the wall is insulated while the right-side is held at  $45^\circ\text{C}$  by a coolant. Calculate the maximum temperature in the wall under steady conditions.*

#### Solution

Let  $z$  be the distance measured from the left-face. The use of Eq. (9.2-18) with  $q_o = 0$  gives the temperature distribution as

$$\begin{aligned} T &= T_L + \frac{\mathfrak{R} L^2}{2k} \left[ 1 - \left( \frac{z}{L} \right)^2 \right] \\ &= 45 + \frac{(1 \times 10^4)(0.5)^2}{2(20)} \left[ 1 - \left( \frac{z}{0.5} \right)^2 \right] \end{aligned} \quad (1)$$

Simplification of Eq. (1) leads to

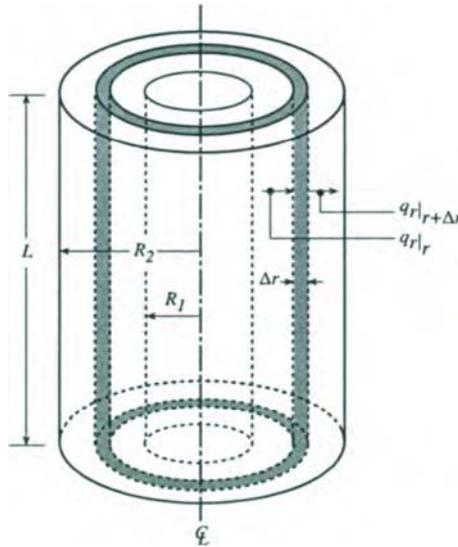
$$T = 107.5 - 250 z^2 \quad (2)$$

Note that  $dT/dz = 0$  at  $z = 0$ . Therefore, the maximum temperature occurs at the insulated surface and its value is  $107.5^\circ\text{C}$ .

### 9.2.2 Conduction in Cylindrical Coordinates

#### 9.2.2.1 Hollow cylinder

Consider one-dimensional transfer of energy in the  $r$ -direction through a hollow cylinder of inner and outer radii of  $R_1$  and  $R_2$ , respectively, as shown in Figure 9.7. Let  $\mathfrak{R}$  be the rate of energy generation per unit volume within the cylinder.



**Figure 9.7** One-dimensional conduction through a hollow cylinder with internal generation.

Since  $T = T(r)$ , Table C.5 in Appendix C indicates that the only non-zero energy flux component is  $e_r$  and it is given by

$$e_r = q_r = -k \frac{dT}{dr} \tag{9.2-22}$$

For a cylindrical differential volume element of thickness  $\Delta r$  as shown in Figure 9.7, the inventory rate equation for energy, Eq. (9.2-1), is expressed as

$$2\pi L (rq_r)|_r - 2\pi L (rq_r)|_{r+\Delta r} + 2\pi r \Delta r L \mathfrak{R} = 0 \tag{9.2-23}$$

Dividing each term by  $2\pi L \Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(rq_r)|_r - (rq_r)|_{r+\Delta r}}{\Delta r} + r \mathfrak{R} = 0 \tag{9.2-24}$$

or,

$$\frac{1}{r} \frac{d}{dr} (rq_r) = \mathfrak{R} \tag{9.2-25}$$

Substitution of Eq. (9.2-22) into Eq. (9.2-25) gives the governing equation for temperature as

$$\boxed{-\frac{1}{r} \frac{d}{dr} \left( rk \frac{dT}{dr} \right) = \mathfrak{R}} \quad (9.2-26)$$

Integration of Eq. (9.2-26) gives

$$k \frac{dT}{dr} = -\frac{1}{r} \int_0^r \mathfrak{R}(u) u \, du + \frac{C_1}{r} \quad (9.2-27)$$

where  $u$  is a dummy variable of integration and  $C_1$  is an integration constant. Integration of Eq. (9.2-27) once more leads to

$$\boxed{\int_0^T k(T) \, dT = -\int_0^r \frac{1}{r} \left[ \int_0^r \mathfrak{R}(u) u \, du \right] dr + C_1 \ln r + C_2} \quad (9.2-28)$$

Evaluation of the constants  $C_1$  and  $C_2$  requires the boundary conditions to be specified.

### Type I boundary condition

The solution of Eq. (9.2-28) subject to the boundary conditions

$$\begin{aligned} \text{at } r = R_1 \quad T = T_1 \\ \text{at } r = R_2 \quad T = T_2 \end{aligned} \quad (9.2-29)$$

is given by

$$\begin{aligned} \int_{T_2}^T k(T) \, dT = \left\{ \int_{T_2}^{T_1} k(T) \, dT - \int_{R_1}^{R_2} \frac{1}{r} \left[ \int_0^r \mathfrak{R}(u) u \, du \right] dr \right\} \frac{\ln(r/R_2)}{\ln(R_1/R_2)} \\ + \int_r^{R_2} \frac{1}{r} \left[ \int_0^r \mathfrak{R}(u) u \, du \right] dr \end{aligned} \quad (9.2-30)$$

Note that when  $\mathfrak{R} = 0$ , Eq. (9.2-30) reduces to Eq. (C) in Table 8.3. Equation (9.2-30) may be further simplified depending on whether the thermal conductivity and/or energy generation per unit volume are constant.

### ■ Case (i) $k = \text{constant}$

In this case Eq. (9.2-30) reduces to

$$\begin{aligned} k(T - T_2) = \left\{ k(T_1 - T_2) - \int_{R_1}^{R_2} \frac{1}{r} \left[ \int_0^r \mathfrak{R}(u) u \, du \right] dr \right\} \frac{\ln(r/R_2)}{\ln(R_1/R_2)} \\ + \int_r^{R_2} \frac{1}{r} \left[ \int_0^r \mathfrak{R}(u) u \, du \right] dr \end{aligned} \quad (9.2-31)$$

When  $\mathfrak{R} = 0$ , Eq. (9.2-31) simplifies to Eq. (D) in Table 8.3.

■ Case (ii)  $k = \text{constant}$ ;  $\mathfrak{R} = \text{constant}$

In this case Eq. (9.2-30) reduces to

$$T = T_2 + \frac{\mathfrak{R} R_2^2}{4k} \left[ 1 - \left( \frac{r}{R_2} \right)^2 \right] + \left\{ T_1 - T_2 - \frac{\mathfrak{R} R_2^2}{4k} \left[ 1 - \left( \frac{R_1}{R_2} \right)^2 \right] \right\} \frac{\ln(r/R_2)}{\ln(R_1/R_2)} \quad (9.2-32)$$

The location of maximum temperature can be obtained from  $dT/dr = 0$  as

$$\left( \frac{r}{R_2} \right)_{T=T_{\max}} = \left\{ \frac{2k(T_1 - T_2) - \frac{1}{2} \left[ 1 - \left( \frac{R_1}{R_2} \right)^2 \right]}{\ln \left( \frac{R_1}{R_2} \right)} \right\}^{1/2} \quad (9.2-33)$$

**Type II boundary condition**

The solution of Eq. (9.2-28) subject to the boundary conditions

$$\begin{aligned} \text{at } r = R_1 & \quad -k \frac{dT}{dz} = q_1 \\ \text{at } r = R_2 & \quad T = T_2 \end{aligned} \quad (9.2-34)$$

is given by

$$\int_{T_2}^T k(T) dT = \int_r^{R_2} \frac{1}{r} \left[ \int_0^r \mathfrak{R}(u) u du \right] dr + \left[ \int_0^{R_1} \mathfrak{R}(u) u du - q_1 R_1 \right] \ln \left( \frac{r}{R_2} \right) \quad (9.2-35)$$

Note that when  $\mathfrak{R} = 0$ , Eq. (9.2-35) reduces to Eq. (C) in Table 8.4.

■ Case (i)  $k = \text{constant}$

In this case Eq. (9.2-35) reduces to

$$k(T - T_2) = \int_r^{R_2} \frac{1}{r} \left[ \int_0^r \mathfrak{R}(u) u du \right] dr + \left[ \int_0^{R_1} \mathfrak{R}(u) u du - q_1 R_1 \right] \ln \left( \frac{r}{R_2} \right) \quad (9.2-36)$$

When  $\mathfrak{R} = 0$ , Eq. (9.2-36) simplifies to Eq. (D) in Table 8.4.

■ Case (ii)  $k = \text{constant}$ ;  $\mathfrak{R} = \text{constant}$

In this case Eq. (9.2-35) simplifies to

$$T = T_2 + \frac{\mathfrak{R} R_2^2}{4k} \left[ 1 - \left( \frac{r}{R_2} \right)^2 \right] + \left( \frac{\mathfrak{R} R_1^2}{2k} - \frac{q_1 R_1}{k} \right) \ln \left( \frac{r}{R_2} \right) \quad (9.2-37)$$

**Macroscopic equation**

The integration of the governing equation, Eq. (9.2-26) over the volume of the system gives the macroscopic energy balance as

$$- \int_0^L \int_0^{2\pi} \int_{R_1}^{R_2} \frac{1}{r} \frac{d}{dr} \left( rk \frac{dT}{dr} \right) r dr d\theta dz = \int_0^L \int_0^{2\pi} \int_{R_1}^{R_2} \mathfrak{R} r dr d\theta dz \quad (9.2-38)$$

Integration of Eq. (9.2-38) yields

$$\underbrace{\left( -k \frac{dT}{dr} \right)_{r=R_2} 2\pi R_2 L + \left( k \frac{dT}{dr} \right)_{r=R_1} 2\pi R_1 L}_{\text{Net rate of energy out}} = \underbrace{2\pi L \int_{R_1}^{R_2} \mathfrak{R} r dr}_{\text{Rate of energy generation}} \quad (9.2-39)$$

Equation (9.2-39) is simply the macroscopic energy balance under steady condition by considering the hollow cylinder as a system.

It is also possible to make use of Newton's law of cooling to express the rate of heat loss from the system. If the heat is lost from both surfaces to the surroundings, Eq. (9.2-39) can be written as

$$R_1 \langle h_A \rangle (T_1 - T_A) + R_2 \langle h_B \rangle (T_2 - T_B) = \int_{R_1}^{R_2} \mathfrak{R} r dr \quad (9.2-40)$$

where  $T_1$  and  $T_2$  are the surface temperatures at  $r = R_1$  and  $r = R_2$ , respectively.

**Example 9.2** *A catalytic reaction is being carried out in a packed bed in the annular space between two concentric cylinders with inner radius  $R_1 = 1.5$  cm and outer radius  $R_2 = 1.8$  cm. The entire surface of the inner cylinder is insulated. The rate of generation of energy per unit volume as a result of a chemical reaction is  $5 \times 10^6$  W/m<sup>3</sup> and it is uniform throughout the annular reactor. The effective thermal conductivity of the bed is 0.5 W/m.K. If the inner surface temperature is measured as 280°C, calculate the temperature of the outer surface.*

**Solution**

The temperature distribution is given by Eq. (9.2-37). Since  $q_1 = 0$ , it reduces to

$$T = T_2 + \frac{\mathfrak{R} R_2^2}{4k} \left[ 1 - \left( \frac{r}{R_2} \right)^2 \right] + \frac{\mathfrak{R} R_1^2}{2k} \ln \left( \frac{r}{R_2} \right) \quad (1)$$

The temperature,  $T_1$ , at  $r = R_1$  is given by

$$T_1 = T_2 + \frac{\Re R_2^2}{4k} \left[ 1 - \left( \frac{R_1}{R_2} \right)^2 \right] + \frac{\Re R_1^2}{2k} \ln \left( \frac{R_1}{R_2} \right) \quad (2)$$

Substitution of the numerical values into Eq. (2) gives

$$280 = T_2 + \frac{(5 \times 10^6)(1.8 \times 10^{-2})^2}{4(0.5)} \left[ 1 - \left( \frac{1.5}{1.8} \right)^2 \right] + \frac{(5 \times 10^6)(1.5 \times 10^{-2})^2}{2(0.5)} \ln \left( \frac{1.5}{1.8} \right) \quad (3)$$

or,

$$T_2 = 237.6^\circ\text{C} \quad (4)$$

### 9.2.2.2 Solid cylinder

Consider a solid cylinder of radius  $R$  with a constant surface temperature of  $T_R$ . The solution obtained for a hollow cylinder, Eq. (9.2-28) is also valid for this case. However, since the temperature must have a finite value at the center, i.e.,  $r = 0$ , then  $C_1$  must be zero and the temperature distribution becomes

$$\int_0^T k(T) dT = - \int_0^r \frac{1}{r} \left[ \int_0^r \Re(u) u du \right] dr + C_2 \quad (9.2-41)$$

The use of the boundary condition

$$\text{at } r = R \quad T = T_R \quad (9.2-42)$$

gives the solution in the form

$$\int_{T_R}^T k(T) dT = \int_r^R \frac{1}{r} \left[ \int_0^r \Re(u) u du \right] dr \quad (9.2-43)$$

#### ■ Case (i) $k = \text{constant}$

Simplification of Eq. (9.2-43) gives

$$k(T - T_R) = \int_r^R \frac{1}{r} \left[ \int_0^r \Re(u) u du \right] dr \quad (9.2-44)$$

#### ■ Case (ii) $k = \text{constant}$ ; $\Re = \text{constant}$

In this case Eq. (9.2-43) simplifies to

$$T = T_R + \frac{\Re R^2}{4k} \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \quad (9.2-45)$$

which implies that the variation of temperature with respect to the radial position is parabolic with the maximum temperature at the center of the pipe.

### Macroscopic equation

The integration of the governing equation, Eq. (9.2-26) over the volume of the system gives the macroscopic energy balance as

$$-\int_0^L \int_0^{2\pi} \int_0^R \frac{1}{r} \frac{d}{dr} \left( r k \frac{dT}{dr} \right) r dr d\theta dz = \int_0^L \int_0^{2\pi} \int_0^R \mathfrak{R} r dr d\theta dz \quad (9.2-46)$$

Integration of Eq. (9.2-46) yields

$$\underbrace{\left( -k \frac{dT}{dr} \right)_{r=R}}_{\text{Rate of energy out}} 2\pi RL = \underbrace{2\pi L \int_0^R \mathfrak{R} r dr}_{\text{Rate of energy generation}} \quad (9.2-47)$$

Equation (9.2-47) is the macroscopic energy balance under steady conditions by considering the solid cylinder as a system. It is also possible to make use of Newton's law of cooling to express the rate of heat loss from the system to the surroundings at  $T_\infty$  with an average heat transfer coefficient  $\langle h \rangle$ . In this case Eq. (9.2-47) reduces to

$$R \langle h \rangle (T_R - T_\infty) = \int_0^R \mathfrak{R} r dr \quad (9.2-48)$$

**Example 9.3** *Rate of heat generation per unit volume,  $\mathfrak{R}_e$ , during the transmission of an electric current through wires is given by*

$$\mathfrak{R}_e = \frac{1}{k_e} \left( \frac{I}{\pi R^2} \right)^2$$

where  $I$  is the current,  $k_e$  is the electrical conductivity, and  $R$  is the radius of the wire.

a) Obtain an expression for the difference between the maximum and the surface temperatures of the wire.

b) Develop a correlation that will permit the selection of the electric current and the wire diameter if the difference between the maximum and the surface temperatures is specified. If the wire must carry a larger current, should the wire have a larger or smaller diameter?

### Solution

#### Assumption

1. The thermal conductivity and the electrical conductivity of the wire are constant.

**Analysis**

a) The temperature distribution is given by Eq. (9.2-45) as

$$T = T_R + \frac{\mathfrak{R}_e R^2}{4k} \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \quad (1)$$

where  $T_R$  is the surface temperature. The maximum temperature occurs at  $r = 0$ , i.e.,

$$T_{\max} = T_R + \frac{\mathfrak{R}_e R^2}{4k} \quad (2)$$

or,

$$T_{\max} - T_R = \frac{\mathfrak{R}_e R^2}{4k} \quad (3)$$

b) Expressing  $\mathfrak{R}_e$  in terms of  $I$  and  $k_e$  gives

$$T_{\max} - T_R = \left( \frac{1}{4\pi k k_e} \right) \frac{I^2}{R^2} \quad (4)$$

Therefore, if  $I$  increases,  $R$  must be increased in order to keep  $T_{\max} - T_R$  constant.

**Example 9.4** Energy is generated in a cylindrical nuclear fuel element of radius  $R_F$  at a rate of

$$\mathfrak{R} = \mathfrak{R}_o(1 + \beta r^2)$$

It is clad in a material of radius  $R_C$  and the outside surface temperature is kept constant at  $T_o$  by a coolant. Determine the steady temperature distribution in the fuel element.

**Solution**

The temperature distribution within the fuel element can be determined from Eq. (9.2-44), i.e.,

$$k_F(T^F - T_i) = \mathfrak{R}_o \int_r^{R_F} \frac{1}{r} \left[ \int_0^r (1 + \beta u^2) u du \right] dr \quad (1)$$

or,

$$T^F = T_i + \frac{\mathfrak{R}_o R_F^2}{4k_F} \left\{ 1 - \left( \frac{r}{R_F} \right)^2 + \frac{\beta R_F^2}{4} \left[ 1 - \left( \frac{r}{R_F} \right)^4 \right] \right\} \quad (2)$$

in which the interface temperature  $T_i$  at  $r = R_F$  is not known. To express  $T_i$  in terms of known quantities, consider the temperature distribution in a cladding. Since there is no internal generation within the cladding, the use of Eq. (D) in Table 8.3 gives

$$\frac{T_o - T^C}{T_o - T_i} = \frac{\ln(r/R_C)}{\ln(R_F/R_C)} \quad (3)$$

The energy flux at  $r = R_F$  is continuous, i.e.,

$$-k_F \frac{dT^F}{dr} = -k_C \frac{dT^C}{dr} \quad (4)$$

Substitution of Eqs. (2) and (3) into Eq. (4) gives

$$T_i = T_o + \frac{\mathfrak{R}_o R_F^2 \ln(R_C/R_F)}{2k_C} \left(1 + \frac{\beta R_F^2}{2}\right) \quad (5)$$

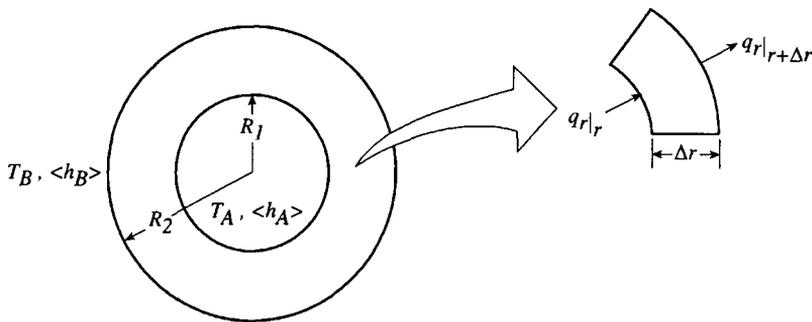
Therefore, the temperature distribution given by Eq. (2) becomes

$$T^F - T_o = \frac{\mathfrak{R}_o R_F^2}{4k_F} \left\{ 1 - \left(\frac{r}{R_F}\right)^2 + \frac{\beta R_F^2}{4} \left[ 1 - \left(\frac{r}{R_F}\right)^4 \right] \right\} + \frac{\mathfrak{R}_o R_F^2 \ln(R_C/R_F)}{2k_C} \left(1 + \frac{\beta R_F^2}{2}\right) \quad (6)$$

## 9.2.3 Conduction in Spherical Coordinates

### 9.2.3.1 Hollow sphere

Consider one-dimensional transfer of energy in the  $r$ -direction through a hollow sphere of inner and outer radii of  $R_1$  and  $R_2$ , respectively, as shown in Figure 9.8. Let  $\mathfrak{R}$  be the rate of generation per unit volume within the sphere.



**Figure 9.8** One-dimensional conduction through a hollow sphere with internal generation.

Since  $T = T(r)$ , Table C.6 in Appendix C indicates that the only non-zero energy flux component is  $e_r$  and it is given by

$$e_r = q_r = -k \frac{dT}{dr} \quad (9.2-49)$$

For a spherical differential volume of thickness  $\Delta r$  as shown in Figure 9.8, the inventory rate equation for energy, Eq. (9.2-1), is expressed as

$$4\pi (r^2 q_r)|_r - 4\pi (r^2 q_r)|_{r+\Delta r} + 4\pi r^2 \Delta r \mathfrak{R} = 0 \tag{9.2-50}$$

Dividing each term by  $4\pi\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(r^2 q_r)|_r - (r^2 q_r)|_{r+\Delta r}}{\Delta r} + r^2 \mathfrak{R} = 0 \tag{9.2-51}$$

or,

$$\frac{1}{r^2} \frac{d}{dr} (r^2 q_r) = \mathfrak{R} \tag{9.2-52}$$

Substitution of Eq. (9.2-49) into Eq. (9.2-52) gives the governing equation for temperature as

$$\boxed{-\frac{1}{r^2} \frac{d}{dr} \left( r^2 k \frac{dT}{dr} \right) = \mathfrak{R}} \tag{9.2-53}$$

Integration of Eq. (9.2-53) gives

$$k \frac{dT}{dr} = -\frac{1}{r^2} \int_0^r \mathfrak{R}(u) u^2 du + \frac{C_1}{r^2} \tag{9.2-54}$$

where  $u$  is the dummy variable of integration. Integration of Eq. (9.2-54) once more leads to

$$\boxed{\int_0^T k(T) dT = -\int_0^r \frac{1}{r^2} \left[ \int_0^r \mathfrak{R}(u) u^2 du \right] dr - \frac{C_1}{r} + C_2} \tag{9.2-55}$$

Evaluation of the constants  $C_1$  and  $C_2$  requires the boundary conditions to be specified.

**Type I boundary condition**

The solution of Eq. (9.2-55) subject to the boundary conditions

$$\begin{aligned} \text{at } r = R_1 \quad T = T_1 \\ \text{at } r = R_2 \quad T = T_2 \end{aligned} \tag{9.2-56}$$

is given by

$$\begin{aligned} \int_{T_2}^T k(T) dT = \left\{ \int_{T_2}^{T_1} k(T) dT - \int_{R_1}^{R_2} \frac{1}{r^2} \left[ \int_0^r \mathfrak{R}(u) u^2 du \right] dr \right\} \frac{\frac{1}{R_2} - \frac{1}{r}}{\frac{1}{R_2} - \frac{1}{R_1}} \\ + \int_r^{R_2} \frac{1}{r^2} \left[ \int_0^r \mathfrak{R}(u) u^2 du \right] dr \end{aligned} \tag{9.2-57}$$

Note that when  $\mathfrak{R} = 0$ , Eq. (9.2-57) reduces to Eq. (C) in Table 8.5. Further simplification of Eq. (9.2-57) depends on the functional forms of  $k$  and  $\mathfrak{R}$ .

■ Case (i)  $k = \text{constant}$

In this case Eq. (9.2-57) reduces to

$$k(T - T_2) = \left\{ k(T_1 - T_2) - \int_{R_1}^{R_2} \frac{1}{r^2} \left[ \int_0^r \mathfrak{R}(u) u^2 du \right] dr \right\} \frac{\frac{1}{R_2} - \frac{1}{r}}{\frac{1}{R_2} - \frac{1}{R_1}} + \int_r^{R_2} \frac{1}{r^2} \left[ \int_0^r \mathfrak{R}(u) u^2 du \right] dr \quad (9.2-58)$$

When  $\mathfrak{R} = 0$ , Eq. (9.2-58) reduces to Eq. (D) in Table 8.5.

■ Case (ii)  $k = \text{constant}$ ;  $\mathfrak{R} = \text{constant}$

In this case Eq. (9.2-57) simplifies to

$$T = T_2 + \left\{ T_1 - T_2 - \frac{\mathfrak{R} R_2^2}{6k} \left[ 1 - \left( \frac{R_1}{R_2} \right)^2 \right] \right\} \frac{\frac{1}{R_2} - \frac{1}{r}}{\frac{1}{R_2} - \frac{1}{R_1}} + \frac{\mathfrak{R} R_2^2}{6k} \left[ 1 - \left( \frac{r}{R_2} \right)^2 \right] \quad (9.2-59)$$

**Type II boundary condition**

The solution of Eq. (9.2-55) subject to the boundary conditions

$$\begin{aligned} \text{at } r = R_1 & \quad -k \frac{dT}{dz} = q_1 \\ \text{at } r = R_2 & \quad T = T_2 \end{aligned} \quad (9.2-60)$$

is given by

$$\int_{T_2}^T k(T) dT = \int_r^{R_2} \frac{1}{r^2} \left[ \int_0^r \mathfrak{R}(u) u^2 du \right] dr + \left[ q_1 R_1^2 - \int_0^{R_1} \mathfrak{R}(u) u^2 du \right] \left( \frac{1}{r} - \frac{1}{R_2} \right) \quad (9.2-61)$$

Note that when  $\mathfrak{R} = 0$ , Eq. (9.2-61) reduces to Eq. (C) in Table 8.6. Further simplification of Eq. (9.2-61) depends on the functional forms of  $k$  and  $\mathfrak{R}$ .

■ Case (i)  $k = \text{constant}$

In this case Eq. (9.2-61) reduces to

$$k(T - T_2) = \int_r^{R_2} \frac{1}{r^2} \left[ \int_0^r \mathfrak{R}(u)u^2 du \right] dr + \left[ q_1 R_1^2 - \int_0^{R_1} \mathfrak{R}(u)u^2 du \right] \left( \frac{1}{r} - \frac{1}{R_2} \right) \tag{9.2-62}$$

Note that when  $\mathfrak{R} = 0$ , Eq. (9.2-62) reduces to Eq. (D) in Table 8.6

■ Case (ii)  $k = \text{constant}; \mathfrak{R} = \text{constant}$

In this case Eq. (9.2-61) simplifies to

$$T = T_2 + \frac{\mathfrak{R} R_2^2}{6k} \left[ 1 - \left( \frac{r}{R_2} \right)^2 \right] + \left( \frac{q_1 R_1^2}{k} - \frac{\mathfrak{R} R_1^3}{3k} \right) \left( \frac{1}{r} - \frac{1}{R_2} \right) \tag{9.2-63}$$

**Macroscopic equation**

The integration of the governing equation, Eq. (9.2-53) over the volume of the system gives the macroscopic energy balance as

$$- \int_0^{2\pi} \int_0^\pi \int_{R_1}^{R_2} \frac{1}{r^2} \frac{d}{dr} \left( r^2 k \frac{dT}{dr} \right) r^2 \sin \theta dr d\theta d\phi = \int_0^{2\pi} \int_0^\pi \int_{R_1}^{R_2} \mathfrak{R} r^2 \sin \theta dr d\theta d\phi \tag{9.2-64}$$

Integration of Eq. (9.2-64) yields

$$\underbrace{\left( -k \frac{dT}{dr} \right)_{r=R_2} 4\pi R_2^2 + \left( k \frac{dT}{dr} \right)_{r=R_1} 4\pi R_1^2}_{\text{Net rate of energy out}} = \underbrace{4\pi \int_{R_1}^{R_2} \mathfrak{R} r^2 dr}_{\text{Rate of energy generation}} \tag{9.2-65}$$

Equation (9.2-65) is the macroscopic energy balance under steady conditions by considering the hollow sphere as a system.

It is also possible to make use of the Newton’s law of cooling to express the rate of heat loss from the system. If heat is lost from both surfaces, Eq. (9.2-65) can be written as

$$R_1^2 \langle h_A \rangle (T_1 - T_A) + R_2^2 \langle h_B \rangle (T_2 - T_B) = \int_{R_1}^{R_2} \mathfrak{R} r^2 dr \tag{9.2-66}$$

where  $T_1$  and  $T_2$  are the surface temperatures at  $r = R_1$  and  $r = R_2$ , respectively.

### 9.2.3.2 Solid sphere

Consider a solid sphere of radius  $R$  with a constant surface temperature of  $T_R$ . The solution obtained for a hollow sphere, Eq. (9.2-55) is also valid for this case. However, since the temperature must have a finite value at the center, i.e.,  $r = 0$ , then  $C_1$  must be zero and the temperature distribution becomes

$$\int_0^T k(T) dT = - \int_0^r \frac{1}{r^2} \left[ \int_0^r \Re(u) u^2 du \right] dr + C_2 \quad (9.2-67)$$

The use of the boundary condition

$$\text{at } r = R \quad T = T_R \quad (9.2-68)$$

gives the solution in the form

$$\int_{T_R}^T k(T) dT = \int_r^R \frac{1}{r^2} \left[ \int_0^r \Re(u) u^2 du \right] dr \quad (9.2-69)$$

#### ■ Case (i) $k = \text{constant}$

Simplification of Eq. (9.2-69) gives

$$k(T - T_R) = \int_r^R \frac{1}{r^2} \left[ \int_0^r \Re(u) u^2 du \right] dr \quad (9.2-70)$$

#### ■ Case (ii) $k = \text{constant}; \Re = \text{constant}$

In this case Eq. (9.2-69) simplifies to

$$T = T_R + \frac{\Re R^2}{6k} \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \quad (9.2-71)$$

which implies that the variation of temperature with respect to the radial position is parabolic with the maximum temperature at the center of the sphere.

### Macroscopic equation

The integration of the governing equation, Eq. (9.2-53) over the volume of the system gives the macroscopic energy balance as

$$- \int_0^{2\pi} \int_0^\pi \int_0^R \frac{1}{r^2} \frac{d}{dr} \left( r^2 k \frac{dT}{dr} \right) r^2 \sin \theta dr d\theta d\phi = \int_0^{2\pi} \int_0^\pi \int_0^R \Re r^2 \sin \theta dr d\theta d\phi \quad (9.2-72)$$

Integration of Eq. (9.2-72) yields

$$\underbrace{\left( -k \frac{dT}{dr} \right)_{r=R}}_{\text{Rate of energy out}} \quad 4\pi R^2 = \underbrace{4\pi \int_0^R \Re r^2 dr}_{\text{Rate of energy generation}} \quad (9.2-73)$$

Equation (9.2-73) is the macroscopic energy balance under steady conditions by considering the solid sphere as a system. It is also possible to make use of Newton's law of cooling to express the rate of heat loss from the system to the surroundings at  $T_\infty$  with an average heat transfer coefficient  $\langle h \rangle$ . In this case Eq. (9.2-73) reduces to

$$R^2 \langle h \rangle (T_R - T_\infty) = \int_0^R \mathfrak{R} r^2 dr \quad (9.2-74)$$

**Example 9.5** Consider Example 3.2 in which energy generation as a result of fission within a spherical reactor of radius  $R$  is given as

$$\mathfrak{R} = \mathfrak{R}_o \left[ 1 - \left( \frac{r}{R} \right)^2 \right]$$

Cooling fluid at a temperature of  $T_\infty$  flows over a reactor with an average heat transfer coefficient of  $\langle h \rangle$ . Determine the temperature distribution and the rate of heat loss from the reactor surface.

### Solution

The temperature distribution within the reactor can be calculated from Eq. (9.2-70). Note that

$$\begin{aligned} \int_0^r \mathfrak{R}(u) u^2 du &= \mathfrak{R}_o \int_0^r \left[ 1 - \left( \frac{u}{R} \right)^2 \right] u^2 du \\ &= \mathfrak{R}_o \left( \frac{r^3}{3} - \frac{r^5}{5R^2} \right) \end{aligned} \quad (1)$$

Substitution of Eq. (1) into Eq. (9.2-70) gives

$$k(T - T_R) = \mathfrak{R}_o \int_r^R \frac{1}{r^2} \left( \frac{r^3}{3} - \frac{r^5}{5R^2} \right) dr \quad (2)$$

Evaluation of the integration gives the temperature distribution as

$$T = T_R + \frac{7}{60} \frac{\mathfrak{R}_o R^2}{k} - \frac{\mathfrak{R}_o R^2}{2k} \left[ \frac{1}{3} \left( \frac{r}{R} \right)^2 - \frac{1}{10} \left( \frac{r}{R} \right)^4 \right] \quad (3)$$

This result, however, contains an unknown quantity  $T_R$ . Therefore, it is necessary to express  $T_R$  in terms of the known quantities, i.e.,  $T_\infty$  and  $\langle h \rangle$ .

One way of calculating the surface temperature,  $T_R$ , is to use the macroscopic energy balance given by Eq. (9.2-74), i.e.,

$$R^2 \langle h \rangle (T_R - T_\infty) = \mathfrak{R}_o \int_0^R \left[ 1 - \left( \frac{r}{R} \right)^2 \right] r^2 dr \quad (4)$$

Equation (4) gives the surface temperature as

$$T_R = T_\infty + \frac{2}{15} \frac{\Re_o R}{\langle h \rangle} \quad (5)$$

Another way of calculating the surface temperature is to equate Newton's law of cooling and Fourier's law of heat conduction at the surface of the sphere, i.e.,

$$\langle h \rangle (T_R - T_\infty) = -k \left. \frac{dT}{dr} \right|_{r=R} \quad (6)$$

From Eq. (3)

$$\left. \frac{dT}{dr} \right|_{r=R} = -\frac{2 \Re_o R^2}{15 k} \quad (7)$$

Substituting Eq. (7) into Eq. (6) and solving for  $T_R$  results in Eq. (5).

Therefore, the temperature distribution within the reactor in terms of the known quantities is given by

$$T = T_\infty + \frac{2}{15} \frac{\Re_o R}{\langle h \rangle} + \frac{7}{60} \frac{\Re_o R^2}{k} - \frac{\Re_o R^2}{2k} \left[ \frac{1}{3} \left( \frac{r}{R} \right)^2 - \frac{1}{10} \left( \frac{r}{R} \right)^4 \right] \quad (8)$$

The rate of heat loss can be calculated from Eq. (9.2-73) as

$$\begin{aligned} \dot{Q}_{loss} &= 4\pi \Re_o \int_0^R \left[ 1 - \left( \frac{r}{R} \right)^2 \right] r^2 dr \\ &= \frac{8\pi}{15} \Re_o R^3 \end{aligned} \quad (9)$$

Note that the calculation of the rate of heat loss does not require the temperature distribution to be known.

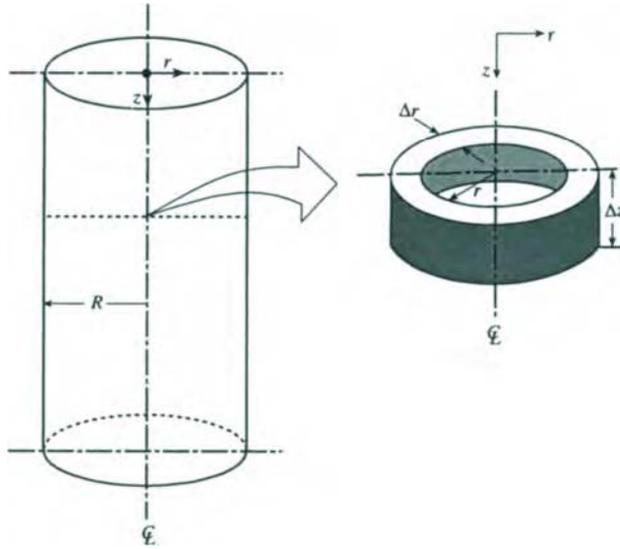
## 9.3 HEAT TRANSFER WITH CONVECTION

### 9.3.1 Laminar Flow Forced Convection in a Pipe

Consider the laminar flow of an incompressible Newtonian fluid in a circular pipe under the action of a pressure gradient as shown in Figure 9.9. The velocity distribution is given by Eqs. (9.1-79) and (9.1-84) as

$$v_z = 2 \langle v_z \rangle \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \quad (9.3-1)$$

Suppose that the fluid, which is at a uniform temperature of  $T_o$  for  $z < 0$ , is started to be heated for  $z > 0$  and we want to develop the governing equation for temperature.



**Figure 9.9** Forced convection heat transfer in a pipe.

In general,  $T = T(r, z)$  and from Table C.5 in Appendix C, the non-zero energy flux components are

$$e_r = -k \frac{\partial T}{\partial r} \tag{9.3-2}$$

$$e_z = -k \frac{\partial T}{\partial z} + (\rho \hat{C}_P T) v_z \tag{9.3-3}$$

Since there is no generation of energy, Eq. (9.2-1) simplifies to

$$(\text{Rate of energy in}) - (\text{Rate of energy out}) = 0 \tag{9.3-4}$$

For a cylindrical differential volume element of thickness  $\Delta r$  and length  $\Delta z$ , as shown in Figure 9.9, Eq. (9.3-4) is expressed as

$$(e_r|_r 2\pi r \Delta z + e_z|_z 2\pi r \Delta r) - [e_r|_{r+\Delta r} 2\pi(r + \Delta r) \Delta z + e_z|_{z+\Delta z} 2\pi r \Delta r] = 0 \tag{9.3-5}$$

Dividing Eq. (9.3-5) by  $2\pi \Delta r \Delta z$  and taking the limit as  $\Delta r \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(re_r)|_r - (re_r)|_{r+\Delta r}}{\Delta r} + \lim_{\Delta z \rightarrow 0} r \frac{e_z|_z - e_z|_{z+\Delta z}}{\Delta z} = 0 \tag{9.3-6}$$

or,

$$\frac{1}{r} \frac{\partial (re_r)}{\partial r} + \frac{\partial e_z}{\partial z} = 0 \tag{9.3-7}$$

Substitution of Eqs. (9.3-2) and (9.3-3) into Eq. (9.3-7) yields

$$\underbrace{\rho \hat{C}_P v_z \frac{\partial T}{\partial z}}_{\text{Convection in } z\text{-direction}} = \underbrace{\frac{k}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right)}_{\text{Conduction in } r\text{-direction}} + \underbrace{k \frac{\partial^2 T}{\partial z^2}}_{\text{Conduction in } z\text{-direction}} \quad (9.3-8)$$

Note that in the  $z$ -direction energy is transported both by convection and conduction. As stated by Eq. (2.4-8), conduction can be considered negligible with respect to convection when  $\text{Pe}_H \gg 1$ . Under these circumstances, Eq. (9.3-8) reduces to

$$\boxed{\rho \hat{C}_P v_z \frac{\partial T}{\partial z} = \frac{k}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right)} \quad (9.3-9)$$

As an engineer, we are interested in the variation of the bulk fluid temperature,  $T_b$ , rather than the local temperature,  $T$ . For forced convection heat transfer in a circular pipe of radius  $R$ , the bulk fluid temperature defined by Eq. (4.1-2) takes the form

$$T_b = \frac{\int_0^{2\pi} \int_0^R v_z T r \, dr d\theta}{\int_0^{2\pi} \int_0^R v_z r \, dr d\theta} \quad (9.3-10)$$

Note that while the fluid temperature,  $T$ , depends on both the radial and the axial coordinates, the bulk temperature,  $T_b$ , depends only on the axial direction.

To determine the governing equation for the bulk temperature, it is necessary to integrate Eq. (9.3-9) over the cross-sectional area of the pipe, i.e.,

$$\rho \hat{C}_P \int_0^{2\pi} \int_0^R v_z \frac{\partial T}{\partial z} r \, dr d\theta = k \int_0^{2\pi} \int_0^R \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) r \, dr d\theta \quad (9.3-11)$$

Since  $v_z \neq v_z(z)$ , the integral on the left-side of Eq. (9.3-11) can be rearranged as

$$\begin{aligned} \int_0^{2\pi} \int_0^R v_z \frac{\partial T}{\partial z} r \, dr d\theta &= \int_0^{2\pi} \int_0^R \frac{\partial(v_z T)}{\partial z} r \, dr d\theta \\ &= \frac{d}{dz} \left( \int_0^{2\pi} \int_0^R v_z T r \, dr d\theta \right) \end{aligned} \quad (9.3-12)$$

Substitution of Eq. (9.3-10) into Eq. (9.3-12) yields

$$\begin{aligned} \int_0^{2\pi} \int_0^R v_z \frac{\partial T}{\partial z} r \, dr d\theta &= \frac{d}{dz} \left( \underbrace{T_b \int_0^{2\pi} \int_0^R v_z r \, dr d\theta}_{\langle v_z \rangle \pi R^2} \right) \\ &= \frac{\dot{m}}{\rho} \frac{dT_b}{dz} \end{aligned} \quad (9.3-13)$$

where  $\dot{m}$  is the mass flow rate given by

$$\dot{m} = \rho \langle v_z \rangle \pi R^2 \quad (9.3-14)$$

On the other hand, since  $\partial T / \partial r = 0$  as a result of the symmetry condition at the center of the tube, the integral on the right-side of Eq. (9.3-11) takes the form

$$\int_0^{2\pi} \int_0^R \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) r \, dr \, d\theta = 2\pi R \left. \frac{\partial T}{\partial r} \right|_{r=R} \quad (9.3-15)$$

Substitution of Eqs. (9.3-13) and (9.3-15) into Eq. (9.3-11) gives the governing equation for the bulk temperature in the form

$$\boxed{\dot{m} \hat{C}_P \frac{dT_b}{dz} = \pi D k \left. \frac{\partial T}{\partial r} \right|_{r=R}} \quad (9.3-16)$$

The solution of Eq. (9.3-16) requires the boundary conditions associated with the problem to be known. The two most commonly used boundary conditions are the *constant wall temperature* and *constant wall heat flux*.

### Constant wall temperature

Constant wall temperature occurs in evaporators and condensers in which phase change takes place on one side of the surface. The heat flux at the wall can be represented either by Fourier's law of heat conduction or by Newton's law of cooling, i.e.,

$$q_r|_{r=R} = k \left. \frac{\partial T}{\partial r} \right|_{r=R} = h (T_w - T_b) \quad (9.3-17)$$

It is implicitly implied in writing Eq. (9.3-17) that the temperature increases in the radial direction. Substitution of Eq. (9.3-17) into Eq. (9.3-16) and rearrangement yields

$$\dot{m} \hat{C}_P \int_{T_{b,in}}^{T_b} \frac{dT_b}{T_w - T_b} = \pi D \int_0^z h \, dz \quad (9.3-18)$$

Since the wall temperature,  $T_w$ , is constant, integration of Eq. (9.3-18) yields

$$\dot{m} \hat{C}_P \ln \left( \frac{T_w - T_b}{T_w - T_{b,in}} \right) = \pi D \langle h \rangle_z z \quad (9.3-19)$$

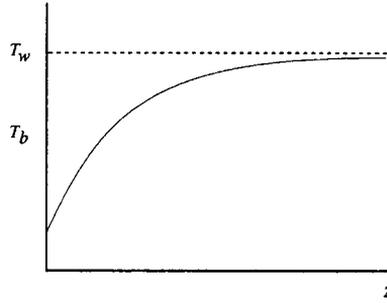
in which  $\langle h \rangle_z$  is the average heat transfer coefficient from the entrance to the point  $z$  defined by

$$\langle h \rangle_z = \frac{1}{z} \int_0^z h \, dz \quad (9.3-20)$$

If Eq. (9.3-19) is solved for  $T_b$ , the result is

$$T_b = T_w - (T_w - T_{b,in}) \exp \left[ - \left( \frac{\pi D \langle h \rangle_z}{\dot{m} \hat{C}_P} \right) z \right] \quad (9.3-21)$$

which indicates that the bulk fluid temperature varies exponentially with the axial direction as shown in Figure 9.10.



**Figure 9.10** Variation of the bulk temperature with the axial direction for a constant wall temperature.

Evaluation of Eq. (9.3-19) over the total length,  $L$ , of the pipe gives

$$\dot{m} \hat{C}_P \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) = \pi D \langle h \rangle L \quad (9.3-22)$$

where

$$\langle h \rangle = \frac{1}{L} \int_0^L h dz \quad (9.3-23)$$

If Eq. (9.3-22) is solved for  $T_{b_{out}}$ , the result is

$$T_{b_{out}} = T_w - (T_w - T_{b_{in}}) \exp \left[ - \left( \frac{\pi D \langle h \rangle}{\dot{m} \hat{C}_P} \right) L \right] \quad (9.3-24)$$

Equation (9.3-24) can be expressed in terms of dimensionless numbers with the help of Eq. (3.4-5), i.e.,

$$\begin{aligned} \text{St}_H &= \frac{\text{Nu}}{\text{Re Pr}} = \frac{\langle h \rangle}{\rho \langle v_z \rangle \hat{C}_P} \\ &= \frac{\langle h \rangle}{[\dot{m}/(\pi D^2/4)] \hat{C}_P} \end{aligned} \quad (9.3-25)$$

The use of Eq. (9.3-25) in Eq. (9.3-24) gives

$$T_{b_{out}} = T_w - (T_w - T_{b_{in}}) \exp \left[ - \frac{4 \text{Nu}(L/D)}{\text{Re Pr}} \right] \quad (9.3-26)$$

As an engineer, we are interested in the rate of heat transferred to the fluid, i.e.,

$$\dot{Q} = \dot{m} \hat{C}_P (T_{b_{out}} - T_{b_{in}}) = \dot{m} \hat{C}_P [(T_w - T_{b_{in}}) - (T_w - T_{b_{out}})] \quad (9.3-27)$$

Substitution of Eq. (9.3-22) into Eq. (9.3-27) results in

$$\dot{Q} = (\pi DL)\langle h \rangle \left[ \frac{(T_w - T_{b_{in}}) - (T_w - T_{b_{out}})}{\ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right)} \right] \quad (9.3-28)$$

Note that Eq. (9.3-28) can be expressed in the form

$$\dot{Q} = A_H \langle h \rangle (\Delta T)_{ch} = (\pi DL)\langle h \rangle \Delta T_{LM} \quad (9.3-29)$$

which is identical with Eqs. (3.2-7) and (4.5-29).

### Constant wall heat flux

Constant wall heat flux type boundary condition is encountered when electrical resistance is wrapped around the pipe. Since the heat flux at the wall is constant, then

$$q_r|_{r=R} = k \left. \frac{\partial T}{\partial r} \right|_{r=R} = q_w = \text{constant} \quad (9.3-30)$$

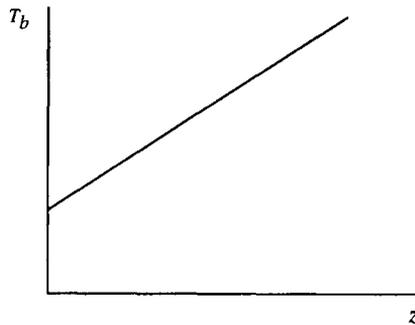
Substitution of Eq. (9.3-30) into Eq. (9.3-16) gives

$$\frac{dT_b}{dz} = \frac{\pi D q_w}{\dot{m} \hat{C}_P} = \text{constant} \quad (9.3-31)$$

Integration of Eq. (9.3-31) gives the variation of the bulk temperature in the axial direction as

$$T_b = T_{b_{in}} + \left( \frac{\pi D q_w}{\dot{m} \hat{C}_P} \right) z \quad (9.3-32)$$

Therefore, the bulk fluid temperature varies linearly in the axial direction as shown in Figure 9.11.



**Figure 9.11** Variation of the bulk temperature with the axial direction for a constant wall heat flux.

Evaluation of Eq. (9.3-32) over the total length gives the bulk temperature at the exit of the pipe as

$$\begin{aligned} T_{b_{out}} &= T_{b_{in}} + \left( \frac{\pi D q_w}{\dot{m} \hat{C}_P} \right) L \\ &= T_{b_{in}} + \frac{4 q_w L}{k \text{Re Pr}} \end{aligned} \quad (9.3-33)$$

The rate of heat transferred to the fluid is given by

$$\dot{Q} = \dot{m} \hat{C}_P (T_{b_{out}} - T_{b_{in}}) \quad (9.3-34)$$

Substitution of Eq. (9.3-33) into Eq. (9.3-34) yields

$$\dot{Q} = (\pi D L) q_w \quad (9.3-35)$$

### 9.3.1.1 Thermally developed flow

As stated in Section 8.1, when the fluid velocity is no longer dependent on the axial direction  $z$ , the flow is said to be hydrodynamically fully developed. In the case of heat transfer, if the ratio

$$\frac{T - T_b}{T_w - T_b} \quad (9.3-36)$$

does not vary along the axial direction, then the temperature profile is said to be fully developed.

It is important to note that although the fluid temperature,  $T$ , bulk fluid temperature,  $T_b$ , and wall temperature,  $T_w$ , may change along the axial direction, the ratio given in Eq. (9.3-36) is independent of the axial coordinate<sup>2</sup>, i.e.,

$$\frac{\partial}{\partial z} \left( \frac{T - T_b}{T_w - T_b} \right) = 0 \quad (9.3-37)$$

Equation (9.3-37) indicates that

$$\frac{\partial T}{\partial z} = \left( \frac{T_w - T}{T_w - T_b} \right) \frac{dT_b}{dz} + \left( \frac{T - T_b}{T_w - T_b} \right) \frac{dT_w}{dz} \quad (9.3-38)$$

**Example 9.6** For a thermally developed flow of a fluid with constant physical properties, show that the heat transfer coefficient is constant.

<sup>2</sup>In the literature, the condition for the *thermally developed flow* is also given in the form

$$\frac{\partial}{\partial z} \left( \frac{T_w - T}{T_w - T_b} \right) = 0$$

Note that

$$\frac{T_w - T}{T_w - T_b} = 1 - \frac{T - T_b}{T_w - T_b}$$

**Solution**

For a thermally developed flow, the ratio given in Eq. (9.3-36) depends only on the radial coordinate  $r$ , i.e.,

$$\frac{T - T_b}{T_w - T_b} = f(r) \quad (1)$$

Differentiation of Eq. (1) with respect to  $r$  gives

$$\frac{\partial T}{\partial r} = (T_w - T_b) \frac{df}{dr} \quad (2)$$

which is valid at all points within the flow field. Evaluation of Eq. (2) at the surface of the pipe yields

$$\left. \frac{\partial T}{\partial r} \right|_{r=R} = (T_w - T_b) \left. \frac{df}{dr} \right|_{r=R} \quad (3)$$

On the other hand, the heat flux at the wall is expressed as

$$q_r|_{r=R} = k \left. \frac{\partial T}{\partial r} \right|_{r=R} = h(T_w - T_b) \quad (4)$$

Substitution of Eq. (3) into Eq. (4) gives

$$h = k \left. \frac{df}{dr} \right|_{r=R} = \text{constant} \quad (5)$$

**Example 9.7** For a thermally developed flow, show that the temperature gradient in the axial direction,  $\partial T/\partial z$ , remains constant for a constant wall heat flux.

**Solution**

The heat flux at the wall is given by

$$q_r|_{r=R} = h(T_w - T_b) = \text{constant} \quad (1)$$

Since  $h$  is constant for a thermally developed flow, Eq. (1) implies that

$$T_w - T_b = \text{constant} \quad (2)$$

or,

$$\frac{dT_w}{dz} = \frac{dT_b}{dz} \quad (3)$$

Therefore, Eq. (9.3-38) simplifies to

$$\frac{\partial T}{\partial z} = \frac{dT_b}{dz} = \frac{dT_w}{dz} \quad (4)$$

Since  $dT_b/dz$  is constant according to Eq. (9.3-31),  $\partial T/\partial z$  also remains constant, i.e.,

$$\frac{\partial T}{\partial z} = \frac{dT_b}{dz} = \frac{dT_w}{dz} = \frac{\pi D q_w}{m \hat{C}_P} = \text{constant} \quad (5)$$

### 9.3.1.2 Nusselt number for a thermally developed flow

Substitution of Eq. (9.3-1) into Eq. (9.3-9) gives

$$2\rho\hat{C}_P\langle v_z \rangle \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \frac{\partial T}{\partial z} = \frac{k}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \quad (9.3-39)$$

It should always be kept in mind that the purpose of solving the above equation for temperature distribution is to obtain a correlation to use in the design of heat transfer equipment, such as, heat exchangers and evaporators. As shown in Chapter 4, heat transfer correlations are expressed in terms of the Nusselt number. Therefore, Eq. (9.3-39) will be solved for a thermally developed flow for two different types of boundary conditions, i.e., constant wall heat flux and constant wall temperature, to determine the Nusselt number.

#### Constant wall heat flux

In the case of a constant wall heat flux, as shown in Example 9.7, the temperature gradient in the axial direction is constant and expressed in the form

$$\frac{\partial T}{\partial z} = \frac{\pi D q_w}{\dot{m} \hat{C}_P} = \frac{\pi D q_w}{[\rho \langle v_z \rangle (\pi R^2)] \hat{C}_P} = \text{constant} \quad (9.3-40)$$

Since we are interested in the determination of the Nusselt number, it is appropriate to express  $\partial T/\partial z$  in terms of the Nusselt number. Note that the Nusselt number is given by

$$\text{Nu} = \frac{hD}{k} = \frac{[q_w/(T_w - T_b)] D}{k} \quad (9.3-41)$$

Therefore, Eq. (9.3-40) reduces to

$$\frac{\partial T}{\partial z} = \frac{\text{Nu} (T_w - T_b) k}{\rho \hat{C}_P R^2 \langle v_z \rangle} \quad (9.3-42)$$

Substitution of Eq. (9.3-42) into Eq. (9.3-39) yields

$$\frac{2}{R^2} \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \text{Nu} (T_w - T_b) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \quad (9.3-43)$$

In terms of the dimensionless variables

$$\theta = \frac{T - T_b}{T_w - T_b} \quad (9.3-44)$$

$$\xi = \frac{r}{R} \quad (9.3-45)$$

Eq. (9.3-43) takes the form

$$2 \text{Nu} (1 - \xi^2) = \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{d\theta}{d\xi} \right) \quad (9.3-46)$$

It is important to note that  $\theta$  depends only on  $\xi$  (or,  $r$ ).

The boundary conditions associated with Eq. (9.3-46) are

$$\text{at } \xi = 0 \quad \frac{d\theta}{d\xi} = 0 \quad (9.3-47)$$

$$\text{at } \xi = 1 \quad \theta = 1 \quad (9.3-48)$$

Integration of Eq. (9.3-46) with respect to  $\xi$  gives

$$\xi \frac{d\theta}{d\xi} = \left( \xi^2 - \frac{\xi^4}{2} \right) \text{Nu} + C_1 \quad (9.3-49)$$

where  $C_1$  is an integration constant. Application of Eq. (9.3-47) indicates that  $C_1 = 0$ . Integration of Eq. (9.3-49) once more with respect to  $\xi$  and the use of the boundary condition given by Eq. (9.3-48) gives

$$\theta = 1 - \frac{\text{Nu}}{8} (3 - 4\xi^2 + \xi^4) \quad (9.3-50)$$

On the other hand, the bulk temperature in dimensionless form can be expressed as

$$\theta_b = \frac{T_b - T_b}{T_w - T_b} = 0 = \frac{\int_0^1 (1 - \xi^2) \theta \xi d\xi}{\int_0^1 (1 - \xi^2) \xi d\xi} \quad (9.3-51)$$

Substitution of Eq. (9.3-50) into Eq. (9.3-51) and integration gives the Nusselt number as

$$\boxed{\text{Nu} = \frac{48}{11}} \quad (9.3-52)$$

### Constant wall temperature

When the wall temperature is constant, Eq. (9.3-38) indicates that

$$\frac{\partial T}{\partial z} = \left( \frac{T_w - T}{T_w - T_b} \right) \frac{dT_b}{dz} \quad (9.3-53)$$

The variation of  $T_b$  as a function of the axial position can be obtained from Eq. (9.3-21) as

$$\frac{dT_b}{dz} = \frac{\pi D \langle h \rangle_z}{\dot{m} \hat{C}_P} \underbrace{(T_w - T_{b,in}) \exp \left[ - \left( \frac{\pi D \langle h \rangle_z}{\dot{m} \hat{C}_P} \right) z \right]}_{(T_w - T_b)} \quad (9.3-54)$$

Since the heat transfer coefficient is constant for a thermally developed flow, Eq. (9.3-54) becomes

$$\frac{dT_b}{dz} = \frac{\pi D h (T_w - T_b)}{\dot{m} \hat{C}_P} = \frac{4 h (T_w - T_b)}{D \langle v_z \rangle \rho \hat{C}_P} \quad (9.3-55)$$

The use of Eq. (9.3-55) in Eq. (9.3-53) yields

$$\frac{\partial T}{\partial z} = \frac{4h(T_w - T)}{D\langle v_z \rangle \rho \hat{C}_P} \quad (9.3-56)$$

Substitution of Eq. (9.3-56) into Eq. (9.3-39) gives

$$\frac{8}{D^2} \left( \frac{hD}{k} \right) \left[ 1 - \left( \frac{r}{R} \right)^2 \right] (T_w - T) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \quad (9.3-57)$$

In terms of the dimensionless variables defined by Eqs. (9.3-44) and (9.3-45), Eq. (9.3-57) becomes

$$2 \text{Nu} (1 - \xi^2)(1 - \theta) = \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{d\theta}{d\xi} \right) \quad (9.3-58)$$

The boundary conditions associated with Eq. (9.3-58) are

$$\text{at } \xi = 0 \quad \frac{d\theta}{d\xi} = 0 \quad (9.3-59)$$

$$\text{at } \xi = 1 \quad \theta = 1 \quad (9.3-60)$$

Note that the use of the substitution

$$u = 1 - \theta \quad (9.3-61)$$

reduces Eqs. (9.3-58)-(9.3-61) to

$$-2 \text{Nu} (1 - \xi^2) u = \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{du}{d\xi} \right) \quad (9.3-62)$$

$$\text{at } \xi = 0 \quad \frac{du}{d\xi} = 0 \quad (9.3-63)$$

$$\text{at } \xi = 1 \quad u = 0 \quad (9.3-64)$$

Equation (9.3-62) can be solved for Nu by the method of Stodola and Vianello as explained in Section B.3.4.1 in Appendix B.

A reasonable first guess for  $u$  which satisfies the boundary conditions is

$$u_1 = 1 - \xi^2 \quad (9.3-65)$$

Substitution of Eq. (9.3-65) into the left-side of Eq. (9.3-62) gives

$$\frac{d}{d\xi} \left( \xi \frac{du}{d\xi} \right) = -2 \text{Nu} (\xi - 2\xi^3 + \xi^5) \quad (9.3-66)$$

The solution of Eq. (9.3-66) is

$$u = \text{Nu} \underbrace{\left( \frac{11 - 18\xi^2 + 9\xi^4 - 2\xi^6}{36} \right)}_{f_1(\xi)} \quad (9.3-67)$$

Therefore, the first approximation to the Nusselt number is

$$\text{Nu}^{(1)} = \frac{\int_0^1 \xi(1 - \xi^2)^2 f_1(\xi) d\xi}{\int_0^1 \xi(1 - \xi^2) f_1^2(\xi) d\xi} \quad (9.3-68)$$

Substitution of  $f_1(\xi)$  from Eq. (9.3-67) into Eq. (9.3-68) and evaluation of the integrals gives

$$\text{Nu} = 3.663 \quad (9.3-69)$$

On the other hand, the value of the Nusselt number, as calculated by Graetz (1883, 1885) and later independently by Nusselt (1910), is 3.66. Therefore, for a thermally developed laminar flow in a circular pipe with constant wall temperature  $\text{Nu} = 3.66$  for all practical purposes.

**Example 9.8** *Water flows through a circular pipe of 5 cm internal diameter with an average velocity of 0.01 m/s. Determine the length of the pipe to increase the water temperature from 20°C to 60°C for the following conditions:*

- a) *Steam condenses on the outer surface of the pipe so as to keep the surface temperature at 100°C.*
- b) *Electrical wires are wrapped around the outer surface of the pipe to provide a constant wall heat flux of 1500 W/m<sup>2</sup>.*

### Solution

#### Physical properties

*The mean bulk temperature is  $(20 + 60)/2 = 40^\circ\text{C}$  (313 K).*

$$\text{For water at 313 K : } \begin{cases} \rho = 992 \text{ kg/m}^3 \\ \mu = 654 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ k = 632 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ \text{Pr} = 4.32 \end{cases}$$

#### Assumptions

1. *Steady-state conditions prevail.*
2. *Flow is hydrodynamically and thermally fully developed.*

#### Analysis

*The Reynolds number is*

$$\begin{aligned} \text{Re} &= \frac{D\langle v_z \rangle \rho}{\mu} \\ &= \frac{(0.05)(0.01)(992)}{654 \times 10^{-6}} = 758 \quad \Rightarrow \quad \text{Laminar flow} \end{aligned}$$

a) Since the wall temperature is constant, from Eq. (9.3-26)

$$\begin{aligned} L &= \frac{D \operatorname{Re} \operatorname{Pr}}{4 \operatorname{Nu}} \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) \\ &= \frac{(0.05)(758)(4.32)}{4(3.66)} \ln \left( \frac{100 - 20}{100 - 60} \right) = 7.8 \text{ m} \end{aligned}$$

b) For a constant heat flux at the wall, the use of Eq. (9.3-33) gives

$$\begin{aligned} L &= \frac{(T_{b_{out}} - T_{b_{in}}) k \operatorname{Re} \operatorname{Pr}}{4 q_w} \\ &= \frac{(60 - 20)(632 \times 10^{-3})(758)(4.32)}{4(1500)} = 13.8 \text{ m} \end{aligned}$$

### 9.3.2 Viscous Heating in a Couette Flow

Viscous heating becomes an important problem during flow of liquids in lubrication, viscometry and extrusion. Let us consider Couette flow of a Newtonian fluid between two large parallel plates as shown in Figure 9.12. The surfaces at  $x = 0$  and  $x = B$  are maintained at  $T_o$  and  $T_1$ , respectively, with  $T_o > T_1$ .

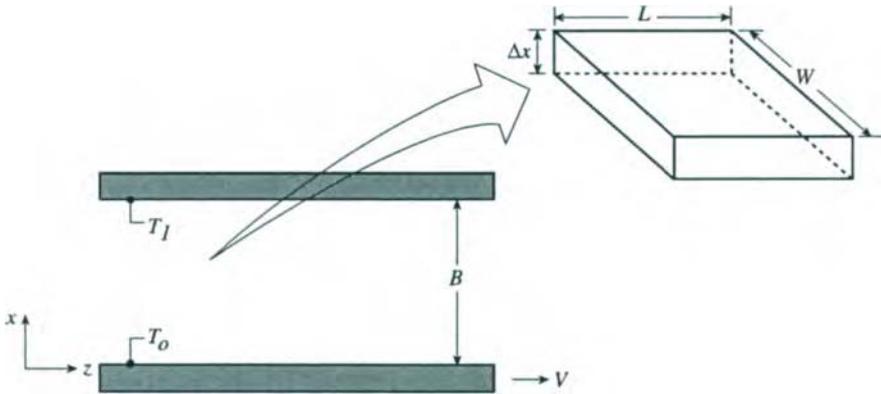


Figure 9.12 Couette flow with heat transfer.

Rate of energy generation per unit volume as a result of viscous dissipation is given by<sup>3</sup>

$$\mathfrak{R} = \mu \left( \frac{dv_z}{dx} \right)^2 \quad (9.3-70)$$

<sup>3</sup>The origin of this term comes from  $-(\tau : \nabla v)$ , which represents the irreversible degradation of mechanical energy into thermal energy in the equation of energy. For a more detailed discussion on the subject, see Bird *et. al.* (1960).

The velocity distribution for this problem is given by Eq. (8.1-12) as

$$\frac{v_z}{V} = 1 - \frac{x}{B} \quad (9.3-71)$$

The use of Eq. (9.3-71) in Eq. (9.3-70) gives the rate of energy generation per unit volume as

$$\mathfrak{R} = \frac{\mu V^2}{B^2} \quad (9.3-72)$$

The boundary conditions for the temperature, i.e.,

$$\text{at } x = 0 \quad T = T_o \quad (9.3-73)$$

$$\text{at } x = B \quad T = T_1 \quad (9.3-74)$$

suggest that  $T = T(x)$ . Therefore, Table C.4 in Appendix C indicates that the only non-zero energy flux component is  $e_x$  and it is given by

$$e_x = q_x = -k \frac{dT}{dx} \quad (9.3-75)$$

For a rectangular volume element of thickness  $\Delta x$ , as shown in Figure 9.12, Eq. (9.2-1) is expressed as

$$q_x|_x WL - q_x|_{x+\Delta x} WL + \left( \frac{\mu V^2}{B^2} \right) WL \Delta x = 0 \quad (9.3-76)$$

Dividing each term by  $WL \Delta x$  and taking the limit as  $\Delta x \rightarrow 0$  gives

$$\lim_{\Delta x \rightarrow 0} \frac{q_x|_x - q_x|_{x+\Delta x}}{\Delta x} + \frac{\mu V^2}{B^2} = 0 \quad (9.3-77)$$

or,

$$-\frac{dq_x}{dx} + \frac{\mu V^2}{B^2} = 0 \quad (9.3-78)$$

Substitution of Eq. (9.3-75) into Eq. (9.3-78) gives the governing equation for temperature as

$$\boxed{k \frac{d^2 T}{dx^2} + \frac{\mu V^2}{B^2} = 0} \quad (9.3-79)$$

Note that in the development of Eq. (9.3-79) both viscosity and thermal conductivity are assumed independent of temperature. The physical significance and the order of magnitude of the terms in Eq. (9.3-79) are given in Table 9.1. Therefore, the ratio of the viscous dissipation to conduction, which is known as the *Brinkman number*, is given by

$$\text{Br} = \frac{\text{Viscous dissipation}}{\text{Conduction}} = \frac{\mu V^2/B^2}{k(T_o - T_1)/B^2} = \frac{\mu V^2}{k(T_o - T_1)} \quad (9.3-80)$$

**Table 9.1** The physical significance and the order of magnitude of the terms in Eq. (9.3-79).

Term	Physical Significance	Order of Magnitude
$k \frac{d^2 T}{dx^2}$	Conduction	$\frac{k(T_o - T_1)}{B^2}$
$\frac{\mu V^2}{B^2}$	Viscous dissipation	$\frac{\mu V^2}{B^2}$

Before solving Eq. (9.3-79), it is convenient to express the governing equation and the boundary conditions in dimensionless form. Introduction of the dimensionless quantities

$$\theta = \frac{T - T_1}{T_o - T_1} \quad (9.3-81)$$

$$\xi = \frac{x}{B} \quad (9.3-82)$$

reduces Eqs. (9.3-79), (9.3-73) and (9.3-74) to

$$\frac{d^2 \theta}{d\xi^2} = -\text{Br} \quad (9.3-83)$$

$$\text{at } \xi = 0 \quad \theta = 1 \quad (9.3-84)$$

$$\text{at } \xi = 1 \quad \theta = 0 \quad (9.3-85)$$

Integration of Eq. (9.3-83) twice gives

$$\theta = -\frac{\text{Br}}{2} \xi^2 + C_1 \xi + C_2 \quad (9.3-86)$$

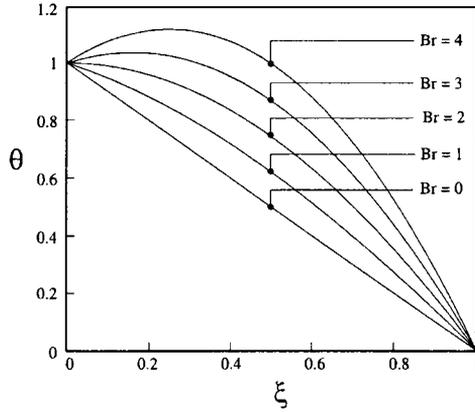
Application of the boundary conditions, Eqs. (9.3-84) and (9.3-85), gives the solution as

$$\theta = -\frac{\text{Br}}{2} \xi^2 + \left( \frac{\text{Br}}{2} - 1 \right) \xi + 1 \quad (9.3-87)$$

Note that when  $\text{Br} = 0$ , i.e., no viscous dissipation, Eq. (9.3-87) reduces to Eq. (8.3-10). The variation of  $\theta$  as a function of  $\xi$  with  $\text{Br}$  as a parameter is shown in Figure 9.13.

In engineering calculations, it is more appropriate to express the solution in terms of the Nusselt number. Calculation of the Nusselt number, on the other hand, requires the evaluation of the bulk temperature defined by

$$T_b = \frac{\int_0^W \int_0^B v_z T \, dx dy}{\int_0^W \int_0^B v_z \, dx dy} = \frac{\int_0^B v_z T \, dx}{\int_0^B v_z \, dx} \quad (9.3-88)$$



**Figure 9.13** Variation of  $\theta$  as a function of  $\xi$  with Br as a parameter.

In dimensionless form, Eq. (9.3-88) becomes

$$\theta_b = \frac{T_b - T_1}{T_o - T_1} = \frac{\int_0^1 \phi \theta d\xi}{\int_0^1 \phi d\xi} \tag{9.3-89}$$

where

$$\phi = \frac{v_z}{V} \tag{9.3-90}$$

Substitution of Eqs. (9.3-71) and (9.3-87) into Eq. (9.3-89) gives

$$\theta_b = \frac{\text{Br} + 8}{12} \tag{9.3-91}$$

**Calculation of the Nusselt number for the bottom plate**

The heat flux at the bottom plate is expressed as

$$-k \left. \frac{dT}{dx} \right|_{x=0} = \langle h \rangle_o (T_o - T_b) \tag{9.3-92}$$

Therefore, the Nusselt number becomes

$$\text{Nu}_o = \frac{\langle h \rangle_o (2B)}{k} = 2B \frac{-(dT/dx)_{x=0}}{T_o - T_b} \tag{9.3-93}$$

Note that the term  $2B$  in the definition of the Nusselt number represents the hydraulic equivalent diameter for parallel plates. In dimensionless form Eq. (9.3-93) becomes

$$\text{Nu}_o = \frac{2(d\theta/d\xi)_{\xi=0}}{\theta_b - 1} \quad (9.3-94)$$

The use of Eq. (9.3-87) in Eq. (9.3-94) gives

$$\boxed{\text{Nu}_o = 12 \left( \frac{\text{Br} - 2}{\text{Br} - 4} \right)} \quad (9.3-95)$$

Note that  $\text{Nu}_o$  takes the following values depending on the value of  $\text{Br}$  :

$$\text{Nu}_o = \begin{cases} 0 & \text{Br} = 2 \\ < 0 & 2 < \text{Br} < 4 \\ \infty & \text{Br} = 4 \end{cases} \quad (9.3-96)$$

When  $\text{Br} = 2$ , the temperature gradient at the lower plate is zero, i.e., adiabatic surface. When  $2 < \text{Br} < 4$ , as can be seen from Figure 9.13, temperature reaches a maximum within the flow field. For example, for  $\text{Br} = 3$ ,  $\theta$  reaches the maximum value of 1.042 at  $\xi = 0.167$  and heat transfer takes place from the fluid to the lower plate. When  $\text{Br} = 4$ ,  $\theta_b = 1$  from Eq. (9.3-91) and, as a result of very high viscous dissipation,  $T_b$  becomes uniform at the value of  $T_o$ . Since the driving force, i.e.,  $T_o - T_b$ , is zero,  $\text{Nu}_o$  is undefined under these circumstances.

### Calculation of the Nusselt number for the upper plate

The heat flux at the upper plate is

$$k \left. \frac{dT}{dx} \right|_{x=B} = \langle h \rangle_1 (T_1 - T_b) \quad (9.3-97)$$

Therefore, the Nusselt number becomes

$$\begin{aligned} \text{Nu}_1 &= \frac{\langle h \rangle_1 (2B)}{k} = 2B \frac{(dT/dx)_{x=B}}{T_1 - T_b} \\ &= - \frac{2(d\theta/d\xi)_{\xi=1}}{\theta_b} \end{aligned} \quad (9.3-98)$$

Substitution of Eq. (9.3-87) into Eq. (9.3-98) gives

$$\boxed{\text{Nu}_1 = 12 \left( \frac{\text{Br} + 2}{\text{Br} + 8} \right)} \quad (9.3-99)$$

## 9.4 MASS TRANSFER WITHOUT CONVECTION

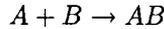
Under steady conditions, the conservation statement for species  $\mathcal{A}$  is expressed by

$$\left( \begin{array}{c} \text{Rate of} \\ \text{species } \mathcal{A} \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{species } \mathcal{A} \text{ out} \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{species } \mathcal{A} \text{ generation} \end{array} \right) = 0 \quad (9.4-1)$$

In this section we restrict our analysis to cases in which convection is negligible and mass transfer takes place mainly by diffusion.

### 9.4.1 Diffusion in a Liquid With Homogeneous Reaction

Gas  $\mathcal{A}$  dissolves in liquid  $\mathcal{B}$  and diffuses into the liquid phase as shown in Figure 9.14. As it diffuses, species  $\mathcal{A}$  undergoes an irreversible chemical reaction with species  $\mathcal{B}$  to form  $\mathcal{AB}$ , i.e.,



The rate of reaction is expressed by

$$r = k c_A$$

We are interested in the determination of concentration distribution within the liquid phase and the rate of depletion of species  $\mathcal{A}$ .

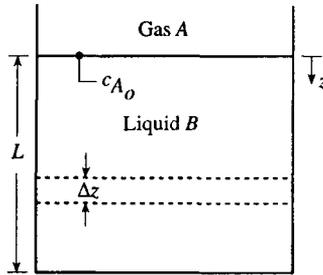


Figure 9.14 Diffusion and reaction in a liquid.

The problem will be analyzed with the following assumptions:

1. Steady-state conditions prevail.
2. The convective flux is negligible with respect to the molecular flux, i.e.,  $v_z^* \simeq 0$ .
3. The total concentration is constant, i.e.,

$$c = c_A + c_B + c_{AB} \simeq c_B$$

4. The concentration of  $\mathcal{AB}$  does not interfere with the diffusion of  $\mathcal{A}$  through  $\mathcal{B}$ , i.e.,  $\mathcal{A}$  molecules, for the most part, hit molecules  $\mathcal{B}$  and hardly ever hit molecules  $\mathcal{AB}$ . This is known as the *pseudo-binary behavior*.

Since  $c_A = c_A(z)$ , Table C.8 in Appendix C indicates that the only non-zero molar flux component is  $N_{A_z}$  and it is given by

$$N_{A_z} = J_{A_z}^* = -\mathcal{D}_{AB} \frac{dc_A}{dz} \quad (9.4-2)$$

For a differential volume element of thickness  $\Delta z$ , as shown in Figure 9.14, Eq. (9.4-1) is expressed as

$$N_{A_z}|_z A - N_{A_z}|_{z+\Delta z} A + \mathfrak{R}_A A \Delta z = 0 \quad (9.4-3)$$

Dividing Eq. (9.4-3) by  $A \Delta z$  and taking the limit as  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{N_{A_z}|_z - N_{A_z}|_{z+\Delta z}}{\Delta z} + \mathfrak{R}_A = 0 \quad (9.4-4)$$

or,

$$-\frac{dN_{A_z}}{dz} + \mathfrak{R}_A = 0 \quad (9.4-5)$$

The use of Eq. (5.3-26) gives the rate of depletion of species  $\mathcal{A}$  per unit volume as

$$\mathfrak{R}_A = -k c_A \quad (9.4-6)$$

Substitution of Eqs. (9.4-2) and (9.4-6) into Eq. (9.4-5) yields

$$\boxed{\mathcal{D}_{AB} \frac{d^2 c_A}{dz^2} - k c_A = 0} \quad (9.4-7)$$

The boundary conditions associated with the problem are

$$\text{at } z = 0 \quad c_A = c_{A_0} \quad (9.4-8)$$

$$\text{at } z = L \quad \frac{dc_A}{dz} = 0 \quad (9.4-9)$$

The value of  $c_{A_0}$  in Eq. (9.4-8) can be determined from Henry's law. The boundary condition given by Eq. (9.4-9) indicates that since species  $\mathcal{A}$  cannot diffuse through the bottom of the container, i.e., impermeable wall, then, the molar flux and the concentration gradient of species  $\mathcal{A}$  are zero.

The physical significance and the order of magnitude of the terms in Eq. (9.4-7) are given in Table 9.2. Therefore, the ratio of the rate of reaction to the rate of diffusion is given by

$$\frac{\text{Rate of reaction}}{\text{Rate of diffusion}} = \frac{k c_{A_0}}{\mathcal{D}_{AB} c_{A_0} / L^2} = \frac{k L^2}{\mathcal{D}_{AB}} \quad (9.4-10)$$

**Table 9.2** The physical significance and the order of magnitude of the terms in Eq. (9.4-7).

Term	Physical Significance	Order of Magnitude
$D_{AB} \frac{d^2 c_A}{dz^2}$	Rate of diffusion	$D_{AB} \frac{c_{A_0}}{L^2}$
$k c_A$	Rate of reaction	$k c_{A_0}$

and the Thiele modulus,  $\Lambda$ , is defined by

$$\Lambda = \sqrt{\frac{kL^2}{D_{AB}}} \quad (9.4-11)$$

Introduction of the dimensionless quantities

$$\theta = \frac{c_A}{c_{A_0}} \quad (9.4-12)$$

$$\xi = \frac{z}{L} \quad (9.4-13)$$

reduces Eqs. (9.4-7)-(9.4-9) to the form

$$\frac{d^2\theta}{d\xi^2} = \Lambda^2\theta \quad (9.4-14)$$

$$\text{at } \xi = 0 \quad \theta = 1 \quad (9.4-15)$$

$$\text{at } \xi = 1 \quad \frac{d\theta}{d\xi} = 0 \quad (9.4-16)$$

Note that Eqs. (9.4-14)-(9.4-16) are exactly equivalent to Eqs. (8.2-85)-(8.2-87). Therefore, the solution is

$$\theta = \frac{\cosh[\Lambda(1-\xi)]}{\cosh \Lambda} \quad (9.4-17)$$

It is interesting to observe how the Thiele modulus affects the concentration distribution. Figure 9.15 shows variation of  $\theta$  as a function of  $\xi$  with  $\Lambda$  being a parameter. Since the Thiele modulus indicates the rate of reaction with respect to the rate of diffusion,  $\Lambda = 0$  implies no chemical reaction and hence,  $\theta = 1$  ( $c_A = c_{A_0}$ ) for all  $\xi$ . Therefore, for very small values of  $\Lambda$ ,  $\theta$  is almost unity throughout the liquid. On the other hand, for large values of  $\Lambda$ , i.e., rate of reaction  $\gg$  rate of diffusion, as soon as species  $\mathcal{A}$  enters the liquid phase, it undergoes a homogeneous reaction with species  $\mathcal{B}$ . As a result, species  $\mathcal{A}$  is depleted before it reaches the bottom of the container. Note that the slope of the tangent to the curve drawn at  $\xi = 1$  has a zero slope, i.e., parallel to the  $\xi$ -axis.

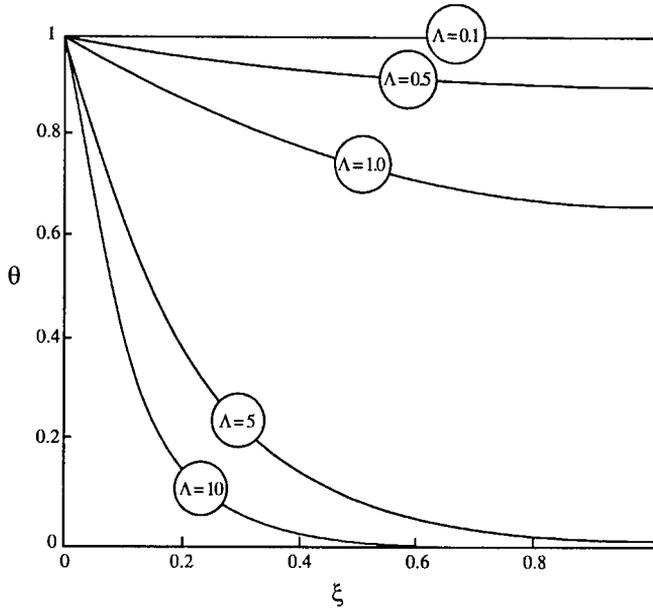


Figure 9.15 Variation of  $\theta$  as a function of  $\xi$  with  $\Lambda$  being a parameter.

#### 9.4.1.1 Macroscopic equation

Integration of the microscopic level equations over the volume of the system gives the equations at the macroscopic level. Integration of Eq. (9.4-7) over the volume of the system gives

$$\int_0^L \int_0^{2\pi} \int_0^R \mathcal{D}_{AB} \frac{d^2 c_A}{dz^2} r \, dr d\theta dz = \int_0^L \int_0^{2\pi} \int_0^R k c_A r \, dr d\theta dz \quad (9.4-18)$$

Carrying out the integrations yields

$$\underbrace{\pi R^2 \left( -\mathcal{D}_{AB} \frac{dc_A}{dz} \Big|_{z=0} \right)}_{\text{Rate of moles of species } \mathcal{A} \text{ entering into the liquid}} = \underbrace{\pi R^2 k \int_0^L c_A dz}_{\text{Rate of depletion of species } \mathcal{A} \text{ by homogeneous chem. rxn.}} \quad (9.4-19)$$

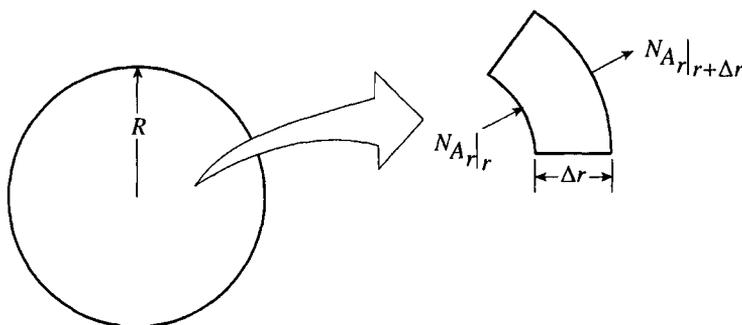
Note that Eq. (9.4-19) is the macroscopic inventory rate equation for species  $\mathcal{A}$  by considering the liquid in the tank as a system. Substitution of Eq. (9.4-17) into Eq. (9.4-19) gives the molar rate of depletion of species  $\mathcal{A}$ ,  $\dot{n}_A$ , as

$$\dot{n}_A = \frac{\pi R^2 \mathcal{D}_{AB} c_{A_0} \tanh \Lambda}{L} \quad (9.4-20)$$

### 9.4.2 Diffusion in a Spherical Particle With Homogeneous Reaction

Consider a homogeneous spherical aggregate of bacteria of radius  $R$  as shown in Figure 9.16. Species  $\mathcal{A}$  diffuses into a bacteria and undergoes an irreversible first-order reaction. The concentration of species  $\mathcal{A}$  at the surface of the bacteria,  $c_{A_R}$  is known. We want to determine the rate of consumption of species  $\mathcal{A}$ . The problem will be analyzed with the following assumptions:

1. Steady-state conditions prevail.
2. Convective flux is negligible with respect to the molecular flux, i.e.,  $v_z^* \simeq 0$ .
3. The total concentration is constant.



**Figure 9.16** Diffusion and homogeneous reaction inside a spherical particle.

Since  $c_A = c_A(r)$ , Table C.9 in Appendix C indicates that the only non-zero molar flux component is  $N_{A_r}$  and it is given by

$$N_{A_r} = J_{A_r}^* = -\mathcal{D}_{AB} \frac{dc_A}{dr} \quad (9.4-21)$$

For a spherical differential volume element of thickness  $\Delta r$ , as shown in Figure 9.16, Eq. (9.4-1) is expressed in the form

$$N_{A_r}|_r 4\pi r^2 - N_{A_r}|_{r+\Delta r} 4\pi (r + \Delta r)^2 + 4\pi r^2 \Delta r \mathfrak{R}_A = 0 \quad (9.4-22)$$

Dividing Eq. (9.4-22) by  $4\pi \Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(r^2 N_{A_r})|_r - (r^2 N_{A_r})|_{r+\Delta r}}{\Delta r} + r^2 \mathfrak{R}_A = 0 \quad (9.4-23)$$

or,

$$-\frac{d(r^2 N_{A_r})}{dr} + r^2 \mathfrak{R}_A = 0 \quad (9.4-24)$$

The use of Eq. (5.3-26) gives the rate of depletion of species  $A$  per unit volume as

$$\mathfrak{R}_A = -k c_A \quad (9.4-25)$$

Substitution of Eqs. (9.4-21) and (9.4-25) into Eq. (9.4-24) gives

$$\boxed{\frac{D_{AB}}{r^2} \frac{d}{dr} \left( r^2 \frac{dc_A}{dr} \right) - k c_A = 0} \quad (9.4-26)$$

in which the diffusion coefficient is considered constant. The boundary conditions associated with Eq. (9.4-26) are

$$\text{at } r = 0 \quad \frac{dc_A}{dr} = 0 \quad (9.4-27)$$

$$\text{at } r = R \quad c_A = c_{AR} \quad (9.4-28)$$

The physical significance and the order of magnitude of the terms in Eq. (9.4-26) are given in Table 9.3.

**Table 9.3** The physical significance and the order of magnitude of the terms in Eq. (9.4-26).

Term	Physical Significance	Order of Magnitude
$\frac{D_{AB}}{r^2} \frac{d}{dr} \left( r^2 \frac{dc_A}{dr} \right)$	Rate of diffusion	$D_{AB} \frac{c_{AR}}{R^2}$
$k c_A$	Rate of reaction	$k c_{AR}$

Therefore, the ratio of the rate of reaction to the rate of diffusion is given by

$$\frac{\text{Rate of reaction}}{\text{Rate of diffusion}} = \frac{k c_{AR}}{D_{AB} c_{AR}/R^2} = \frac{k R^2}{D_{AB}} \quad (9.4-29)$$

and the Thiele modulus,  $\Lambda$ , is defined by

$$\Lambda = \sqrt{\frac{k R^2}{D_{AB}}} \quad (9.4-30)$$

Introduction of the dimensionless quantities

$$\theta = \frac{c_A}{c_{AR}} \quad (9.4-31)$$

$$\xi = \frac{r}{R} \quad (9.4-32)$$

reduces Eqs. (9.4-26)-(9.4-28) to

$$\frac{1}{\xi^2} \frac{d}{d\xi} \left( \xi^2 \frac{d\theta}{d\xi} \right) - \Lambda^2 \theta = 0 \quad (9.4-33)$$

$$\text{at } \xi = 0 \quad \frac{d\theta}{d\xi} = 0 \quad (9.4-34)$$

$$\text{at } \xi = 1 \quad \theta = 1 \quad (9.4-35)$$

Problems in spherical coordinates are converted to rectangular coordinates by the use of the following transformation

$$\theta = \frac{u(\xi)}{\xi} \quad (9.4-36)$$

From Eq. (9.4-36), note that

$$\frac{d\theta}{d\xi} = \frac{1}{\xi} \frac{du}{d\xi} - \frac{u}{\xi^2} \quad (9.4-37)$$

$$\xi^2 \frac{d\theta}{d\xi} = \xi \frac{du}{d\xi} - u \quad (9.4-38)$$

$$\frac{d}{d\xi} \left( \xi^2 \frac{d\theta}{d\xi} \right) = \frac{du}{d\xi} + \xi \frac{d^2u}{d\xi^2} - \frac{du}{d\xi} = \xi \frac{d^2u}{d\xi^2} \quad (9.4-39)$$

Substitution of Eqs. (9.4-36) and (9.4-39) into Eq. (9.4-33) yields

$$\frac{d^2u}{d\xi^2} - \Lambda^2 u = 0 \quad (9.4-40)$$

On the other hand, the boundary conditions, Eqs. (9.4-34) and (9.4-35), become

$$\text{at } \xi = 0 \quad u = 0 \quad (9.4-41)$$

$$\text{at } \xi = 1 \quad u = 1 \quad (9.4-42)$$

The solution of Eq. (9.4-40) is

$$\theta = K_1 \sinh(\Lambda\xi) + K_2 \cosh(\Lambda\xi) \quad (9.4-43)$$

where  $K_1$  and  $K_2$  are constants. Application of the boundary conditions, Eqs. (9.4-41) and (9.4-42), gives the solution as

$$u = \frac{\sinh(\Lambda\xi)}{\sinh \Lambda} \quad (9.4-44)$$

or,

$$\boxed{\frac{c_A}{c_{AR}} = \frac{R}{r} \frac{\sinh[\Lambda(r/R)]}{\sinh \Lambda}} \quad (9.4-45)$$

### 9.4.2.1 Macroscopic equation

Integration of the governing differential equation, Eq. (9.4-26), over the spherical aggregate of bacteria gives

$$\int_0^{2\pi} \int_0^\pi \int_0^R \frac{D_{AB}}{r^2} \frac{d}{dr} \left( r^2 \frac{dc_A}{dr} \right) r^2 \sin \theta \, dr d\theta d\phi = \int_0^{2\pi} \int_0^\pi \int_0^R k c_A r^2 \sin \theta \, dr d\theta d\phi \quad (9.4-46)$$

Carrying out the integrations yields

$$\underbrace{4\pi R^2 D_{AB} \frac{dc_A}{dr} \Big|_{r=R}}_{\text{Rate of moles of species } \mathcal{A} \text{ entering into the bacteria}} = \underbrace{4\pi k \int_0^R c_A r^2 \, dr}_{\text{Rate of consumption of species } \mathcal{A} \text{ by homogeneous chem. rxn.}} \quad (9.4-47)$$

Substitution of Eq. (9.4-45) into Eq. (9.4-47) gives the molar rate of consumption of species  $\mathcal{A}$ ,  $\dot{n}_A$ , as

$$\dot{n}_A = -4\pi R D_{AB} c_{A_r} (1 - \Lambda \tanh \Lambda) \quad (9.4-48)$$

The minus sign in Eq. (9.4-48) indicates that the flux is in the negative  $r$ -direction, i.e., towards the center of the sphere.

## 9.5 MASS TRANSFER WITH CONVECTION

### 9.5.1 Laminar Forced Convection in a Pipe

Consider the laminar flow of an incompressible Newtonian liquid ( $\mathcal{B}$ ) in a circular pipe under the action of a pressure gradient as shown in Figure 9.17. The velocity distribution is given by Eqs. (9.1-79) and (9.1-84) as

$$v_z = 2 \langle v_z \rangle \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \quad (9.5-1)$$

Suppose that the liquid has a uniform species  $\mathcal{A}$  concentration of  $c_{A_0}$  for  $z < 0$ . For  $z > 0$ , species  $\mathcal{A}$  concentration starts to change as a function of  $r$  and  $z$  as a result of mass transfer from the walls of the pipe. We want to develop the governing equation for species  $\mathcal{A}$  concentration. Liquid viscosity is assumed to be unaffected by mass transfer.

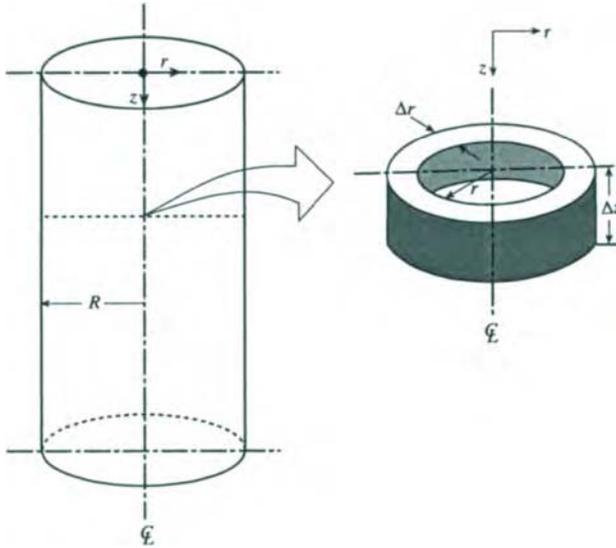


Figure 9.17 Forced convection mass transfer in a pipe.

From Table C.8 in Appendix C, the non-zero mass flux components for species  $A$  are

$$W_{A_r} = -\rho D_{AB} \frac{\partial \omega_A}{\partial r} \tag{9.5-2}$$

$$W_{A_z} = -\rho D_{AB} \frac{\partial \omega_A}{\partial z} + \rho_A v_z \tag{9.5-3}$$

For a dilute liquid solution, the total density is almost constant and Eqs. (9.5-2) and (9.5-3) become

$$W_{A_r} = -D_{AB} \frac{\partial \rho_A}{\partial r} \tag{9.5-4}$$

$$W_{A_z} = -D_{AB} \frac{\partial \rho_A}{\partial z} + \rho_A v_z \tag{9.5-5}$$

Dividing Eqs. (9.5-4) and (9.5-5) by the molecular weight of species  $A$ ,  $M_A$ , gives

$$N_{A_r} = -D_{AB} \frac{\partial c_A}{\partial r} \tag{9.5-6}$$

$$N_{A_z} = -D_{AB} \frac{\partial c_A}{\partial z} + c_A v_z \tag{9.5-7}$$

Since there is no generation of species  $A$ , Eq. (9.4-1) simplifies to

$$\left( \begin{array}{c} \text{Rate of} \\ \text{species } A \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{species } A \text{ out} \end{array} \right) = 0 \tag{9.5-8}$$

For a cylindrical differential volume element of thickness  $\Delta r$  and length  $\Delta z$ , as shown in Figure 9.17, Eq. (9.5-8) is expressed as

$$(N_{A_r}|_r 2\pi r \Delta z + N_{A_z}|_z 2\pi r \Delta r) - [N_{A_r}|_{r+\Delta r} 2\pi(r + \Delta r) \Delta z + N_{A_z}|_{z+\Delta z} 2\pi r \Delta r] = 0 \quad (9.5-9)$$

Dividing Eq. (9.5-9) by  $2\pi \Delta r \Delta z$  and taking the limit as  $\Delta r \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta r \rightarrow 0} \frac{(rN_{A_r})|_r - (rN_{A_r})|_{r+\Delta r}}{\Delta r} + \lim_{\Delta z \rightarrow 0} r \frac{N_{A_z}|_z - N_{A_z}|_{z+\Delta z}}{\Delta z} = 0 \quad (9.5-10)$$

or,

$$\frac{1}{r} \frac{\partial(rN_{A_r})}{\partial r} + \frac{\partial N_{A_z}}{\partial z} = 0 \quad (9.5-11)$$

Substitution of Eqs. (9.5-6) and (9.5-7) into Eq. (9.5-11) yields

$$\underbrace{v_z \frac{\partial c_A}{\partial z}}_{\text{Convection in } z\text{-direction}} = \underbrace{\frac{D_{AB}}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right)}_{\text{Diffusion in } r\text{-direction}} + \underbrace{D_{AB} \frac{\partial^2 c_A}{\partial z^2}}_{\text{Diffusion in } z\text{-direction}} \quad (9.5-12)$$

Note that in the  $z$ -direction mass of species  $\mathcal{A}$  is transported both by convection and diffusion. As stated by Eq. (2.4-8), diffusion can be considered negligible with respect to convection when  $\text{Pe}_M \gg 1$ . Under these circumstances, Eq. (9.5-12) reduces to

$$\boxed{v_z \frac{\partial c_A}{\partial z} = \frac{D_{AB}}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right)} \quad (9.5-13)$$

As an engineer, we are interested in the variation of the bulk concentration of species  $\mathcal{A}$ ,  $c_{A_b}$ , rather than the local concentration,  $c_A$ . For forced convection mass transfer in a circular pipe of radius  $R$ , the bulk concentration defined by Eq. (4.1-3) takes the form

$$c_{A_b} = \frac{\int_0^{2\pi} \int_0^R v_z c_A r \, dr d\theta}{\int_0^{2\pi} \int_0^R v_z r \, dr d\theta} \quad (9.5-14)$$

In general, the concentration of species  $\mathcal{A}$ ,  $c_A$ , may depend on both the radial and axial coordinates. However, the bulk concentration of species  $\mathcal{A}$ ,  $c_{A_b}$ , depends only on the axial direction.

To determine the governing equation for the bulk concentration of species  $\mathcal{A}$ , it is necessary to integrate Eq. (9.5-13) over the cross-sectional area of the tube, i.e.,

$$\int_0^{2\pi} \int_0^R v_z \frac{\partial c_A}{\partial z} r \, dr d\theta = D_{AB} \int_0^{2\pi} \int_0^R \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right) r \, dr d\theta \quad (9.5-15)$$

Since  $v_z \neq v_z(z)$ , the integral on the left-side of Eq. (9.5-15) can be rearranged as

$$\begin{aligned} \int_0^{2\pi} \int_0^R v_z \frac{\partial c_A}{\partial z} r \, dr d\theta &= \int_0^{2\pi} \int_0^R \frac{\partial(v_z c_A)}{\partial z} r \, dr d\theta \\ &= \frac{d}{dz} \left( \int_0^{2\pi} \int_0^R v_z c_A r \, dr d\theta \right) \end{aligned} \quad (9.5-16)$$

Substitution of Eq. (9.5-14) into Eq. (9.5-16) yields

$$\begin{aligned} \int_0^{2\pi} \int_0^R v_z \frac{\partial c_A}{\partial z} r \, dr d\theta &= \frac{d}{dz} \left( c_{A_b} \underbrace{\int_0^{2\pi} \int_0^R v_z r \, dr d\theta}_Q \right) \\ &= Q \frac{dc_{A_b}}{dz} \end{aligned} \quad (9.5-17)$$

where  $Q$  is the volumetric flow rate.

On the other hand, since  $\partial c_A / \partial r = 0$  as a result of the symmetry condition at the center of the tube, the integral on the right-side of Eq. (9.5-15) takes the form

$$\int_0^{2\pi} \int_0^R \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right) r \, dr d\theta = \pi D \left. \frac{\partial c_A}{\partial r} \right|_{r=R} \quad (9.5-18)$$

Substitution of Eqs. (9.5-17) and (9.5-18) into Eq. (9.5-15) gives the governing equation for the bulk concentration in the form

$$\boxed{Q \frac{dc_{A_b}}{dz} = \pi D \mathcal{D}_{AB} \left. \frac{\partial c_A}{\partial r} \right|_{r=R}} \quad (9.5-19)$$

The solution of Eq. (9.5-19) requires the boundary conditions associated with the problem to be known.

### Constant wall concentration

If the inner surface of the pipe is coated with species  $\mathcal{A}$ , the molar flux of species  $\mathcal{A}$  on the surface can be represented by

$$\mathcal{D}_{AB} \left. \frac{\partial c_A}{\partial r} \right|_{r=R} = k_c (c_{A_w} - c_{A_b}) \quad (9.5-20)$$

It is implicitly implied in writing Eq. (9.5-20) that the concentration increases in the radial direction. Substitution of Eq. (9.5-20) into Eq. (9.5-19) and rearrangement yields

$$Q \int_{c_{A_b, \text{in}}}^{c_{A_b}} \frac{dc_{A_b}}{c_{A_w} - c_{A_b}} = \pi D \int_0^z k_c \, dz \quad (9.5-21)$$

Since the wall concentration,  $c_{A_w}$ , is constant, integration of Eq. (9.5-21) yields

$$Q \ln \left( \frac{c_{A_w} - c_{A_{b_{in}}}}{c_{A_w} - c_{A_b}} \right) = \pi D \langle k_c \rangle_z z \quad (9.5-22)$$

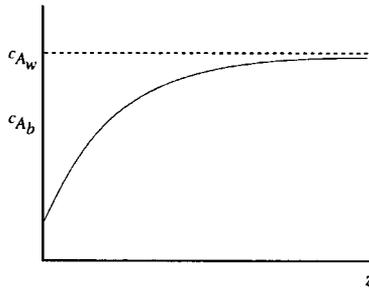
in which  $\langle k_c \rangle_z$  is the average mass transfer coefficient from the entrance to the point  $z$  defined by

$$\langle k_c \rangle_z = \frac{1}{z} \int_0^z k_c dz \quad (9.5-23)$$

If Eq. (9.5-22) is solved for  $c_{A_b}$ , the result is

$$c_{A_b} = c_{A_w} - (c_{A_w} - c_{A_{b_{in}}}) \exp \left[ - \left( \frac{\pi D \langle k_c \rangle_z}{Q} \right) z \right] \quad (9.5-24)$$

which indicates that the bulk concentration of species  $A$  varies exponentially with the axial direction as shown in Figure 9.18.



**Figure 9.18** Variation of the bulk concentration of species  $A$  with the axial direction for a constant wall concentration.

Evaluation of Eq. (9.5-22) over the total length,  $L$ , of the pipe gives

$$Q \ln \left( \frac{c_{A_w} - c_{A_{b_{in}}}}{c_{A_w} - c_{A_{b_{out}}}} \right) = \pi D \langle k_c \rangle L \quad (9.5-25)$$

where

$$\langle k_c \rangle = \frac{1}{L} \int_0^L k_c dz \quad (9.5-26)$$

If Eq. (9.5-25) is solved for  $c_{A_{b_{out}}}$ , the result is

$$c_{A_{b_{out}}} = c_{A_w} - (c_{A_w} - c_{A_{b_{in}}}) \exp \left[ - \left( \frac{\pi D \langle k_c \rangle}{Q} \right) L \right] \quad (9.5-27)$$

Equation (9.5-27) can be expressed in terms of dimensionless numbers with the help of Eq. (3.4-6). The result is

$$\begin{aligned} St_M &= \frac{Sh}{Re Sc} = \frac{\langle k_c \rangle}{\langle v_z \rangle} \\ &= \frac{\langle k_c \rangle}{Q/(\pi D^2/4)} \end{aligned} \quad (9.5-28)$$

The use of Eq. (9.5-28) in Eq. (9.5-27) gives

$$c_{A_{b_{out}}} = c_{A_w} - (c_{A_w} - c_{A_{b_{in}}}) \exp \left[ -\frac{4 Sh(L/D)}{Re Sc} \right] \quad (9.5-29)$$

As an engineer, we are interested in the rate of moles of species  $\mathcal{A}$  transferred to the fluid, i.e.,

$$\dot{n}_A = Q(c_{A_{b_{out}}} - c_{A_{b_{in}}}) = Q \left[ (c_{A_w} - c_{A_{b_{in}}}) - (c_{A_w} - c_{A_{b_{out}}}) \right] \quad (9.5-30)$$

Substitution of Eq. (9.5-25) into Eq. (9.5-30) results in

$$\dot{n}_A = (\pi DL) \langle k_c \rangle \left[ \frac{(c_{A_w} - c_{A_{b_{in}}}) - (c_{A_w} - c_{A_{b_{out}}})}{\ln \left( \frac{c_{A_w} - c_{A_{b_{in}}}}{c_{A_w} - c_{A_{b_{out}}}} \right)} \right] \quad (9.5-31)$$

Note that Eq. (9.5-31) can be expressed in the form

$$\dot{n}_A = A_M \langle k_c \rangle (\Delta c_A)_{ch} = (\pi DL) \langle k_c \rangle (\Delta c_A)_{LM} \quad (9.5-32)$$

which is identical with Eqs. (3.3-7) and (4.5-34).

### Constant wall mass flux

Consider a circular pipe with a porous wall. If species  $\mathcal{A}$  were forced through the porous wall at a specified rate per unit area, then the molar flux of species  $\mathcal{A}$  on the pipe surface remains constant, i.e.,

$$N_{A_r}|_{r=R} = \mathcal{D}_{AB} \left. \frac{\partial c_A}{\partial r} \right|_{r=R} = N_{A_w} = \text{constant} \quad (9.5-33)$$

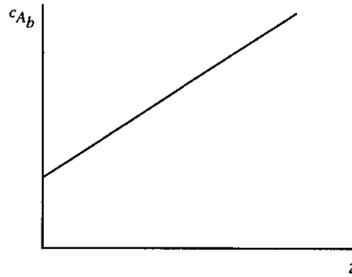
Substitution of Eq. (9.5-33) into Eq. (9.5-19) gives

$$\frac{dc_{A_b}}{dz} = \frac{\pi D N_{A_w}}{Q} = \text{constant} \quad (9.5-34)$$

Integration of Eq. (9.5-34) gives the variation of the bulk concentration of species  $\mathcal{A}$  in the axial direction as

$$c_{A_b} = c_{A_{b_{in}}} + \left( \frac{\pi D N_{A_w}}{Q} \right) z \quad (9.5-35)$$

Therefore, the bulk concentration of species  $\mathcal{A}$  varies linearly in the axial direction as shown in Figure 9.19.



**Figure 9.19** Variation of the bulk concentration of species  $\mathcal{A}$  with the axial direction for a constant wall heat flux.

Evaluation of Eq. (9.5-35) over the total length gives the bulk concentration of species  $\mathcal{A}$  at the exit of the pipe as

$$\begin{aligned} c_{A_{b_{out}}} &= c_{A_{b_{in}}} + \left( \frac{\pi D N_{A_w}}{Q} \right) L \\ &= c_{A_{b_{in}}} + \frac{4 N_{A_w} L}{\mathcal{D}_{AB} \text{Re} \text{Sc}} \end{aligned} \quad (9.5-36)$$

The rate of moles of species  $\mathcal{A}$  transferred is given by

$$\dot{n}_A = Q (c_{A_{b_{out}}} - c_{A_{b_{in}}}) \quad (9.5-37)$$

Substitution of Eq. (9.5-36) into Eq. (9.5-37) yields

$$\boxed{\dot{n}_A = (\pi D L) N_{A_w}} \quad (9.5-38)$$

### 9.5.1.1 Fully developed concentration profile

If the ratio

$$\frac{c_A - c_{A_b}}{c_{A_w} - c_{A_b}} \quad (9.5-39)$$

does not vary along the axial direction, then the concentration profile is said to be fully developed.

It is important to note that although the local concentration,  $c_A$ , the bulk concentration,  $c_{A_b}$ , and the wall concentration,  $c_{A_w}$ , may change along the axial direction, the ratio given in Eq. (9.5-39) is independent of the axial coordinate<sup>4</sup>, i.e.,

$$\frac{\partial}{\partial z} \left( \frac{c_A - c_{A_b}}{c_{A_w} - c_{A_b}} \right) = 0 \quad (9.5-40)$$

Equation (9.5-40) indicates that

$$\frac{\partial c_A}{\partial z} = \left( \frac{c_{A_w} - c_A}{c_{A_w} - c_{A_b}} \right) \frac{dc_{A_b}}{dz} + \left( \frac{c_A - c_{A_b}}{c_{A_w} - c_{A_b}} \right) \frac{dc_{A_w}}{dz} \quad (9.5-41)$$

**Example 9.10** Consider the flow of a fluid with constant physical properties. Show that the mass transfer coefficient is constant when the concentration profile is fully developed.

### Solution

For a fully developed concentration profile, the ratio given in Eq. (9.5-39) depends only on the radial coordinate  $r$ , i.e.,

$$\frac{c_A - c_{A_b}}{c_{A_w} - c_{A_b}} = f(r) \quad (1)$$

Differentiation of Eq. (1) with respect to  $r$  gives

$$\frac{\partial c_A}{\partial r} = (c_{A_w} - c_{A_b}) \frac{df}{dr} \quad (2)$$

which is valid at all points within the flow field. Evaluation of Eq. (2) at the surface of the pipe yields

$$\left. \frac{\partial c_A}{\partial r} \right|_{r=R} = (c_{A_w} - c_{A_b}) \left. \frac{df}{dr} \right|_{r=R} \quad (3)$$

On the other hand, the molar flux of species  $A$  at the pipe surface is expressed as

$$N_{A_w} = \mathcal{D}_{AB} \left. \frac{\partial c_A}{\partial r} \right|_{r=R} = k_c (c_{A_w} - c_{A_b}) \quad (4)$$

<sup>4</sup>In the literature, the condition for the fully developed concentration profile is also given in the form

$$\frac{\partial}{\partial z} \left( \frac{c_{A_w} - c_A}{c_{A_w} - c_{A_b}} \right) = 0$$

Note that

$$\frac{c_{A_w} - c_A}{c_{A_w} - c_{A_b}} = 1 - \frac{c_A - c_{A_b}}{c_{A_w} - c_{A_b}}$$

Substitution of Eq. (3) into Eq. (4) gives

$$k_c = \mathcal{D}_{AB} \left( \frac{df}{dr} \right)_{r=R} = \text{constant} \quad (5)$$

**Example 9.11** When the concentration profile is fully developed, show that the concentration gradient in the axial direction,  $\partial c_A / \partial z$ , remains constant for a constant wall mass flux.

### Solution

The molar flux of species  $A$  at the surface of the pipe is given by

$$N_{A,r}|_{r=R} = k_c (c_{A_w} - c_{A_b}) = \text{constant} \quad (1)$$

Since  $k_c$  is constant for a fully developed concentration profile, Eq. (1) implies that

$$c_{A_w} - c_{A_b} = \text{constant} \quad (2)$$

or,

$$\frac{dc_{A_w}}{dz} = \frac{dc_{A_b}}{dz} \quad (3)$$

Therefore, Eq. (9.5-41) simplifies to

$$\frac{\partial c_A}{\partial z} = \frac{dc_{A_b}}{dz} = \frac{dc_{A_w}}{dz} \quad (4)$$

Since  $dc_{A_b}/dz$  is constant according to Eq. (9.5-34),  $\partial c_A / \partial z$  also remains constant, i.e.,

$$\frac{\partial c_A}{\partial z} = \frac{dc_{A_b}}{dz} = \frac{dc_{A_w}}{dz} = \frac{\pi D N_{A_w}}{Q} = \text{constant} \quad (5)$$

#### 9.5.1.2 Sherwood number for a fully developed concentration profile

Substitution of Eq. (9.5-1) into Eq. (9.5-13) gives

$$2 \langle v_z \rangle \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \frac{\partial c_A}{\partial z} = \frac{\mathcal{D}_{AB}}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right) \quad (9.5-42)$$

It should always be kept in mind that the purpose of solving the above equation for concentration distribution is to obtain a correlation to calculate the number of moles of species  $A$  transferred between the phases. As shown in Chapter 4, mass transfer correlations are expressed in terms of the Sherwood number. Therefore, Eq. (9.5-42) will be solved for a fully developed concentration profile for two different types of boundary conditions, i.e., constant wall mass flux and constant wall concentration, to determine the Sherwood number.

**Constant wall mass flux**

As shown in Example 9.11, in the case of a constant wall mass flux, the concentration gradient in the axial direction is constant and expressed in the form

$$\frac{\partial c_A}{\partial z} = \frac{\pi D N_{A_w}}{Q} = \text{constant} \quad (9.5-43)$$

Since we are interested in the determination of the Sherwood number, it is appropriate to express  $\partial c_A/\partial z$  in terms of the Sherwood number. Note that the Sherwood number is given by

$$\text{Sh} = \frac{k_c D}{\mathcal{D}_{AB}} = \frac{[N_{A_w}/(c_{A_w} - c_{A_b})] D}{\mathcal{D}_{AB}} \quad (9.5-44)$$

Therefore, Eq. (9.5-43) reduces to

$$\frac{\partial c_A}{\partial z} = \frac{\text{Sh}(c_{A_w} - c_{A_b}) \mathcal{D}_{AB}}{R^2 \langle v_z \rangle} \quad (9.5-45)$$

Substitution of Eq. (9.5-45) into Eq. (9.5-42) yields

$$\frac{2}{R^2} \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \text{Sh}(c_{A_w} - c_{A_b}) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right) \quad (9.5-46)$$

In terms of the dimensionless variables

$$\theta = \frac{c_A - c_{A_b}}{c_{A_w} - c_{A_b}} \quad (9.5-47)$$

$$\xi = \frac{r}{R} \quad (9.5-48)$$

Eq. (9.5-46) takes the form

$$2 \text{Sh}(1 - \xi^2) = \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{d\theta}{d\xi} \right) \quad (9.5-49)$$

It is important to note that  $\theta$  depends only on  $\xi$  (or,  $r$ ).

The boundary conditions associated with Eq. (9.5-49) are

$$\text{at } \xi = 0 \quad \frac{d\theta}{d\xi} = 0 \quad (9.5-50)$$

$$\text{at } \xi = 1 \quad \theta = 1 \quad (9.5-51)$$

Note that Eqs.(9.5-49)-(9.5-51) are identical with Eqs. (9.3-46)-(9.3-48) with only exception that  $\text{Nu}$  is replaced by  $\text{Sh}$ . Therefore, the solution is

$$\theta = 1 - \frac{\text{Sh}}{8} (3 - 4\xi^2 + \xi^4) \quad (9.5-52)$$

On the other hand, the bulk concentration in dimensionless form can be expressed as

$$\theta_b = \frac{c_{A_b} - c_{A_b}}{c_{A_w} - c_{A_b}} = 0 = \frac{\int_0^1 (1 - \xi^2) \theta \xi d\xi}{\int_0^1 (1 - \xi^2) \xi d\xi} \quad (9.5-53)$$

Substitution of Eq. (9.5-52) into Eq. (9.5-53) gives the Sherwood number as

$$\boxed{\text{Sh} = \frac{48}{11}} \quad (9.5-54)$$

### Constant wall concentration

When the wall concentration is constant, Eq. (9.5-41) indicates that

$$\frac{\partial c_A}{\partial z} = \left( \frac{c_{A_w} - c_A}{c_{A_w} - c_{A_b}} \right) \frac{dc_{A_b}}{dz} \quad (9.5-55)$$

The variation of  $c_{A_b}$  as a function of the axial position can be obtained from Eq. (9.5-24) as

$$\frac{dc_{A_b}}{dz} = \frac{\pi D \langle k_c \rangle_z}{Q} \underbrace{(c_{A_w} - c_{A_{b_{in}}})}_{(c_{A_w} - c_{A_b})} \exp \left[ - \left( \frac{\pi D \langle k_c \rangle_z}{Q} \right) z \right] \quad (9.5-56)$$

Since the mass transfer coefficient is constant for a fully developed concentration profile, Eq. (9.5-56) becomes

$$\frac{dc_{A_b}}{dz} = \frac{\pi D k_c (c_{A_w} - c_{A_b})}{Q} = \frac{4 k_c (c_{A_w} - c_{A_b})}{D \langle v_z \rangle} \quad (9.5-57)$$

The use of Eq. (9.5-57) in Eq. (9.5-55) yields

$$\frac{\partial c_A}{\partial z} = \frac{4 k_c (c_{A_w} - c_A)}{D \langle v_z \rangle} \quad (9.5-58)$$

Substitution of Eq. (9.5-58) into Eq. (9.5-42) gives

$$\frac{8}{D^2} \left( \frac{k_c D}{\mathcal{D}_{AB}} \right) \left[ 1 - \left( \frac{r}{R} \right)^2 \right] (c_{A_w} - c_A) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_A}{\partial r} \right) \quad (9.5-59)$$

In terms of the dimensionless variables defined by Eqs. (9.5-47) and (9.5-48), Eq. (9.5-59) becomes

$$2 \text{Sh} (1 - \xi^2) (1 - \theta) = \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{d\theta}{d\xi} \right) \quad (9.5-60)$$

The boundary conditions associated with Eq. (9.5-60) are

$$\text{at } \xi = 0 \quad \frac{d\theta}{d\xi} = 0 \quad (9.5-61)$$

$$\text{at } \xi = 1 \quad \theta = 1 \quad (9.5-62)$$

The use of the substitution

$$u = 1 - \theta \quad (9.5-63)$$

reduces Eqs. (9.5-60)-(9.5-62) to

$$-2 \text{Sh} (1 - \xi^2) u = \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{du}{d\xi} \right) \quad (9.5-64)$$

$$\text{at } \xi = 0 \quad \frac{du}{d\xi} = 0 \quad (9.5-65)$$

$$\text{at } \xi = 1 \quad u = 0 \quad (9.5-66)$$

Equation (9.3-61) can be solved for Sh by the method of Stodola and Vianello as explained in Section B.3.4.1 in Appendix B.

A reasonable first guess for  $u$  which satisfies the boundary conditions is

$$u_1 = 1 - \xi^2 \quad (9.5-67)$$

Substitution of Eq. (9.5-67) into the left-side of Eq. (9.5-64) gives

$$\frac{d}{d\xi} \left( \xi \frac{du}{d\xi} \right) = -2 \text{Sh} (\xi - 2\xi^3 + \xi^5) \quad (9.5-68)$$

The solution of Eq. (9.5-68) is

$$u = \text{Sh} \underbrace{\left( \frac{11 - 18\xi^2 + 9\xi^4 - 2\xi^6}{36} \right)}_{f_1(\xi)} \quad (9.5-69)$$

Therefore, the first approximation to the Sherwood number is

$$\text{Sh}^{(1)} = \frac{\int_0^1 \xi (1 - \xi^2)^2 f_1(\xi) d\xi}{\int_0^1 \xi (1 - \xi^2) f_1^2(\xi) d\xi} \quad (9.5-70)$$

Substitution of  $f_1(\xi)$  from Eq. (9.5-69) into Eq. (9.5-70) and evaluation of the integrals gives

$$\text{Sh} = 3.663 \quad (9.5-71)$$

On the other hand, the value of the Sherwood number, as calculated by Graetz (1883, 1885) and Nusselt (1910), is 3.66. Therefore, for a fully developed concentration profile in a circular pipe with a constant wall concentration  $\text{Sh} = 3.66$  for all practical purposes.

### 9.5.1.3 Sherwood number for a fully developed velocity profile

For water flowing in a circular pipe of diameter  $D$  at a Reynolds number of 100 and at a temperature of  $20^\circ\text{C}$ , Skelland (1974) calculated the length of the tube,  $L$ , required for the velocity, temperature and concentration distributions to reach a fully developed profile as

$$L = \begin{cases} 5D & \text{fully developed velocity profile} \\ 35D & \text{fully developed temperature profile} \\ 6000D & \text{fully developed concentration profile} \end{cases} \quad (9.5-72)$$

Therefore, a fully developed concentration profile is generally not attained for fluids with high Schmidt number and the use of Eqs. (9.5-54) and (9.5-71) may lead to erroneous results.

When the velocity profile is fully developed, it is recommended to use the following semi-empirical correlations suggested by Hausen (1943):

$$\boxed{\text{Sh} = 3.66 + \frac{0.668 [(D/L) \text{Re Sc}]}{1 + 0.04 [(D/L) \text{Re Sc}]^{2/3}}} \quad c_{A_w} = \text{constant} \quad (9.5-73)$$

$$\boxed{\text{Sh} = 4.36 + \frac{0.023 [(D/L) \text{Re Sc}]}{1 + 0.0012 [(D/L) \text{Re Sc}]}} \quad N_{A_w} = \text{constant} \quad (9.5-74)$$

In the calculation of the mass transfer rates by the use of Eqs. (9.5-73) and (9.5-74), the appropriate driving force is the log-mean concentration difference.

**Example 9.12** *Pure water at  $25^\circ\text{C}$  flows through a smooth metal pipe of 6 cm internal diameter with an average velocity of  $1.5 \times 10^{-3}$  m/s. Once the fully developed velocity profile is established, the metal pipe is replaced by a pipe, cast from benzoic acid, of the same inside diameter. If the length of the pipe made of a benzoic acid is 2 m, calculate the concentration of benzoic acid in water at the exit of the pipe.*

#### Solution

##### Physical properties

From Example 4.8:

$$\text{For water (B) at } 25^\circ\text{C (298 K)} : \begin{cases} \rho = 1000 \text{ kg/m}^3 \\ \mu = 892 \times 10^{-6} \text{ kg/m}\cdot\text{s} \\ \mathcal{D}_{AB} = 1.21 \times 10^{-9} \text{ m}^2/\text{s} \end{cases}$$

$$\text{Sc} = 737$$

$$\text{Saturation solubility of benzoic acid (A) in water} = 3.412 \text{ kg/m}^3$$

**Analysis**

The Reynolds number is

$$\begin{aligned} \text{Re} &= \frac{D \langle v_z \rangle \rho}{\mu} \\ &= \frac{(6 \times 10^{-2})(1.5 \times 10^{-3})(1000)}{892 \times 10^{-6}} = 101 \quad \Rightarrow \quad \text{Laminar flow} \quad (1) \end{aligned}$$

Note that the term  $(D/L) \text{Re Sc}$  becomes

$$\left(\frac{D}{L}\right) \text{Re Sc} = \left(\frac{6 \times 10^{-2}}{2}\right) (101)(737) = 2233 \quad (2)$$

Since the concentration at the surface of the pipe is constant, the use of Eq. (9.5-73) gives

$$\begin{aligned} \text{Sh} &= 3.66 + \frac{0.668 [(D/L) \text{Re Sc}]}{1 + 0.04 [(D/L) \text{Re Sc}]^{2/3}} \\ &= 3.66 + \frac{0.0668 (2233)}{1 + 0.04 (2233)^{2/3}} = 22.7 \quad (3) \end{aligned}$$

Considering the water in the pipe as a system, a macroscopic mass balance on benzoic acid gives

$$\underbrace{(\pi D^2/4) \langle v_z \rangle}_{\dot{Q}} [(c_{A_b})_{out} - (c_{A_b})_{in}] = \underbrace{(\pi DL) \langle k_c \rangle}_{A_M} \underbrace{\frac{[c_{A_w} - (c_{A_b})_{out}] - [c_{A_w} - (c_{A_b})_{in}]}{\ln \left[ \frac{c_{A_w} - (c_{A_b})_{out}}{c_{A_w} - (c_{A_b})_{in}} \right]}}_{(\Delta c_A)_{LM}} \quad (4)$$

Since  $(c_{A_b})_{in} = 0$ , Eq. (4) simplifies to

$$\begin{aligned} (c_{A_b})_{out} &= c_{A_w} \left[ 1 - \exp \left( -\frac{4L}{D} \frac{\langle k_c \rangle}{\langle v_z \rangle} \right) \right] \\ &= c_{A_w} \left[ 1 - \exp \left( -\frac{4L}{D} \frac{\text{Sh}}{\text{Re Sc}} \right) \right] \quad (5) \end{aligned}$$

Substitution of numerical values into Eq. (5) gives

$$\begin{aligned} (c_{A_b})_{out} &= 3.412 \left\{ 1 - \exp \left[ -\frac{4(2)(22.7)}{(6 \times 10^{-2})(101)(737)} \right] \right\} \\ &= 0.136 \text{ kg/m}^3 \quad (6) \end{aligned}$$

**Comment:** One could also use Eq. (4.5-31) to calculate the Sherwood number, i.e.,

$$\begin{aligned} \text{Sh} &= 1.86 [\text{Re Sc}(D/L)]^{1/3} \\ &= 1.86 (2233)^{1/3} = 24.3 \end{aligned}$$

which is not very much different from 22.7.

### 9.5.2 Diffusion Into a Falling Liquid Film

Consider gas absorption in a wetted-wall column as shown in Figure 9.20. An incompressible Newtonian liquid ( $B$ ) flows in laminar flow over a flat plate of width  $W$  and length  $L$  as a thin film of thickness  $\delta$  under the action of gravity. Gas  $A$  flows in a countercurrent direction to the liquid and we want to determine the amount of  $A$  absorbed by the liquid.

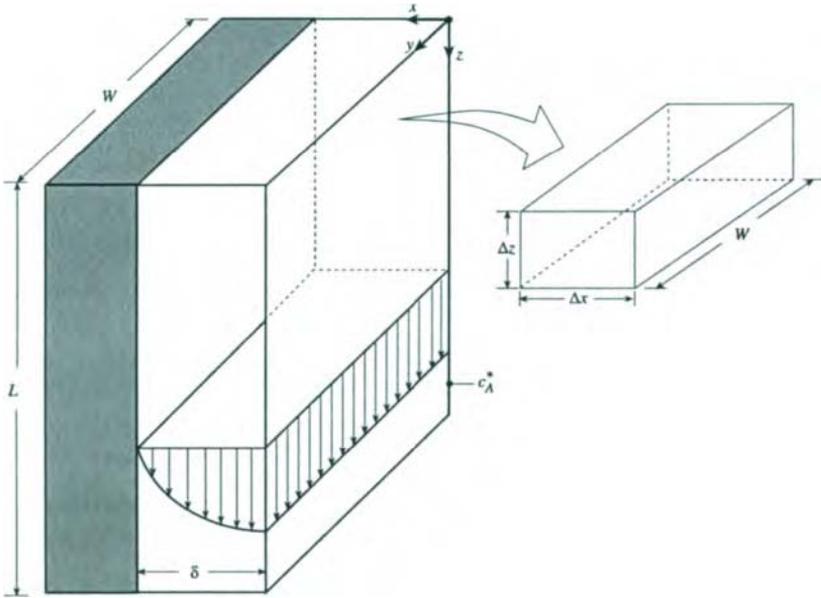


Figure 9.20 Diffusion into a falling liquid film.

The fully developed velocity distribution is given by Eqs. (9.1-57) and (9.1-58) as

$$v_z = v_{\max} \left[ 1 - \left( \frac{x}{\delta} \right)^2 \right] \quad (9.5-75)$$

where

$$v_{\max} = \frac{3}{2} \langle v_z \rangle = \frac{\rho g \delta^2}{2\mu} \quad (9.5-76)$$

Liquid viscosity is assumed to be unaffected by mass transfer.

In general, the concentration of species  $A$  in the liquid phase changes as a function of  $x$  and  $z$ . Therefore, from Table C.7 in Appendix C, the non-zero mass flux components are

$$\mathcal{W}_{A_x} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial x} \quad (9.5-77)$$

$$\mathcal{W}_{A_z} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial z} + \rho_A v_z \quad (9.5-78)$$

For a dilute liquid solution, the total density is almost constant and Eqs. (9.5-77) and (9.5-78) become

$$W_{A_x} = -D_{AB} \frac{\partial \rho_A}{\partial x} \tag{9.5-79}$$

$$W_{A_z} = -D_{AB} \frac{\partial \rho_A}{\partial z} + \rho_A v_z \tag{9.5-80}$$

Dividing Eqs. (9.5-79) and (9.5-80) by the molecular weight of species  $\mathcal{A}$ ,  $\mathcal{M}_A$ , gives

$$N_{A_x} = -D_{AB} \frac{\partial c_A}{\partial x} \tag{9.5-81}$$

$$N_{A_z} = -D_{AB} \frac{\partial c_A}{\partial z} + c_A v_z \tag{9.5-82}$$

Since there is no generation of species  $\mathcal{A}$ , Eq. (9.4-1) simplifies to

$$\left( \begin{array}{c} \text{Rate of} \\ \text{species } \mathcal{A} \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{species } \mathcal{A} \text{ out} \end{array} \right) = 0 \tag{9.5-83}$$

For a rectangular differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , as shown in Figure 9.20, Eq. (9.5-83) is expressed as

$$(N_{A_x}|_x W \Delta z + N_{A_z}|_z W \Delta x) - (N_{A_x}|_{x+\Delta x} W \Delta z + N_{A_z}|_{z+\Delta z} W \Delta x) = 0 \tag{9.5-84}$$

Dividing Eq. (9.5-84) by  $W \Delta x \Delta z$  and taking the limit as  $\Delta x \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta x \rightarrow 0} \frac{N_{A_x}|_x - N_{A_x}|_{x+\Delta x}}{\Delta x} + \lim_{\Delta z \rightarrow 0} \frac{N_{A_z}|_z - N_{A_z}|_{z+\Delta z}}{\Delta z} = 0 \tag{9.5-85}$$

or,

$$\frac{\partial N_{A_x}}{\partial x} + \frac{\partial N_{A_z}}{\partial z} = 0 \tag{9.5-86}$$

Substitution of Eqs. (9.5-81) and (9.5-82) into Eq. (9.5-86) yields

$$\underbrace{v_z \frac{\partial c_A}{\partial z}}_{\text{Convection in } z\text{-direction}} = \underbrace{D_{AB} \frac{\partial^2 c_A}{\partial x^2}}_{\text{Diffusion in } x\text{-direction}} + \underbrace{D_{AB} \frac{\partial^2 c_A}{\partial z^2}}_{\text{Diffusion in } z\text{-direction}} \tag{9.5-87}$$

In the  $z$ -direction, the mass of species  $\mathcal{A}$  is transported by both convection and diffusion. As stated by Eq. (2.4-8), diffusion can be considered negligible with respect to convection when  $Pe_M \gg 1$ . Under these circumstances, Eq. (9.5-87) reduces to

$$\boxed{v_{\max} \left[ 1 - \left( \frac{x}{\delta} \right)^2 \right] \frac{\partial c_A}{\partial z} = D_{AB} \frac{\partial^2 c_A}{\partial x^2}} \tag{9.5-88}$$

The boundary conditions associated with Eq. (9.5-88) are

$$\text{at } z = 0 \quad c_A = c_{A_o} \quad (9.5-89)$$

$$\text{at } x = 0 \quad c_A = c_A^* \quad (9.5-90)$$

$$\text{at } x = \delta \quad \frac{\partial c_A}{\partial x} = 0 \quad (9.5-91)$$

It is assumed that the liquid has a uniform concentration of  $c_{A_o}$  for  $z < 0$ . At the liquid-gas interface, the value of  $c_A^*$  is determined from the solubility data, i.e., Henry's law. Equation (9.5-91) indicates that species  $A$  cannot diffuse through the wall.

The problem will be analyzed for two cases, namely, for long and short contact times.

### 9.5.2.1 Long contact times

The solution of Eq. (9.5-88) subject to the boundary conditions given by Eqs. (9.5-89)-(9.5-91) is first obtained by Johnstone and Pigford (1942). Their series solution expresses the bulk concentration of species  $A$  at  $z = L$  as

$$\frac{c_A^* - (c_{A_b})_L}{c_A^* - c_{A_o}} = 0.7857 e^{-5.1213 \eta} + 0.1001 e^{-39.318 \eta} + 0.03599 e^{-105.64 \eta} + \dots \quad (9.5-92)$$

where

$$\eta = \frac{D_{AB} L}{\delta^2 v_{\max}} = \frac{2 D_{AB} L}{3 \delta^2 \langle v_z \rangle} \quad (9.5-93)$$

As an engineer we are interested in expressing the results in the form of a mass transfer correlation. For this purpose it is first necessary to obtain an expression for the mass transfer coefficient.

For a rectangular differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , as shown in Figure 9.20, the conservation statement given by Eq. (9.5-83) is also expressed as

$$[Q c_{A_b}|_z + k_c (c_A^* - c_{A_b}) W \Delta z] - Q c_{A_b}|_{z+\Delta z} = 0 \quad (9.5-94)$$

Dividing Eq. (9.5-94) by  $\Delta z$  and taking the limit as  $\Delta z \rightarrow 0$  gives

$$Q \lim_{\Delta z \rightarrow 0} \frac{c_{A_b}|_z - c_{A_b}|_{z+\Delta z}}{\Delta z} + k_c (c_A^* - c_{A_b}) W = 0 \quad (9.5-95)$$

or,

$$Q \frac{dc_{A_b}}{dz} = k_c (c_A^* - c_{A_b}) W \quad (9.5-96)$$

Equation (9.5-96) is a separable equation and rearrangement gives

$$Q \int_{c_{A_o}}^{(c_{A_b})_L} \frac{dc_{A_b}}{c_A^* - c_{A_b}} = W \int_0^L k_c dz \quad (9.5-97)$$

Carrying out the integrations yields

$$\langle k_c \rangle = \frac{Q}{WL} \ln \left[ \frac{c_A^* - c_{A_o}}{c_A^* - (c_{A_b})_L} \right] \quad (9.5-98)$$

where the average mass transfer coefficient,  $\langle k_c \rangle$ , is defined by

$$\langle k_c \rangle = \frac{1}{L} \int_0^L k_c dz \quad (9.5-99)$$

The rate of moles of species  $A$  transferred to the liquid is

$$\dot{n}_A = Q [(c_{A_b})_L - c_{A_o}] = Q \{(c_A^* - c_{A_o}) - [c_A^* - (c_{A_b})_L]\} \quad (9.5-100)$$

Elimination of  $Q$  between Eqs. (9.5-98) and (9.5-100) leads to

$$\dot{n}_A = (WL) \langle k_c \rangle \underbrace{\frac{(c_A^* - c_{A_o}) - [c_A^* - (c_{A_b})_L]}{\ln \left[ \frac{c_A^* - c_{A_o}}{c_A^* - (c_{A_b})_L} \right]}}_{(\Delta c_A)_{LM}} \quad (9.5-101)$$

When  $\eta > 0.1$ , all the terms in Eq. (9.5-92), excluding the first, become almost zero, i.e.,

$$\frac{c_A^* - (c_{A_b})_L}{c_A^* - c_{A_o}} = 0.7857 e^{-5.1213 \eta} \quad (9.5-102)$$

The use of Eq. (9.5-102) in Eq. (9.5-98) gives

$$\langle k_c \rangle = \frac{Q}{WL} (5.1213 \eta + 0.241) \quad (9.5-103)$$

Since we restrict our analysis to long contact times, i.e.,  $\eta$  is large, then Eq. (9.5-103) simplifies to

$$\langle k_c \rangle = \frac{Q}{WL} (5.1213 \eta) \quad (9.5-104)$$

Substitution of Eq. (9.5-93) into Eq. (9.5-104) and the use of  $Q = \langle v_z \rangle W \delta$  gives

$$\langle k_c \rangle = 3.41 \frac{D_{AB}}{\delta} \quad (9.5-105)$$

Therefore, the average value of the Sherwood number becomes

$$\text{Sh} = \frac{\langle k_c \rangle \delta}{D_{AB}} = 3.41 \quad (9.5-106)$$

It is also possible to arrive at this result using a different approach (see Problem 9.17). Equation (9.5-106) is usually recommended when

$$\text{Re} = \frac{4 \delta \langle v_z \rangle \rho}{\mu} = \frac{4 \dot{m}}{\mu W} < 100 \quad (9.5-107)$$

Note that the term  $4\delta$  in the definition of the Reynolds number represents the hydraulic equivalent diameter.

### 9.5.2.2 Short contact times

If the solubility of species  $\mathcal{A}$  in the liquid  $\mathcal{B}$  is low, for short contact times, species  $\mathcal{A}$  penetrates only a short distance into the falling liquid film. Under these circumstances, species  $\mathcal{A}$ , for the most part, has the impression that the film is moving throughout with a velocity equal to  $v_{\max}$ . Furthermore, species  $\mathcal{A}$  does not feel the presence of the solid wall at  $x = \delta$ . Hence, if the film were of infinite thickness moving with the velocity  $v_{\max}$ , species  $\mathcal{A}$  would not know the difference.

In the light of the above discussion, Eqs. (9.5-88)-(9.5-91) take the following form

$$v_{\max} \frac{\partial c_A}{\partial z} = \mathcal{D}_{AB} \frac{\partial^2 c_A}{\partial x^2} \quad (9.5-108)$$

$$\text{at } z = 0 \quad c_A = c_{A_o} \quad (9.5-109)$$

$$\text{at } x = 0 \quad c_A = c_A^* \quad (9.5-110)$$

$$\text{at } x = \infty \quad c_A = c_{A_o} \quad (9.5-111)$$

Introduction of the dimensionless concentration  $\phi$  as

$$\phi = \frac{c_A - c_{A_o}}{c_A^* - c_{A_o}} \quad (9.5-112)$$

reduces Eqs. (9.5-108)-(9.5-111) to

$$v_{\max} \frac{\partial \phi}{\partial z} = \mathcal{D}_{AB} \frac{\partial^2 \phi}{\partial x^2} \quad (9.5-113)$$

$$\text{at } z = 0 \quad \phi = 0 \quad (9.5-114)$$

$$\text{at } x = 0 \quad \phi = 1 \quad (9.5-115)$$

$$\text{at } x = \infty \quad \phi = 0 \quad (9.5-116)$$

Since Eqs. (9.5-114) and (9.5-116) are the same and there is no length scale, this parabolic partial differential equation can be solved by the similarity solution as explained in Section B.3.6.2 in Appendix B. The solution is sought in the form

$$\phi = f(\Psi) \quad (9.5-117)$$

where

$$\Psi = \frac{x}{\sqrt{4\mathcal{D}_{AB}z/v_{\max}}} \quad (9.5-118)$$

The chain rule of differentiation gives

$$\begin{aligned}\frac{\partial \phi}{\partial z} &= \frac{df}{d\Psi} \frac{\partial \Psi}{\partial z} \\ &= -\frac{1}{2} \frac{\Psi}{z} \frac{df}{d\Psi}\end{aligned}\quad (9.5-119)$$

$$\begin{aligned}\frac{\partial^2 \phi}{\partial x^2} &= \frac{d^2 f}{d\Psi^2} \left( \frac{\partial \Psi}{\partial x} \right)^2 + \frac{df}{d\Psi} \frac{\partial^2 \Psi}{\partial x^2} \\ &= \frac{v_{\max}}{4 D_{AB} z} \frac{d^2 f}{d\Psi^2}\end{aligned}\quad (9.5-120)$$

Substitution of Eqs. (9.5-119) and (9.5-120) into Eq. (9.5-113) yields

$$\frac{d^2 f}{d\Psi^2} + 2 \Psi \frac{df}{d\Psi} = 0 \quad (9.5-121)$$

The boundary conditions associated with Eq. (9.5-121) are

$$\text{at } \Psi = 0 \quad \phi = 1 \quad (9.5-122)$$

$$\text{at } \Psi = \infty \quad \phi = 0 \quad (9.5-123)$$

The integrating factor for Eq. (9.5-121) is  $\exp(\Psi^2)$ . Multiplication of Eq. (9.5-121) by the integrating factor gives

$$\frac{d}{d\Psi} \left( e^{\Psi^2} \frac{df}{d\Psi} \right) = 0 \quad (9.5-124)$$

which implies that

$$\frac{df}{d\Psi} = K_1 e^{-\Psi^2} \quad (9.5-125)$$

Integration of Eq. (9.5-125) leads to

$$f = K_1 \int_0^{\Psi} e^{-u^2} du + K_2 \quad (9.5-126)$$

where  $u$  is a dummy variable of integration. Application of the boundary condition defined by Eq. (9.5-122) gives  $K_2 = 1$ . On the other hand, the use of the boundary condition defined by Eq. (9.5-123) gives

$$K_1 = -\frac{1}{\int_0^{\infty} e^{-u^2} du} = -\frac{2}{\sqrt{\pi}} \quad (9.5-127)$$

Therefore, the solution becomes

$$f = 1 - \frac{2}{\sqrt{\pi}} \int_0^{\Psi} e^{-u^2} du \quad (9.5-128)$$

or,

$$\boxed{\frac{c_A - c_{A_o}}{c_A^* - c_{A_o}} = 1 - \operatorname{erf}\left(\frac{x}{\sqrt{4D_{AB}z/v_{\max}}}\right)} \quad (9.5-129)$$

where  $\operatorname{erf}(x)$  is the error function defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du \quad (9.5-130)$$

### Macroscopic equation

Integration of the governing equation, Eq. (9.5-108), over the volume of the system gives the macroscopic equation as

$$\int_0^L \int_0^W \int_0^\delta v_{\max} \frac{\partial c_A}{\partial z} dx dy dz = \int_0^L \int_0^W \int_0^\delta D_{AB} \frac{\partial^2 c_A}{\partial x^2} dx dy dz \quad (9.5-131)$$

Evaluation of the integrations yields

$$\underbrace{v_{\max} W \int_0^\delta (c_A|_{z=L} - c_{A_o}) dx}_{\text{Net molar rate of species } \mathcal{A} \text{ entering into the liquid}} = \underbrace{W \int_0^L \left( -D_{AB} \frac{\partial c_A}{\partial x} \right)_{x=0} dz}_{\text{Molar rate of species } \mathcal{A} \text{ entering into the liquid through interface}} \quad (9.5-132)$$

Note that Eq. (9.5-132) is the macroscopic inventory rate equation for the mass of species  $\mathcal{A}$  by considering the falling liquid film as a system. The use of Eq. (9.5-129) in Eq. (9.5-132) gives the rate of moles of species  $\mathcal{A}$  absorbed in the liquid as

$$\boxed{\dot{n}_A = WL(c_A^* - c_{A_o}) \sqrt{\frac{4D_{AB}v_{\max}}{\pi L}}} \quad (9.5-133)$$

The rate of moles of species  $\mathcal{A}$  absorbed by the liquid can be expressed in terms of the average mass transfer coefficient as

$$\dot{n}_A = WL \langle k_c \rangle \left\{ \frac{[c_A^* - (c_{A_b})_L] - (c_A^* - c_{A_o})}{\ln \left[ \frac{c_A^* - (c_{A_b})_L}{c_A^* - c_{A_o}} \right]} \right\} \quad (9.5-134)$$

Since  $\ln(1+x) \simeq x$  for small values of  $x$ , the term in the denominator of Eq. (9.5-134) can be approximated as

$$\begin{aligned} \ln \left[ \frac{c_A^* - (c_{A_b})_L}{c_A^* - c_{A_o}} \right] &= \ln \left[ 1 + \frac{c_{A_o} - (c_{A_b})_L}{c_A^* - c_{A_o}} \right] \\ &\simeq \frac{c_{A_o} - (c_{A_b})_L}{c_A^* - c_{A_o}} \end{aligned} \quad (9.5-135)$$

The use of Eq. (9.5-135) in Eq. (9.5-134) gives

$$\dot{n}_A = WL\langle k_c \rangle (c_A^* - c_{A_o}) \quad (9.5-136)$$

The average mass transfer coefficient can be calculated from Eqs. (9.5-133) and (9.5-136) as

$$\langle k_c \rangle = \sqrt{\frac{4D_{AB}v_{\max}}{\pi L}} \quad (9.5-137)$$

Therefore, the Sherwood number is

$$\text{Sh} = \frac{\langle k_c \rangle \delta}{D_{AB}} = \sqrt{\frac{4\delta^2 v_{\max}}{\pi D_{AB}L}} = 0.691 \left( \frac{\delta}{L} \right)^{1/2} \text{Re}^{1/2} \text{Sc}^{1/2} \quad (9.5-138)$$

Equation (9.5-138) is recommended when

$$1200 > \text{Re} = \frac{4\delta \langle v_z \rangle \rho}{\mu} = \frac{4\dot{m}}{\mu W} > 100$$

It should be kept in mind that the calculated mass of species  $A$  absorbed by the liquid based on Eq. (9.5-133) usually underestimates the actual amount. This is due to the increase in the mass transfer area as a result of ripple formation even at a very small values of  $\text{Re}$ , i.e.,  $\text{Re} > 20$ .

In the literature, Eq. (9.5-137) is also expressed in the form

$$\langle k_c \rangle = \sqrt{\frac{4D_{AB}}{\pi t_{\text{exp}}}} \quad (9.5-139)$$

where the *exposure time*, or, *gas-liquid contact time*, is defined by

$$t_{\text{exp}} = \frac{L}{v_{\max}} \quad (9.5-140)$$

Equation (9.5-139) is also applicable to gas absorption to laminar liquid jets and mass transfer from ascending bubbles, if the penetration distance of the solute is small.

**Example 9.13** A laminar liquid jet issuing at a volumetric flow rate of  $Q$  is used for absorption of gas  $A$ . If the jet has a diameter  $D$  and a length  $L$ , derive an expression for the rate of absorption of species  $A$ .

### Solution

The time of exposure can be defined by

$$t_{\text{exp}} = \frac{L}{\langle v \rangle} = \frac{L}{4Q/\pi D^2} \quad (1)$$

Therefore, Eq. (9.5-139) becomes

$$\langle k_c \rangle = \frac{4}{\pi D} \sqrt{\frac{Q \mathcal{D}_{AB}}{L}} \quad (2)$$

The rate of moles of species  $A$  absorbed by the jet is

$$\dot{n}_A = (\pi D L) \langle k_c \rangle (c_A^* - c_{A_o}) \quad (3)$$

where  $c_{A_o}$  is the initial concentration of species  $A$  in the jet and  $c_A^*$  is the equilibrium solubility of species  $A$  in the liquid. Substitution of Eq. (2) into Eq. (3) gives

$$\dot{n}_A = 4 (c_A^* - c_{A_o}) \sqrt{Q \mathcal{D}_{AB} L} \quad (4)$$

### 9.5.3 Analysis of a Plug Flow Reactor

A plug flow reactor consists of a cylindrical pipe in which concentration, temperature, and reaction rate are assumed to vary only along the axial direction. Analysis of these reactors are usually done with the following assumptions:

- Steady-state conditions prevail.
- Reactor is isothermal.
- There is no mixing in the axial direction.

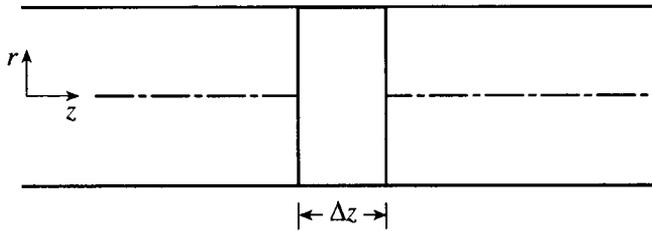


Figure 9.21 Plug flow reactor.

The conservation statement for species  $i$  over a differential volume element of thickness  $\Delta z$ , as shown in Figure 9.21, is expressed as

$$(Q c_i)|_z - (Q c_i)|_{z+\Delta z} + \alpha_i r A \Delta z = 0 \quad (9.5-141)$$

where  $\alpha_i$  is the stoichiometric coefficient of species  $i$  and  $r$  is the chemical reaction rate expression. Dividing Eq. (9.5-141) by  $\Delta z$  and taking the limit as  $\Delta z \rightarrow 0$  gives

$$\lim_{\Delta z \rightarrow 0} \frac{(Q c_i)|_z - (Q c_i)|_{z+\Delta z}}{\Delta z} + \alpha_i r A = 0 \quad (9.5-142)$$

or,

$$\frac{d(Q c_i)}{dz} = \alpha_i r A \quad (9.5-143)$$

It is customary to write Eq. (9.5-143) in terms of  $dV = A dz$  rather than  $dz$ , so that Eq. (9.5-143) becomes

$$\frac{d(Q c_i)}{dV} = \alpha_i r \quad (9.5-144)$$

Equation (9.5-144) can also be expressed in the form

$$\frac{d\dot{n}_i}{dV} = \alpha_i r \quad (9.5-145)$$

where  $\dot{n}_i$  is the molar flow rate of species  $i$ .

The variation of the number of moles of species  $i$  as a function of the molar extent of the reaction is given by Eq. (5.3-10). It is also possible to express this equation as

$$\dot{n}_i = \dot{n}_{i_0} + \alpha_i \dot{\epsilon} \quad (9.5-146)$$

Let us assume that the rate of reaction has the form

$$r = k c_i^n = k \left( \frac{\dot{n}_i}{Q} \right)^n \quad (9.5-147)$$

Substitution of Eq. (9.5-147) into Eq. (145) gives

$$\boxed{\frac{d\dot{n}_i}{dV} = \alpha_i k \left( \frac{\dot{n}_i}{Q} \right)^n} \quad (9.5-148)$$

Integration of Eq. (9.5-148) depends on whether the volumetric flow rate is constant or not.

### 9.5.3.1 Constant volumetric flow rate

When steady-state conditions prevail, the mass flow rate is constant. The volumetric flow rate is the mass flow rate divided by the total mass density, i.e.,

$$Q = \frac{\dot{m}}{\rho} \quad (9.5-149)$$

For most liquid phase reactions the total mass density,  $\rho$ , and hence the volumetric flow rate are constant.

For gas phase reactions, on the other hand, the total mass density is given by the ideal gas equation of state as

$$\rho = \frac{PM}{\mathcal{R}T} \quad (9.5-150)$$

where  $\mathcal{M}$  is the molecular weight of the reacting mixture. Substitution of Eq. (9.5-150) into Eq. (9.5-149) gives

$$Q = \frac{\dot{n} \mathcal{R} T}{P} \quad (9.5-151)$$

Therefore,  $Q$  remains constant when  $\dot{n}$  and  $P$  do not change along the reactor. The conditions for the constancy of  $Q$  are summarized in Table 9.4.

**Table 9.4** Requirements for the constant volumetric flow rate for a plug flow reactor operating under steady and isothermal conditions.

Liquid Phase Reactions	Gas Phase Reactions
Constant total mass density	<ul style="list-style-type: none"> <li>■ No change in the total number of moles during reaction (<math>\bar{\alpha} = 0</math>)</li> <li>■ Negligible pressure drop across the reactor</li> </ul>

When  $Q$  is constant, Eq. (9.5-148) can be rearranged as

$$\int_0^V dV = \frac{Q^n}{\alpha_i k} \int_{\dot{n}_{i_0}}^{\dot{n}_i} \frac{d\dot{n}_i}{\dot{n}_i^n} \quad (9.5-152)$$

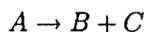
Depending on the values of  $n$  the results are

$$V = \begin{cases} \frac{Q}{\alpha_i k} (c_i - c_{i_0}) & n = 0 \\ \frac{Q}{\alpha_i k} \ln \left( \frac{c_i}{c_{i_0}} \right) & n = 1 \\ \frac{Q}{\alpha_i k} \frac{1}{1-n} \left( \frac{1}{c_i^{1-n}} - \frac{1}{c_{i_0}^{1-n}} \right) & n \geq 2 \end{cases} \quad (9.5-153)$$

### 9.5.3.2 Variable volumetric flow rate

When the volumetric flow rate is not constant, integration of Eq. (9.5-148) is possible only after expressing both  $\dot{n}_i$  and  $Q$  in terms of  $\dot{\epsilon}$ . The following example explains the procedure in detail.

**Example 9.14** *The irreversible gas phase reaction*



is carried out in a constant pressure batch reactor at 400°C and 5 atm pressure. The reaction is first-order and the time required to achieve 60% conversion was found to be 50 min.

Suppose that this reaction is to be carried out in a plug flow reactor which operates isothermally at 400°C and at a pressure of 10 atm. The volumetric flow rate of the feed entering the reactor is 0.05 m<sup>3</sup>/h and it consists of pure A. Calculate the volume of the reactor required to achieve 80% conversion.

### Solution

First, it is necessary to determine the rate constant by using the data given for the batch reactor. The conservation statement for the number of moles of species A, Eq. (7.2-5), reduces to

$$\alpha_A r V = \frac{dn_A}{dt} \quad (1)$$

or,

$$-k c_A V = \frac{dn_A}{dt} \quad (2)$$

Substitution of the identity  $n_A = c_A V$  into Eq. (2) and rearrangement gives

$$-k \int_0^t dt = \int_{n_{A_0}}^{n_A} \frac{dn_A}{dt} \quad (3)$$

Integration gives the rate constant,  $k$ , as

$$k = -\frac{1}{t} \ln \left( \frac{n_A}{n_{A_0}} \right) \quad (4)$$

The fractional conversion,  $X$ , is

$$X = \frac{n_{A_0} - n_A}{n_{A_0}} = 1 - \frac{n_A}{n_{A_0}} \quad (5)$$

Therefore, Eq. (4) can be expressed in terms of the fractional conversion as

$$k = -\frac{\ln(1 - X)}{t} \quad (6)$$

Substitution of the numerical values into Eq. (6) gives

$$k = -\frac{\ln(1 - 0.6)}{(50/60)} = 1.1 \text{ h}^{-1} \quad (7)$$

For a plug flow reactor, Eq. (9.5-148) takes the form

$$\frac{d\dot{n}_A}{dV} = -k \frac{\dot{n}_A}{Q} \quad (8)$$

Since the volumetric flow rate is not constant, i.e.,  $\bar{\alpha} = 1$ , it is necessary to express  $Q$  in terms of  $\dot{\epsilon}$ . The use of Eq. (9.5-146) gives

$$\dot{n}_A = \dot{n}_{A_o} - \dot{\epsilon} \quad (9)$$

$$\dot{n}_B = \dot{\epsilon} \quad (10)$$

$$\dot{n}_C = \dot{\epsilon} \quad (11)$$

Therefore, the total molar flow rate,  $\dot{n}$ , is

$$\dot{n} = \dot{n}_{A_o} + \dot{\epsilon} \quad (12)$$

Substitution of Eq. (12) into Eq. (9.5-151) gives the volumetric flow rate as

$$\begin{aligned} Q &= \frac{\mathcal{R}T}{P} (\dot{n}_{A_o} + \dot{\epsilon}) \\ &= \frac{\mathcal{R}T \dot{n}_{A_o}}{P} \left( 1 + \frac{\dot{\epsilon}}{\dot{n}_{A_o}} \right) = Q_o \left( 1 + \frac{\dot{\epsilon}}{\dot{n}_{A_o}} \right) \end{aligned} \quad (13)$$

where  $Q_o$  is the volumetric flow rate at the inlet of the reactor.

Substitution of Eqs. (9) and (13) into Eq. (8) gives

$$\frac{d\dot{\epsilon}}{dV} = \frac{k \dot{n}_{A_o} [1 - (\dot{\epsilon}/\dot{n}_{A_o})]}{Q_o (1 + \dot{\epsilon}/\dot{n}_{A_o})} \quad (14)$$

The fractional conversion expression for a plug flow reactor is similar to Eq. (5), so

$$X = \frac{\dot{n}_{A_o} - \dot{n}_A}{\dot{n}_{A_o}} = 1 - \frac{\dot{n}_A}{\dot{n}_{A_o}} \quad (15)$$

Substitution of Eq. (9) into Eq. (15) yields

$$X = \frac{\dot{\epsilon}}{\dot{n}_{A_o}} \quad (16)$$

The use of Eq. (16) in Eq. (14) and rearrangement gives

$$\begin{aligned} V &= \frac{Q_o}{k} \int_0^{0.8} \left( \frac{1+X}{1-X} \right) dX \\ &= 2.42 \left( \frac{Q_o}{k} \right) \end{aligned} \quad (17)$$

Substitution of the numerical values into Eq. (17) gives

$$V = \frac{(2.42)(0.05)}{1.1} = 0.11 \text{ m}^3 \quad (18)$$

## NOTATION

$A$	area, $\text{m}^2$
$A_H$	heat transfer area, $\text{m}^2$
$A_M$	mass transfer area, $\text{m}^2$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ}/\text{kg}\cdot\text{K}$
$c$	total concentration, $\text{kmol}/\text{m}^3$
$c_i$	concentration of species $i$ , $\text{kmol}/\text{m}^3$
$D$	pipe diameter, $\text{m}$
$D_{AB}$	diffusion coefficient for system $A$ - $B$ , $\text{m}^2/\text{s}$
$e$	total energy flux, $\text{W}/\text{m}^2$
$F_D$	drag force, $\text{N}$
$f$	friction factor
$g$	acceleration of gravity, $\text{m}/\text{s}^2$
$h$	heat transfer coefficient, $\text{W}/\text{m}^2\cdot\text{K}$
$J^*$	molecular molar flux, $\text{kmol}/\text{m}^2\cdot\text{s}$
$K$	kinetic energy per unit volume, $\text{J}/\text{m}^3$
$k$	reaction rate constant; thermal conductivity, $\text{W}/\text{m}\cdot\text{K}$
$k_c$	mass transfer coefficient, $\text{m}/\text{s}$
$L$	length, $\text{m}$
$\dot{m}$	mass flow rate, $\text{kg}/\text{s}$
$\mathcal{M}$	molecular weight, $\text{kg}/\text{kmol}$
$N$	total molar flux, $\text{kmol}/\text{m}^2\cdot\text{s}$
$\dot{n}$	molar flow rate, $\text{kmol}/\text{s}$
$P$	pressure, $\text{Pa}$
$\mathcal{P}$	modified pressure, $\text{Pa}$
$\dot{Q}$	heat transfer rate, $\text{W}$
$Q$	volumetric flow rate, $\text{m}^3/\text{s}$
$q$	heat flux, $\text{W}/\text{m}^2$
$r$	rate of a chemical reaction, $\text{kmol}/\text{m}^3\cdot\text{s}$
$\mathfrak{R}$	Rate of generation per unit volume
$\mathcal{R}$	gas constant, $\text{J}/\text{mol}\cdot\text{K}$
$T$	temperature, $^\circ\text{C}$ or $\text{K}$
$t$	time, $\text{s}$
$V$	velocity of the plate in Couette flow, $\text{m}/\text{s}$ ; volume, $\text{m}^3$
$v$	velocity, $\text{m}/\text{s}$
$W$	width, $\text{m}$
$\mathcal{W}$	total mass flux, $\text{kg}/\text{m}^2\cdot\text{s}$
$X$	fractional conversion
$x$	rectangular coordinate, $\text{m}$
$z$	rectangular coordinate, $\text{m}$
$\alpha_i$	stoichiometric coefficient of species $i$
$\Delta$	difference

$\Delta H_{rxn}$	heat of reaction, J
$\dot{\epsilon}$	time rate of change of molar extent, kmol/s
$\lambda$	latent heat of vaporization, J
$\nu$	kinematic viscosity, m <sup>2</sup> /s
$\mu$	viscosity, kg/m.s
$\pi$	total momentum flux, N/m <sup>2</sup>
$\rho$	density, kg/m <sup>3</sup>
$\tau_{ij}$	shear stress (flux of $j$ – momentum in the $i$ – direction, N/m <sup>2</sup> )
$\omega$	mass fraction

**Overlines**

$\sim$	per mole
$\hat{\phantom{a}}$	per unit mass
$\bar{\phantom{a}}$	partial molar

**Bracket**

$\langle a \rangle$	average value of $a$
---------------------	----------------------

**Superscripts**

$A$	air
$L$	liquid
$o$	standard state
$sat$	saturation

**Subscripts**

$A, B$	species in binary systems
$b$	bulk
$ch$	characteristic
$exp$	exposure
$i$	species in multicomponent systems
$in$	inlet
$int$	interphase
$LM$	log-mean
$max$	maximum
$out$	out
$ref$	reference
$sys$	system
$w$	wall or surface
$\infty$	free-stream

**Dimensionless Numbers**

Br	Brinkman number
Nu	Nusselt number
Pr	Prandtl number
Re	Reynolds number

$Re_h$	Reynolds number based on the hydraulic equivalent diameter
$Sc$	Schmidt number
$Sh$	Sherwood number
$St_H$	Stanton number for heat transfer
$St_M$	Stanton number for mass transfer

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## PROBLEMS

9.1 The hydrostatic pressure distribution in fluids can be calculated from the equation

$$\frac{dP}{dz} = \rho g_z$$

where

$$g_z = \begin{cases} g & \text{if positive } z \text{ is in the direction of gravity} \\ -g & \text{if positive } z \text{ is in the direction opposite to gravity} \end{cases}$$

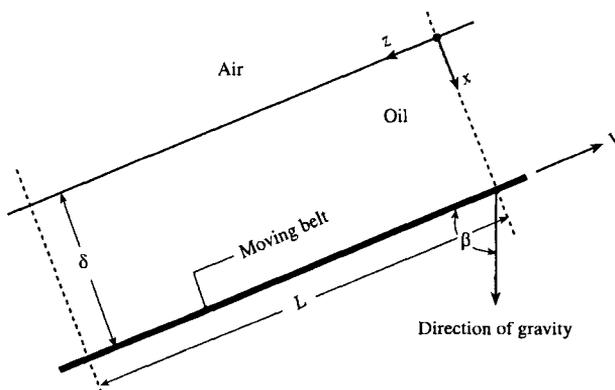
a) If the systolic pressure at the aorta is 120 mmHg, what is the pressure in the neck 25 cm higher and at a position in the legs 90 cm lower? The density of blood is 1.05 g/cm<sup>3</sup>.

b) The lowest point on the earth's surface is located in the western Pacific Ocean, in the Marianas Trench. It is about 11 km below sea level. Estimate the pressure at the bottom of the ocean. Take the density of seawater as 1025 kg/m<sup>3</sup>.

c) The highest point on the earth's surface is the top of Mount Everest, located in the Himalayas on the border of Nepal and China. It is approximately 8900 m above sea level. If the average rate of decrease in air temperature with altitude is 6.5 °C/km, estimate the air pressure at the top of Mount Everest. Assume that the temperature at sea level is 15 °C. Why is it difficult to breathe at high altitudes?

(Answer: a)  $P_{neck} = 100.7 \text{ mmHg}$ ,  $P_{leg} = 189.5 \text{ mmHg}$  b) 1090 atm c) 0.31 atm)

9.2 Oil spills on water can be removed by lowering a moving belt of width  $W$  into the water. The belt moves upward and skims the oil into a reservoir aboard the ship as shown in the figure below.



a) Show that the velocity profile and the volumetric flow rate are given by

$$v_z = \frac{\rho g \delta^2 \cos \beta}{2 \mu} \left[ 1 - \left( \frac{x}{\delta} \right)^2 \right] - V$$

$$Q = \frac{W \rho g \delta^3 \cos \beta}{3 \mu} - WV \delta$$

b) Determine the belt speed that will give a zero volumetric flow rate and specify the design criteria for positive and negative flow rates.

9.3 When the ratio of the radius of the inner pipe to that of the outer pipe is close to unity, a concentric annulus may be considered to be a thin plate slit and its curvature can be neglected. Use this approximation and show that the

modifications of Eqs. (9.1-23) and (9.1-26) for the axial flow in a concentric annulus with inner and outer radii of  $\kappa R$  and  $R$ , respectively, lead to

$$v_z = \frac{(\mathcal{P}_o - \mathcal{P}_L)R^2}{4\mu L} \left\{ 2(1 - \kappa) \left[ \frac{r}{R} - \kappa - \frac{1}{1 - \kappa} \left( \frac{r}{R} - \kappa \right)^2 \right] \right\}$$

$$\dot{Q} = \frac{\pi(\mathcal{P}_o - \mathcal{P}_L)R^4}{8\mu L} \left[ \frac{2(1 - \kappa^2)(1 - \kappa)^2}{3} \right]$$

**9.4** For laminar flow of a Newtonian fluid in a circular pipe the velocity profile is parabolic and Eqs. (9.1-80) and (9.1-84) indicate that

$$\frac{\langle v_z \rangle}{v_{\max}} = 0.5$$

In the case of a turbulent flow, experimentally determined velocity profiles can be represented in the form

$$v_z = v_{\max} \left( 1 - \frac{r}{R} \right)^{1/n}$$

where  $n$  depends on the value of the Reynolds number. Show that the ratio  $\langle v_z \rangle / v_{\max}$  is given as (Whitaker, 1968)

Re	$n$	$\langle v_z \rangle / v_{\max}$
$4 \times 10^3$	6	0.79
$1 \times 10^5$	7	0.82
$3 \times 10^6$	10	0.87

This is the reason why the velocity profile for a turbulent flow is generally considered “flat” in engineering analysis.

**9.5** The steady temperature distribution in a hollow cylinder of inner and outer radii of 50 cm and 80 cm, respectively, is given by

$$T = 5000(4.073 - 6r^2 + \ln r)$$

where  $T$  is in degrees Celsius and  $r$  is in meters. If the thermal conductivity is 5 W/m.K, find the rate of energy generation per unit volume.

(Answer:  $6 \times 10^5$  W/m<sup>3</sup>)

**9.6** Energy generation within a hollow cylinder of inside and outside radii of 60 cm and 80 cm, respectively, is  $10^6$  W/m<sup>3</sup>. If both surfaces are maintained at 55 °C and the thermal conductivity is 15 W/m.K, calculate the maximum temperature under steady conditions.

(Answer: 389.6 °C)

**9.7** The rate of generation per unit volume is sometimes expressed as a function of temperature rather than position. Consider the transmission of an electric current through a wire of radius  $R$ . If the surface temperature is constant at  $T_R$  and the rate of generation per unit volume is given as

$$\mathfrak{R} = \mathfrak{R}_o(1 + aT) \tag{1}$$

a) Show that the governing equation for temperature is given by

$$\frac{d}{dr} \left( r \frac{dT}{dr} \right) + \frac{\mathfrak{R}_o}{k}(1 + aT)r = 0 \tag{2}$$

b) Use the transformation

$$u = 1 + aT \tag{3}$$

and reduce Eq. (2) to the form

$$\frac{d}{dr} \left( r \frac{du}{dr} \right) + \phi r u = 0 \tag{4}$$

where

$$\phi = \frac{\mathfrak{R}_o a}{k} \tag{5}$$

c) Solve Eq. (4) to get

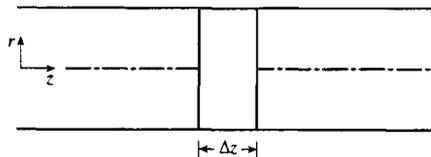
$$\frac{T + (1/a)}{T_R + (1/a)} = \frac{J_o(\sqrt{\phi}r)}{J_o(\sqrt{\phi}R)} \tag{6}$$

d) What happens to Eq. (6) when  $\sqrt{\phi}R = 2.4048$ ?

**9.8** For laminar flow forced convection in a circular pipe with a constant wall temperature, the governing equation for temperature, Eq. (9.3-9), is integrated over the cross-sectional area of the tube in Section 9.3.1 to obtain Eq. (9.3-18), i.e.,

$$\dot{m} \hat{C}_P \frac{dT_b}{dz} = \pi D h (T_w - T_b) \tag{1}$$

a) Now let us assume that the flow is turbulent. Over a differential volume element of thickness  $\Delta z$ , as shown in the figure below, write down the inventory rate equation for energy and show that the result is identical with Eq. (1).



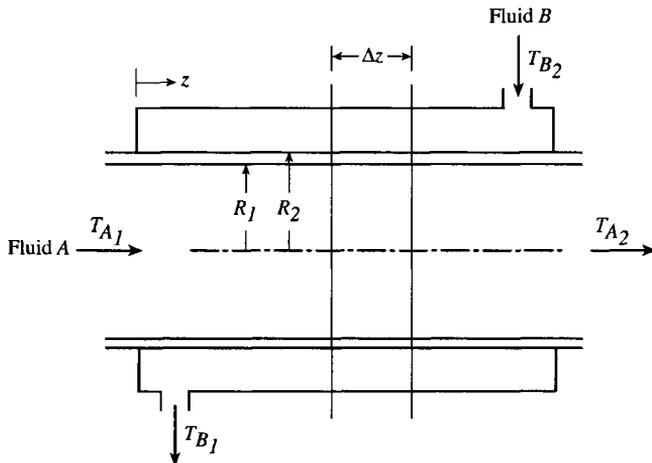
Integrate Eq. (1) to get

$$\dot{m} \hat{C}_P \ln \left( \frac{T_w - T_{b_{in}}}{T_w - T_{b_{out}}} \right) = \pi D \langle h \rangle L \quad (2)$$

b) Water enters the inner pipe ( $D = 23$  mm) of a double-pipe heat exchanger at  $15^\circ\text{C}$  with a mass flow rate of  $0.3$  kg/s. Steam condenses in the annular region so as to keep the wall temperature almost constant at  $112^\circ\text{C}$ . Determine the length of the heat exchanger if the outlet water temperature is  $35^\circ\text{C}$ .

(Answer: b) 1.13 m)

9.9 Consider the heating of fluid  $A$  by fluid  $B$  in a countercurrent double-pipe heat exchanger as shown in the figure below.



a) Show from the macroscopic energy balance that the rate of heat transferred is given by

$$\dot{Q} = (\dot{m} \hat{C}_P)_A (T_{A2} - T_{A1}) = (\dot{m} \hat{C}_P)_B (T_{B2} - T_{B1}) \quad (1)$$

where  $T_A$  and  $T_B$  are the bulk temperatures of the fluids  $A$  and  $B$ , respectively. Indicate your assumptions.

b) Over the differential volume element of thickness  $\Delta z$ , write down the inventory rate equation for energy for the fluids  $A$  and  $B$  separately and show that

$$(\dot{m} \hat{C}_P)_A \frac{dT_A}{dz} = \pi D_1 U_A (T_B - T_A) \quad (2)$$

$$(\dot{m} \hat{C}_P)_B \frac{dT_B}{dz} = \pi D_1 U_A (T_B - T_A) \quad (3)$$

where  $U_A$  is the overall heat transfer coefficient based on the inside radius of the inner pipe given by Eq. (8.2-42), i.e.,

$$U_A = \left[ \frac{1}{\langle h_A \rangle} + \frac{R_1 \ln(R_2/R_1)}{k_w} + \frac{R_1}{\langle h_B \rangle R_2} \right]^{-1} \quad (4)$$

in which  $k_w$  represents the thermal conductivity of the inner pipe.

c) Subtract Eq. (2) from Eq. (3) to obtain

$$\frac{d(T_B - T_A)}{dz} = \left[ \frac{1}{(\dot{m} \hat{C}_P)_B} - \frac{1}{(\dot{m} \hat{C}_P)_A} \right] \pi D_1 U_A (T_B - T_A) \quad (5)$$

d) Combine Eqs. (1) and (5) to get

$$\frac{d(T_B - T_A)}{dz} = \left[ \frac{(T_{B_2} - T_{A_2}) - (T_{B_1} - T_{A_1})}{\dot{Q}} \right] \pi D_1 U_A (T_B - T_A) \quad (6)$$

e) Integrate Eq. (6) and show that the rate of heat transferred is given as

$$\dot{Q} = (\pi D_1 L) U_A \Delta T_{LM} \quad (7)$$

where the logarithmic mean temperature difference is given by

$$\Delta T_{LM} = \frac{(T_{B_2} - T_{A_2}) - (T_{B_1} - T_{A_1})}{\ln \left( \frac{T_{B_2} - T_{A_2}}{T_{B_1} - T_{A_1}} \right)} \quad (8)$$

f) Consider the double-pipe heat exchanger given in Problem 9.8 in which oil is used as the heating medium instead of steam. Oil flows in a countercurrent direction to water and its temperature decreases from 130 °C to 80 °C. If the average heat transfer coefficient for the oil in the annular region is 1100 W/m<sup>2</sup>.K, calculate the length of the heat exchanger.

(Answer: f) 5.2m)

**9.10** You are a design engineer in a petroleum refinery. Oil is cooled from 60 °C to 40 °C in the inner pipe of a double-pipe heat exchanger. Cooling water flows countercurrently to the oil, entering at 15 °C and leaving at 35 °C. The oil tube has an inside diameter of 22 mm and an outside diameter of 25 mm with the inside and outside heat transfer coefficients of 600 and 1400 W/m<sup>2</sup>.K, respectively. It is required to increase the oil flow rate by 40%. Estimate the exit temperatures of both oil and water at the increased flow rate.

(Answer:  $T_{oil} = 43$  °C,  $T_{water} = 39$  °C)

**9.11** Repeat the analysis given in Section 9.3.2 for laminar flow of a Newtonian fluid between two fixed parallel plates under the action of a pressure gradient. The temperatures of the surfaces at  $x = 0$  and  $x = B$  are kept constant at  $T_o$ .

a) Obtain the temperature distribution as

$$T - T_o = \left( \frac{\mathcal{P}_o - \mathcal{P}_L}{L} \right)^2 \frac{B^4}{12 \mu k} \left[ \frac{1}{2} \left( \frac{x}{B} \right) - \frac{3}{2} \left( \frac{x}{B} \right)^2 + 2 \left( \frac{x}{B} \right)^3 - \left( \frac{x}{B} \right)^4 \right]$$

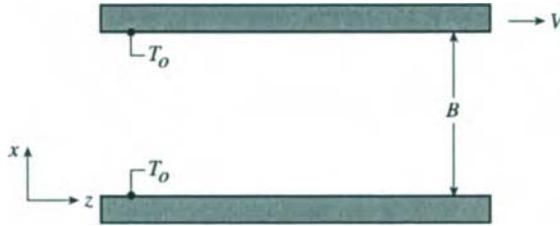
b) Show that the Nusselt number for the upper and lower plates are the same and equal to

$$\text{Nu} = \frac{2B \langle h \rangle}{k} = \frac{35}{2}$$

in which the term  $2B$  represents the hydraulic equivalent diameter.

**9.12** Consider Couette flow of a Newtonian liquid between two large parallel plates as shown in the figure below. As a result of the viscous dissipation, liquid temperature varies in the  $x$ -direction. Although the thermal conductivity and density of the liquid are assumed to be independent of temperature, the variation of the liquid viscosity with temperature is given as

$$\mu = \mu_o \exp \left[ -\beta \left( \frac{T - T_o}{T_o} \right) \right] \quad (1)$$



a) Show that the equations of motion and energy reduce to

$$\frac{d}{dz} \left( \mu \frac{dv_z}{dx} \right) = 0 \quad (2)$$

$$k \frac{d^2 T}{dx^2} + \mu \left( \frac{dv_z}{dx} \right)^2 = 0 \quad (3)$$

b) Integrate Eq. (1) and obtain the velocity distribution in the form

$$\frac{v_z}{V} = \frac{\int_0^x \frac{dx}{\mu}}{\int_0^B \frac{dx}{\mu}} \quad (4)$$

c) Substitute Eq. (4) into Eq. (3) to get

$$\frac{d^2 \theta}{d\xi^2} + \Lambda e^\theta = 0 \quad (5)$$

where the dimensionless quantities are defined by

$$\theta = \frac{\beta(T - T_o)}{T_o} \tag{6}$$

$$\xi = \frac{x}{B} \tag{7}$$

$$\text{Br} = \frac{\mu_o V^2}{k T_o} \tag{8}$$

$$\Lambda = \frac{\text{Br} \beta}{\left(\int_0^1 e^\theta d\xi\right)^2} \tag{9}$$

d) Multiply Eq. (5) by  $2(d\theta/d\xi)$  and integrate the resulting equation to get

$$\frac{d\theta}{d\xi} = \pm \sqrt{2\Lambda} \sqrt{C - e^\theta} \tag{10}$$

where  $C$  is an integration constant.

e) Note that  $\theta$  reaches a maximum value at  $\ln C$ . Therefore, the plus sign must be used in Eq. (10) when  $0 \leq \theta \leq \ln C$ . On the other hand, the negative sign must be used when  $\ln C \leq \theta \leq 1$ . Show that the integration of Eq. (10) leads to

$$\sqrt{2\Lambda} \xi = \int_0^{\ln C} \frac{d\theta}{\sqrt{C - e^\theta}} - \int_{\ln C}^\theta \frac{d\theta}{\sqrt{C - e^\theta}} \tag{11}$$

Solve Eq. (11) to obtain

$$\theta = \ln \left\{ C \operatorname{sech}^2 \left[ \sqrt{\frac{\Lambda C}{8}} (2\xi - 1) \right] \right\} \tag{12}$$

where  $C$  is the solution of

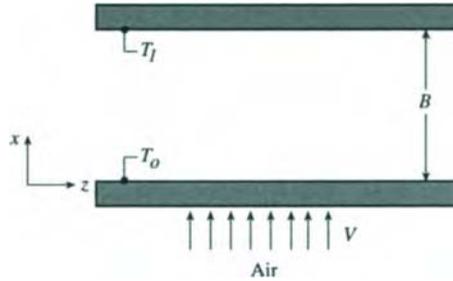
$$C = \cosh^2 \left( \sqrt{\frac{\Lambda C}{8}} \right) \tag{13}$$

f) Substitute Eq. (12) into Eq. (4) and show that the velocity distribution is given by

$$\frac{v_z}{V} = \frac{1}{2} \left\{ 1 + \frac{\tanh \left[ \sqrt{\frac{\Lambda C}{8}} (2\xi - 1) \right]}{\tanh \left( \sqrt{\frac{\Lambda C}{8}} \right)} \right\} \tag{14}$$

For more detailed information on this problem, see Gavis and Laurence (1968).

**9.13** Two large porous plates are separated by a distance  $B$  as shown in the figure below. The temperatures of the lower and the upper plates are  $T_o$  and  $T_1$ , respectively, with  $T_1 > T_o$ . Air at a temperature of  $T_o$  is blown in the  $x$ -direction with a velocity of  $V$ .



a) Show that the inventory rate equation for energy becomes

$$\rho \hat{C}_P V \frac{dT}{dx} = k \frac{d^2T}{dx^2} \quad (1)$$

b) Show that the introduction of the dimensionless variables

$$\theta = \frac{T - T_o}{T_1 - T_o} \quad (2)$$

$$\xi = \frac{x}{B} \quad (3)$$

$$\lambda = \frac{\rho \hat{C}_P V B}{k} \quad (4)$$

reduces Eq. (1) to

$$\frac{d^2\theta}{d\xi^2} - \lambda \frac{d\theta}{d\xi} = 0 \quad (5)$$

c) Solve Eq. (5) and show that the velocity distribution is given as

$$\theta = \frac{1 - e^{\lambda\xi}}{1 - e^\lambda} \quad (6)$$

d) Show that the heat flux at the lower plate is given by

$$q_x|_{x=0} = \frac{\lambda k (T_1 - T_o)}{B(1 - e^\lambda)} \quad (7)$$

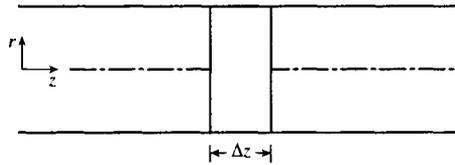
**9.14** Rework the problem given in Section 9.4.1 for a zeroth-order chemical reaction, i.e.,  $r = k_o$ , and show that the concentration profile is given by

$$c_A - c_{A_o} = \frac{k_o L^2}{2\mathcal{D}_{AB}} \left[ \left( \frac{z}{L} \right)^2 - 2 \left( \frac{z}{L} \right) \right]$$

**9.15** For laminar flow forced convection in a circular pipe with a constant wall concentration, the governing equation for concentration of species  $\mathcal{A}$ , Eq. (9.5-13), is integrated over the cross-sectional area of the tube in Section 9.5.1 to obtain Eq. (9.5-21), i.e.,

$$Q \frac{dc_{A_b}}{dz} = \pi D k_c (c_{A_w} - c_{A_b}) \quad (1)$$

a) Now assume that the flow is turbulent. Over a differential volume element of thickness  $\Delta z$ , as shown in the figure below, write down the inventory rate equation for the mass of species  $\mathcal{A}$  and show that the result is identical with Eq. (1).



b) Instead of coating the inner surface of a circular pipe with species  $\mathcal{A}$ , let us assume that the circular pipe is packed with species  $\mathcal{A}$  particles. Over a differential volume element of thickness  $\Delta z$ , write down the inventory rate equation for mass of species  $\mathcal{A}$  and show that the result is

$$Q \frac{dc_{A_b}}{dz} = a_v A k_c (c_{A_w} - c_{A_b}) \quad (2)$$

where  $A$  is the cross-sectional area of the pipe and  $a_v$  is the packing surface area per unit volume. Note that for a circular pipe  $a_v = 4/D$  and  $A = \pi D^2/4$  so that Eq. (2) reduces to Eq. (1).

**9.16** A liquid is being transported in a circular plastic tube of inner and outer radii of  $R_1$  and  $R_2$ , respectively. The dissolved  $O_2$  (species  $\mathcal{A}$ ) concentration in the liquid is  $c_{A_o}$ . Develop an expression relating the increase in  $O_2$  concentration as a function the tubing length as follows:

a) Over a differential volume element of thickness  $\Delta z$ , write down the inventory rate equation for the mass of species  $\mathcal{A}$  and show that the governing equation is

$$Q \frac{dc_{A_b}}{dz} = \frac{2\pi D_{AB}}{\ln(R_2/R_1)} (c_{A_\infty} - c_{A_b}) \quad (1)$$

where  $D_{AB}$  is the diffusion coefficient of  $O_2$  in a plastic tube and  $c_{A_\infty}$  is the concentration of  $O_2$  in air surrounding the tube. In the development of Eq. (1), note that the molar rate of  $O_2$  transfer through the tubing can be represented by Eq. (B) in Table 8.9.

b) Show that the integration of Eq. (1) leads to

$$c_{A_b} = c_{A_\infty} - (c_{A_\infty} - c_{A_o}) \exp \left[ - \frac{2\pi D_{AB} z}{Q \ln(R_2/R_1)} \right] \quad (2)$$

**9.17** Using the solution given by Johnstone and Pigford (1942), the Sherwood number is calculated as 3.41 for long contact times in Section 9.5.4.2. Obtain the same result by using an alternative approach as follows:

a) In terms of the following dimensionless quantities

$$\phi = \frac{c_A^* - c_A}{c_A^* - c_{A_0}} \quad (1)$$

$$\xi = \frac{x}{\delta} \quad (2)$$

$$\eta = \frac{D_{AB}z}{v_{\max}\delta^2} \quad (3)$$

show that Eqs. (9.5-88)-(9.5-91) reduce to

$$(1 - \xi^2) \frac{\partial \phi}{\partial \eta} = \frac{\partial^2 \phi}{\partial \xi^2} \quad (4)$$

$$\text{at } \eta = 0 \quad \phi = 1 \quad (5)$$

$$\text{at } \xi = 0 \quad \phi = 0 \quad (6)$$

$$\text{at } \xi = 1 \quad \frac{\partial \phi}{\partial \xi} = 0 \quad (7)$$

b) Use the method of separation of variables by proposing a solution in the form

$$\phi(\eta, \xi) = F(\eta) G(\xi) \quad (8)$$

and show that the solution is given by

$$\phi = \sum_{n=1}^{\infty} A_n e^{-\lambda_n^2 \eta} G_n(\xi) \quad (9)$$

where

$$A_n = \frac{\int_0^1 (1 - \xi^2) G_n(\xi) d\xi}{\int_0^1 (1 - \xi^2) G_n^2(\xi) d\xi} \quad (10)$$

and  $G_n(\xi)$  are the eigenfunctions of the equation

$$\frac{d^2 G_n}{d\xi^2} + (1 - \xi^2) \lambda_n^2 G_n = 0 \quad (11)$$

c) Show that the Sherwood number is given by

$$\text{Sh} = \frac{k_c \delta}{D_{AB}} = \frac{(\partial \phi / \partial \xi)_{\xi=0}}{\phi_b} \quad (12)$$

in which  $\phi_b$  is the dimensionless bulk temperature defined by

$$\phi_b = \frac{3}{2} \int_0^1 (1 - \xi^2) \phi \, d\xi \tag{13}$$

d) Substitute Eq. (9) into Eq. (12) to get

$$\text{Sh} = \frac{2 \sum_{n=1}^{\infty} A_n e^{-\lambda_n^2 \eta} (dG_n/d\xi)_{\xi=0}}{3 \sum_{n=1}^{\infty} (A_n/\lambda_n^2) e^{-\lambda_n^2 \eta} (dG_n/d\xi)_{\xi=0}} \tag{14}$$

For large values of  $\eta$  show that Eq. (14) reduces to

$$\text{Sh} = \frac{2}{3} \lambda_1^2 \tag{15}$$

e) Use the method of Stodola and Vianello and show that the first approximation gives

$$\lambda_1^2 = 5.122 \tag{16}$$

**Hint:** Use  $G_1 = \xi(\xi - 2)$  as a trial function.

**9.18** Use Eq. (9.5-129) and show that  $c_A \simeq c_{A_0}$  when

$$\frac{x}{\sqrt{4 \mathcal{D}_{AB} z / v_{\max}}} = 2$$

Therefore, conclude that the penetration distance for concentration,  $\delta_c$ , is given by

$$\delta_c(z) = 4 \sqrt{\frac{\mathcal{D}_{AB} z}{v_{\max}}}$$

**9.19**  $\text{H}_2\text{S}$  is being absorbed by pure water flowing down a vertical wall with a volumetric flow rate of  $6.5 \times 10^{-6} \text{ m}^3/\text{s}$  at  $20^\circ\text{C}$ . The height and the width of the plate are 2 m and 0.8 m, respectively. If the diffusion coefficient of  $\text{H}_2\text{S}$  in water is  $1.3 \times 10^{-9} \text{ m}^2/\text{s}$  and its solubility is  $0.1 \text{ kmol}/\text{m}^3$ , calculate the rate of absorption of  $\text{H}_2\text{S}$  into water.

**(Answer:  $6.5 \times 10^{-7} \text{ kmol}/\text{s}$ )**

**9.20** Water at  $25^\circ\text{C}$  flows down a wetted wall column of 5 cm diameter and 1.5 m height at a volumetric flow rate of  $8.5 \times 10^{-6} \text{ m}^3/\text{s}$ . Pure  $\text{CO}_2$  at a pressure of 1 atm flows in the countercurrent direction. If the solubility of  $\text{CO}_2$  is  $0.0336 \text{ kmol}/\text{m}^3$ , determine the rate of absorption of  $\text{CO}_2$  into water.

**(Answer:  $1.87 \times 10^{-7} \text{ kmol}/\text{s}$ )**

**9.21** Consider an industrial absorber in which gas bubbles ( $\mathcal{A}$ ) rise through a liquid ( $\mathcal{B}$ ) column. Bubble diameters usually range from 0.2 to 0.6 cm while bubble velocities range from 15 to 35 cm/s (Astarita, 1967). Making use of Eq. (9.5-139) show that the range for the average mass transfer coefficient is

$$0.018 < \langle k_c \rangle < 0.047 \text{ cm/s}$$

**Hint:** A reasonable estimate for  $\mathcal{D}_{AB}$  is  $10^{-5} \text{ cm}^2/\text{s}$ .

**9.22** Consider a gas film of thickness  $\delta$ , composed of species  $\mathcal{A}$  and  $\mathcal{B}$  adjacent to a flat catalyst particle in which gas  $\mathcal{A}$  diffuses at steady-state through the film to the catalyst surface (positive  $z$ -direction) where the isothermal first-order heterogeneous reaction  $A \rightarrow B$  occurs. As  $\mathcal{B}$  leaves the surface it decomposes by isothermal first-order heterogeneous reaction,  $B \rightarrow A$ . The gas composition at  $z = 0$ , i.e.,  $x_{A_0}$  and  $x_{B_0}$ , is known.

a) Show that the equations representing the conservation of mass for species  $\mathcal{A}$  and  $\mathcal{B}$  are given by

$$\frac{dN_{A_z}}{dz} = \mathfrak{R}_A \quad (1)$$

$$\frac{dN_{B_z}}{dz} = \mathfrak{R}_B \quad (2)$$

where

$$\mathfrak{R}_A = -\mathfrak{R}_B = k c x_B \quad (3)$$

b) Using the heterogeneous reaction rate expression at the surface of the catalyst, conclude that

$$N_{A_z} = -N_{B_z} \quad 0 \leq z \leq \delta \quad (4)$$

c) Since  $x_A + x_B = 1$  everywhere in  $0 \leq z \leq \delta$ , solution of the one of the conservation equations is sufficient to determine the concentration distribution within the film. Show that the governing equation for the mole fraction of species  $\mathcal{B}$  is

$$\frac{d^2 x_B}{dz^2} - \left( \frac{k}{\mathcal{D}_{AB}} \right) x_B = 0 \quad (5)$$

subject to the boundary conditions

$$\text{at } z = 0 \quad x_B = x_{B_0} \quad (6)$$

$$\text{at } z = \delta \quad x_B = 1 + \frac{N_{B_z}}{c k^s} \quad (7)$$

where  $k^s$  is the surface reaction rate constant.

d) Show that the solution of Eq. (5) is given by

$$x_B = x_{B_0} \cosh(\Lambda \xi) + \phi \sinh(\Lambda \xi) \quad (8)$$

where

$$\phi = \frac{1 - x_{B_o} \cosh \Lambda + \frac{x_{B_o} - \cosh \Lambda}{(\lambda/\Lambda) \sinh \Lambda + \cosh \Lambda}}{\sinh \Lambda} \quad (9)$$

$$\Lambda = \sqrt{\frac{k \delta^2}{\mathcal{D}_{AB}}} \quad (10)$$

$$\lambda = \frac{k^s \delta}{\mathcal{D}_{AB}} \quad (11)$$

e) For an instantaneous heterogeneous reaction, show that Eq. (8) reduces to

$$x_B = x_{B_o} \cosh(\Lambda \xi) + \left( \frac{1 - x_{B_o} \cosh \Lambda}{\sinh \Lambda} \right) \sinh(\Lambda \xi) \quad (12)$$

f) If there is no homogeneous reaction, show that Eq. (8) takes the form

$$x_B = x_{B_o} + \left( \frac{\lambda}{\lambda + 1} \right) (1 - x_{B_o}) \xi \quad (13)$$

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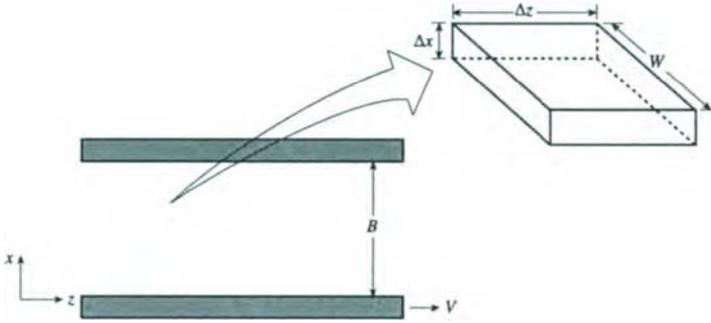
## Chapter 10

# Unsteady-State Microscopic Balances Without Generation

The presence of the accumulation term in the inventory rate equation complicates the mathematical problem since the resulting equation is a partial differential equation even if the transport takes place in one-direction. The solution of partial differential equations not only depends on the structure of the equation itself, but also on the boundary conditions. Systematic treatment of momentum, energy, and mass transport based on the types of the partial differential equation as well as the boundary conditions is a formidable task and beyond the scope of this text. Therefore, only some representative examples on momentum, energy, and mass transport will be covered in this chapter.

### 10.1 MOMENTUM TRANSPORT

Consider an incompressible Newtonian fluid contained between two large parallel plates of area  $A$ , separated by a distance  $B$  as shown in Figure 10.1. The system is initially at rest but at time  $t = 0$ , the lower plate is set in motion in the  $z$ -direction at a constant velocity  $V$  while the upper plate is kept stationary. It is required to determine the development of velocity profile as a function of position and time.



**Figure 10.1** Unsteady Couette flow between parallel plates.

Postulating  $v_z = v_z(t, x)$  and  $v_x = v_y = 0$ , Table C.1 in Appendix C indicates that the only non-zero shear-stress component is  $\tau_{xz}$ . Therefore, the components of the total momentum flux are expressed as

$$\pi_{xz} = \tau_{xz} + (\rho v_z) v_x = \tau_{xz} = -\mu \frac{\partial v_z}{\partial x} \quad (10.1-1)$$

$$\pi_{yz} = \tau_{yz} + (\rho v_z) v_y = 0 \quad (10.1-2)$$

$$\pi_{zz} = \tau_{zz} + (\rho v_z) v_z = \rho v_z^2 \quad (10.1-3)$$

The conservation statement for momentum is expressed as

$$\left( \begin{array}{c} \text{Rate of} \\ \text{momentum in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{momentum out} \end{array} \right) = \left( \begin{array}{c} \text{Rate of momentum} \\ \text{accumulation} \end{array} \right) \quad (10.1-4)$$

For a rectangular differential volume element of thickness  $\Delta x$ , length  $\Delta z$  and width  $W$ , as shown in Figure 10.1, Eq. (10.1-4) is expressed as

$$\begin{aligned} & (\pi_{zz}|_z W \Delta x + \pi_{xz}|_x W \Delta z) - (\pi_{zz}|_{z+\Delta z} W \Delta x + \pi_{xz}|_{x+\Delta x} W \Delta z) \\ & = \frac{\partial}{\partial t} [W \Delta x \Delta z \rho v_z] \end{aligned} \quad (10.1-5)$$

Dividing Eq. (10.1-5) by  $W \Delta x \Delta z$  and taking the limit as  $\Delta x \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\rho \frac{\partial v_z}{\partial t} = \lim_{\Delta x \rightarrow 0} \frac{\pi_{xz}|_x - \pi_{xz}|_{x+\Delta x}}{\Delta x} + \lim_{\Delta z \rightarrow 0} \frac{\pi_{zz}|_z - \pi_{zz}|_{z+\Delta z}}{\Delta z} \quad (10.1-6)$$

or,

$$\rho \frac{\partial v_z}{\partial t} = -\frac{\partial \pi_{xz}}{\partial x} - \frac{\partial \pi_{zz}}{\partial z} \quad (10.1-7)$$

Substitution of Eqs. (10.1-1) and (10.1-3) into Eq. (10.1-7) and noting that  $\partial v_z / \partial z = 0$  yields

$$\rho \frac{\partial v_z}{\partial t} = \mu \frac{\partial^2 v_z}{\partial x^2} \tag{10.1-8}$$

The initial and the boundary conditions associated with Eq. (10.1-8) are

$$\text{at } t = 0 \quad v_z = 0 \tag{10.1-9}$$

$$\text{at } x = 0 \quad v_z = V \tag{10.1-10}$$

$$\text{at } x = B \quad v_z = 0 \tag{10.1-11}$$

The physical significance and the order of magnitude of the terms in Eq. (10.1-8) are given in Table 10.1.

**Table 10.1** The physical significance and the order of magnitude of the terms in Eq. (10.1-8).

Term	Physical Significance	Order of Magnitude
$\mu \frac{\partial^2 v_z}{\partial x^2}$	Viscous force	$\frac{\mu V}{B^2}$
$\rho \frac{\partial v_z}{\partial t}$	Rate of momentum accumulation	$\frac{\rho V}{t}$

Therefore, the ratio of the viscous force to the rate of momentum accumulation is given by

$$\frac{\text{Viscous force}}{\text{Rate of momentum accumulation}} = \frac{\mu V / B^2}{\rho V / t} = \frac{\nu t}{B^2} \tag{10.1-12}$$

Introduction of the dimensionless quantities

$$\theta = \frac{v_z}{V} \tag{10.1-13}$$

$$\xi = \frac{x}{B} \tag{10.1-14}$$

$$\tau = \frac{\nu t}{B^2} \tag{10.1-15}$$

reduces Eqs. (10.1-8)-(10.1-11) to

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} \tag{10.1-16}$$

$$\text{at } \tau = 0 \quad \theta = 0 \tag{10.1-17}$$

$$\text{at } \xi = 0 \quad \theta = 1 \quad (10.1-18)$$

$$\text{at } \xi = 1 \quad \theta = 0 \quad (10.1-19)$$

Since the boundary condition at  $\xi = 0$  is not homogeneous, the method of separation of variables cannot be directly applied to obtain the solution. To circumvent this problem, propose a solution in the form

$$\theta(\tau, \xi) = \theta_\infty(\xi) - \theta_t(\tau, \xi) \quad (10.1-20)$$

in which  $\theta_\infty(\xi)$  is the steady-state solution, i.e.,

$$\frac{d^2\theta_\infty}{d\xi^2} = 0 \quad (10.1-21)$$

with the following boundary conditions

$$\text{at } \xi = 0 \quad \theta_\infty = 1 \quad (10.1-22)$$

$$\text{at } \xi = 1 \quad \theta_\infty = 0 \quad (10.1-23)$$

The steady-state solution is

$$\theta_\infty = 1 - \xi \quad (10.1-24)$$

which is identical with Eq. (8.1-12). On the other hand, the transient contribution  $\theta_t(\tau, \xi)$  satisfies Eq. (10.1-16), i.e.,

$$\frac{\partial\theta_t}{\partial\tau} = \frac{\partial^2\theta_t}{\partial\xi^2} \quad (10.1-25)$$

From Eqs. (10.1-20) and (10.1-24),  $\theta_t = 1 - \xi - \theta$ . Therefore, the initial and the boundary conditions associated with Eq. (10.1-25) become

$$\text{at } \tau = 0 \quad \theta_t = 1 - \xi \quad (10.1-26)$$

$$\text{at } \xi = 0 \quad \theta_t = 0 \quad (10.1-27)$$

$$\text{at } \xi = 1 \quad \theta_t = 0 \quad (10.1-28)$$

Note that the boundary conditions at  $\xi = 0$  and  $\xi = 1$  are now homogeneous and this parabolic partial differential equation can be solved by the method of separation of variables as described in Section B.6.1 in Appendix B.

The separation of variables method assumes that the solution can be represented as a product of two functions of the form

$$\theta_t(\tau, \xi) = F(\tau) G(\xi) \quad (10.1-29)$$

Substitution of Eq. (10.1-29) into Eq. (10.1-25) and rearrangement gives

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2G}{d\xi^2} \quad (10.1-30)$$

While the left-side of Eq. (10.1-30) is a function of  $\tau$  only, the right-side is dependent only on  $\xi$ . This is possible only if both sides of Eq. (10.1-30) are equal to a constant, say  $-\lambda^2$ , i.e.,

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2G}{d\xi^2} = -\lambda^2 \quad (10.1-31)$$

The choice of a negative constant is due to the fact that the solution will decay to zero as time increases. The choice of a positive constant would give a solution that becomes infinite as time increases.

Equation (10.1-31) results in two ordinary differential equations. The equation for  $F$  is given by

$$\frac{dF}{d\tau} + \lambda^2 F = 0 \quad (10.1-32)$$

The solution of Eq. (10.1-32) is

$$F(\tau) = e^{-\lambda^2 \tau} \quad (10.1-33)$$

On the other hand, the equation for  $G$  is

$$\frac{d^2G}{d\xi^2} + \lambda^2 G = 0 \quad (10.1-34)$$

and it is subject to the boundary conditions

$$\text{at } \xi = 0 \quad G = 0 \quad (10.1-35)$$

$$\text{at } \xi = 1 \quad G = 0 \quad (10.1-36)$$

Note that Eq. (10.1-34) is a Sturm-Liouville equation with a weight function of unity. The solution of Eq. (10.1-34) is

$$G(\xi) = A \sin(\lambda\xi) + B \cos(\lambda\xi) \quad (10.1-37)$$

where  $A$  and  $B$  are constants. Application of Eq. (10.1-35) gives  $B = 0$ . The use of the boundary condition defined by Eq. (10.1-36) results in

$$A \sin \lambda = 0 \quad (10.1-38)$$

For a nontrivial solution, the eigenvalues are given by

$$\sin \lambda = 0 \quad \Rightarrow \quad \lambda_n = n\pi \quad n = 1, 2, 3, \dots \quad (10.1-39)$$

Therefore, the transient solution is

$$\theta_t = \sum_{n=1}^{\infty} C_n e^{-n^2 \pi^2 \tau} \sin(n\pi\xi) \quad (10.1-40)$$

The unknown coefficients  $C_n$  can be determined by using the initial condition in Eq. (10.1-26). The result is

$$1 - \xi = \sum_{n=0}^{\infty} C_n \sin(n\pi\xi) \tag{10.1-41}$$

Since the eigenfunctions are simply orthogonal, multiplication of Eq. (10.1-41) by  $\sin(m\pi\xi)$  and integration from  $\xi = 0$  to  $\xi = 1$  gives

$$\int_0^1 (1 - \xi) \sin(m\pi\xi) d\xi = \sum_{n=1}^{\infty} C_n \int_0^1 \sin(m\pi\xi) \sin(n\pi\xi) d\xi \tag{10.1-42}$$

Note that the integral on the right side of Eq. (10.1-42) is zero when  $n \neq m$  and nonzero when  $n = m$ . Therefore, when  $n = m$  the summation drops out and Eq. (10.1-42) reduces to the form

$$\int_0^1 (1 - \xi) \sin(n\pi\xi) d\xi = C_n \int_0^1 \sin^2(n\pi\xi) d\xi \tag{10.1-43}$$

Evaluation of the integrals gives

$$C_n = \frac{2}{n\pi} \tag{10.1-44}$$

The transient solution takes the form

$$\theta_t = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} e^{-n^2\pi^2\tau} \sin(n\pi\xi) \tag{10.1-45}$$

Substitution of the steady-state and the transient solutions, Eqs. (10.1-24) and (10.1-45), into Eq. (10.1-20) gives the solution as

$$\theta = 1 - \xi - \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} e^{-n^2\pi^2\tau} \sin(n\pi\xi) \tag{10.1-46}$$

The volumetric flow rate can be determined by integrating the velocity distribution over the cross-sectional area of the plate, i.e.,

$$\begin{aligned} Q &= \int_0^W \int_0^B v_z dx dy \\ &= WBV \int_0^1 \theta d\xi \end{aligned} \tag{10.1-47}$$

Substitution of Eq. (10.1-46) into Eq. (10.1-47) gives

$$Q = WBV \left\{ \frac{1}{2} - \frac{4}{\pi^2} \sum_{k=0}^{\infty} \frac{1}{(2k+1)^2} \exp[-(2k+1)^2\pi^2\tau] \right\} \tag{10.1-48}$$

Note that when  $\tau \rightarrow \infty$ ,  $Q \rightarrow WBV/2$  which is identical with Eq. (8.1-15).

### 10.1.1 Solution for Short Times

Once the lower plate is set in motion, only the thin layer adjacent to the lower plate feels the motion of the plate during the initial stages. This thin layer does not feel the presence of the stationary plate at  $x = B$  at all. For a fluid particle within this layer, the upper plate is at infinity. Therefore, the governing equation together with the initial and boundary conditions are expressed as

$$\rho \frac{\partial v_z}{\partial t} = \mu \frac{\partial^2 v_z}{\partial x^2} \quad (10.1-49)$$

$$\text{at } t = 0 \quad v_z = 0 \quad (10.1-50)$$

$$\text{at } x = 0 \quad v_z = V \quad (10.1-51)$$

$$\text{at } x = \infty \quad v_z = 0 \quad (10.1-52)$$

In the literature, this problem is generally known as *Stokes' first problem*<sup>1</sup>. Note that there is no length scale in this problem. Since the boundary condition at  $x = \infty$  is the same as the initial condition, the problem can be solved by the similarity analysis. The solution of this problem is given in Section B.3.6.2 in Appendix B and the solution is

$$\boxed{\frac{v_z}{V} = 1 - \operatorname{erf}\left(\frac{x}{\sqrt{4\nu t}}\right)} \quad (10.1-53)$$

The drag force exerted on the plate is given by

$$\begin{aligned} F_D &= A \left( -\mu \frac{\partial v_z}{\partial x} \Big|_{x=0} \right) \\ &= \frac{A\mu V}{\sqrt{\pi\nu t}} \end{aligned} \quad (10.1-54)$$

Finally, note that when  $x/\sqrt{4\nu t} = 2$ , Eq. (10.1-53) becomes

$$\frac{v_z}{V} = 1 - \operatorname{erf}(2) = 1 - 0.995 = 0.005$$

indicating that  $v_z \simeq 0$ . Therefore, the penetration distance for momentum,  $\delta$ , is given by

$$\delta = 4\sqrt{\nu t} \quad (10.1-55)$$

The penetration distance changes with the square root of the momentum diffusivity and is independent of the plate velocity. The momentum diffusivities for water and air at 20°C are  $1 \times 10^{-6}$  and  $15.08 \times 10^{-6} \text{ m}^2/\text{s}$ , respectively. The penetration distances for water and air after one minute are 3.1 cm and 12 cm, respectively.

<sup>1</sup>Some authors refer to this problem as the *Rayleigh problem*.

## 10.2 ENERGY TRANSPORT

The conservation statement for energy reduces to

$$\left( \begin{array}{c} \text{Rate of} \\ \text{energy in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{energy out} \end{array} \right) = \left( \begin{array}{c} \text{Rate of energy} \\ \text{accumulation} \end{array} \right) \quad (10.2-1)$$

As in Section 8.2, our analysis will be restricted to the application of Eq. (10.2-1) to conduction in solids and stationary liquids. The solutions of almost all imaginable conduction problems in different coordinate systems with various initial and boundary conditions are given by Carslaw and Jaeger (1959). For this reason, only some representative problems will be presented in this section.

The Biot number is given by Eq. (7.1-14) as

$$\text{Bi} = \frac{(\text{Difference in driving force})_{\text{solid}}}{(\text{Difference in driving force})_{\text{fluid}}} \quad (10.2-2)$$

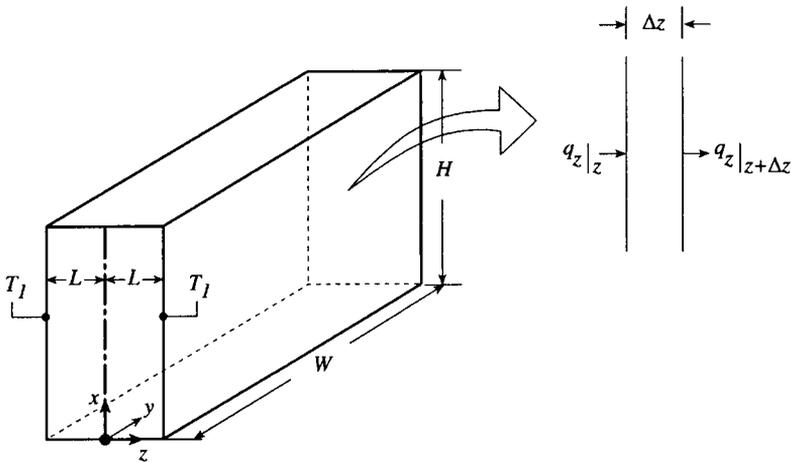
In the case of heat transfer, the temperature distribution is considered uniform within the solid phase when  $\text{Bi}_H \ll 1$ . This obviously brings up the question, "What should the value of  $\text{Bi}_H$  be so that the condition  $\text{Bi}_H \ll 1$  is satisfied?" In the literature, it is generally assumed that the internal resistance to heat transfer is negligible and the temperature distribution within the solid is almost uniform when  $\text{Bi}_H < 0.1$ . Under these conditions, the so-called *lumped-parameter analysis* is possible as can be seen in the solution of problems in Section 7.5. When  $0.1 < \text{Bi}_H < 40$ , the internal and external resistances to heat transfer have almost the same order of magnitude. The external resistance to heat transfer is considered negligible when  $\text{Bi}_H > 40$ .

### 10.2.1 Heating of a Rectangular Slab

Consider a rectangular slab of thickness  $2L$  as shown in Figure 10.2. Initially the slab temperature is uniform at a value of  $T_o$ . At  $t = 0$ , the temperatures of the surfaces at  $z = \pm L$  are increased to  $T_1$ . To calculate the amount of heat transferred into the slab, it is first necessary to determine the temperature profile within the slab as a function of position and time.

If  $2L/H \ll 1$  and  $2L/W \ll 1$ , then it is possible to assume that the conduction is one-dimensional and postulate that  $T = T(t, z)$ . In that case, Table C.4 in Appendix C indicates that the only non-zero energy flux component is  $e_z$  and it is given by

$$e_z = q_z = -k \frac{\partial T}{\partial z} \quad (10.2-3)$$



**Figure 10.2** Unsteady-state conduction through a rectangular slab.

For a rectangular differential volume element of thickness  $\Delta z$ , as shown in Figure 10.2, Eq. (10.2-1) is expressed as

$$q_z|_z WH - q_z|_{z+\Delta z} WH = \frac{\partial}{\partial t} [WH\Delta z \rho \hat{C}_P (T - T_{ref})] \quad (10.2-4)$$

Following the notation introduced by Bird *et al.* (1960), “in” and “out” directions are taken in the  $+z$ -direction. Dividing Eq. (10.2-4) by  $WH\Delta z$  and letting  $\Delta z \rightarrow 0$  gives

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = \lim_{\Delta z \rightarrow 0} \frac{q_z|_z - q_z|_{z+\Delta z}}{\Delta z} \quad (10.2-5)$$

or,

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = - \frac{\partial q_z}{\partial z} \quad (10.2-6)$$

Substitution of Eq. (10.2-3) into Eq. (10.2-6) gives the governing equation for temperature as

$$\boxed{\rho \hat{C}_P \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2}} \quad (10.2-7)$$

All physical properties are assumed to be independent of temperature in the development of Eq. (10.2-7). The initial and boundary conditions associated with Eq. (10.2-7) are

$$\begin{array}{lll} \text{at } t = 0 & T = T_o & \text{for all } z \\ \text{at } z = L & T = T_1 & t > 0 \\ \text{at } z = -L & T = T_1 & t > 0 \end{array} \quad (10.2-8)$$

Note that  $z = 0$  represents a plane of symmetry across which there is no net flux, i.e.,  $\partial T/\partial z = 0$ . Therefore, it is also possible to express the initial and boundary conditions as

$$\begin{aligned} \text{at } t = 0 \quad T &= T_o & \text{for all } z \\ \text{at } z = 0 \quad \frac{\partial T}{\partial z} &= 0 & t > 0 \\ \text{at } z = L \quad T &= T_1 & t > 0 \end{aligned} \tag{10.2-9}$$

The boundary condition at  $z = 0$  can also be interpreted as an insulated surface. As a result, Eqs. (10.2-7) and (10.2-9) also represent the following problem statement: "A slab of thickness  $L$  is initially at a uniform temperature of  $T_o$ . One side of the slab is perfectly insulated while the other surface is kept at a constant temperature of  $T_1$  with  $T_1 > T_o$  for  $t > 0$ ."

The physical significance and the order of magnitude of the terms in Eq. (10.2-7) are given in Table 10.2.

**Table 10.2** The physical significance and the order of magnitude of the terms in Eq. (10.2-7).

Term	Physical Significance	Order of Magnitude
$k \frac{\partial^2 \langle T \rangle}{\partial z^2}$	Rate of conduction	$\frac{k(T_1 - T_o)}{L^2}$
$\rho \hat{C}_P \frac{\partial T}{\partial t}$	Rate of energy accumulation	$\frac{\rho \hat{C}_P (T_1 - T_o)}{t}$

Therefore, the ratio of the rate of conduction to the rate of energy accumulation is given by

$$\frac{\text{Rate of conduction}}{\text{Rate of energy accumulation}} = \frac{k(T_1 - T_o)/L^2}{\rho \hat{C}_P (T_1 - T_o)/t} = \frac{\alpha t}{L^2} \tag{10.2-10}$$

In the literature, the term  $\alpha t/L^2$  is usually referred to as the *Fourier number*,  $Fo$ .

Introduction of the dimensionless quantities

$$\theta = \frac{T_1 - T}{T_1 - T_o} \tag{10.2-11}$$

$$\xi = \frac{z}{L} \tag{10.2-12}$$

$$\tau = \frac{\alpha t}{L^2} \tag{10.2-13}$$

reduces Eqs. (10.2-7) and (10.2-8) to

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} \tag{10.2-14}$$

$$\begin{aligned}
 &\text{at } \tau = 0 && \theta = 1 \\
 &\text{at } \xi = 1 && \theta = 0 \\
 &\text{at } \xi = -1 && \theta = 0
 \end{aligned}
 \tag{10.2-15}$$

Since the governing equation as well as the boundary conditions in the  $\xi$ -direction are homogeneous, this parabolic partial differential equation can be solved by the method of separation of variables as explained in Section B.6.1 in Appendix B.

The solution can be represented as a product of two functions of the form

$$\theta(\tau, \xi) = F(\tau) G(\xi) \tag{10.2-16}$$

so that Eq. (10.2-14) reduces to

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2G}{d\xi^2} \tag{10.2-17}$$

While the left-side of Eq. (10.2-17) is a function of  $\tau$  only, the right-side is dependent only on  $\xi$ . This is possible only if both sides of Eq. (10.2-17) are equal to a constant, say  $-\lambda^2$ , i.e.,

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2G}{d\xi^2} = -\lambda^2 \tag{10.2-18}$$

The choice of a negative constant is due to the fact that the solution will decay to zero as time increases. The choice of a positive constant would give a solution that becomes infinite as time increases.

Equation (10.2-18) results in two ordinary differential equations. The equation for  $F$  is given by

$$\frac{dF}{d\tau} + \lambda^2 F = 0 \tag{10.2-19}$$

The solution of Eq. (10.2-19) is

$$F(\tau) = e^{-\lambda^2 \tau} \tag{10.2-20}$$

On the other hand, the equation for  $G$  is

$$\frac{d^2G}{d\xi^2} + \lambda^2 G = 0 \tag{10.2-21}$$

and it is subject to the boundary conditions

$$\text{at } \xi = 1 \quad G = 0 \tag{10.2-22}$$

$$\text{at } \xi = -1 \quad G = 0 \tag{10.2-23}$$

Note that Eq. (10.2-21) is a Sturm-Liouville equation with a weight function of unity. The solution of Eq. (10.2-21) is

$$G(\xi) = A \sin(\lambda \xi) + B \cos(\lambda \xi) \tag{10.2-24}$$

where  $A$  and  $B$  are constants. Since the problem is symmetric around the  $z$ -axis, then  $\theta$ , and hence  $G$ , must be even functions<sup>2</sup> of  $\xi$ . Therefore,  $A = 0$ . Application of the boundary condition defined by Eq. (10.2-22) gives

$$B \cos \lambda = 0 \tag{10.2-25}$$

For a nontrivial solution, the eigenvalues are given by

$$\cos \lambda = 0 \quad \Rightarrow \quad \lambda_n = \left( n + \frac{1}{2} \right) \pi \quad n = 0, 1, 2, \dots \tag{10.2-26}$$

Therefore, the general solution is

$$\theta = \sum_{n=0}^{\infty} C_n e^{-(n+\frac{1}{2})^2 \pi^2 \tau} \cos \left[ \left( n + \frac{1}{2} \right) \pi \xi \right] \tag{10.2-27}$$

The unknown coefficients  $C_n$  can be determined by using the initial condition in Eq. (10.2-15). The result is

$$1 = \sum_{n=0}^{\infty} C_n \cos \left[ \left( n + \frac{1}{2} \right) \pi \xi \right] \tag{10.2-28}$$

Since the eigenfunctions are simply orthogonal, multiplication of Eq. (10.2-28) by  $\cos \left[ \left( m + \frac{1}{2} \right) \pi \xi \right]$  and integration from  $\xi = 0$  to  $\xi = 1$  gives

$$\int_0^1 \cos \left[ \left( m + \frac{1}{2} \right) \pi \xi \right] d\xi = \sum_{n=0}^{\infty} C_n \int_0^1 \cos \left[ \left( n + \frac{1}{2} \right) \pi \xi \right] \cos \left[ \left( m + \frac{1}{2} \right) \pi \xi \right] d\xi \tag{10.2-29}$$

Note that the integral on the right side of Eq. (10.2-29) is zero when  $n \neq m$  and nonzero when  $n = m$ . Therefore, when  $n = m$  the summation drops out and Eq. (10.2-29) reduces to the form

$$\int_0^1 \cos \left[ \left( n + \frac{1}{2} \right) \pi \xi \right] d\xi = C_n \int_0^1 \cos^2 \left[ \left( n + \frac{1}{2} \right) \pi \xi \right] d\xi \tag{10.2-30}$$

Evaluation of the integrals gives

$$C_n = 2 \frac{\sin \left[ \left( n + \frac{1}{2} \right) \pi \right]}{\left( n + \frac{1}{2} \right) \pi} \tag{10.2-31}$$

Since  $\sin \left( n + \frac{1}{2} \right) \pi = (-1)^n$ , the solution becomes

$$\theta = 2 \sum_{n=0}^{\infty} \frac{(-1)^n}{\left( n + \frac{1}{2} \right) \pi} e^{-(n+\frac{1}{2})^2 \pi^2 \tau} \cos \left[ \left( n + \frac{1}{2} \right) \pi \xi \right] \tag{10.2-32}$$

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<sup>2</sup>A function  $f(x)$  is said to be an *odd function* if  $f(-x) = -f(x)$  and an *even function* if  $f(-x) = f(x)$ .

**Example 10.1** A copper slab ( $\alpha = 117 \times 10^{-6} \text{ m}^2/\text{s}$ ) of 10 cm thick is initially at a temperature of  $20^\circ\text{C}$ . If it is dipped in a boiling water at atmospheric pressure, estimate the time it takes for the center of the slab to reach  $40^\circ\text{C}$ . Repeat the problem also for a 10 cm thick stainless steel slab ( $\alpha = 3.91 \times 10^{-6} \text{ m}^2/\text{s}$ ).

### Solution

The use of Eq. (10.2-32) gives

$$\frac{T_1 - T_c}{T_1 - T_o} = 2 \sum_{n=0}^{\infty} \frac{(-1)^n}{\left(n + \frac{1}{2}\right) \pi} \exp \left[ - \left( n + \frac{1}{2} \right)^2 \frac{\pi^2 \alpha t}{L^2} \right] \quad (1)$$

where  $T_c$  is the temperature at the center, i.e., the value of  $T$  at  $\xi = 0$ .

Copper:

Substitution of the values into Eq. (1) gives

$$\frac{100 - 40}{100 - 20} = 2 \sum_{n=0}^{\infty} \frac{(-1)^n}{\left(n + \frac{1}{2}\right) \pi} \exp \left[ - \left( n + \frac{1}{2} \right)^2 \frac{\pi^2 (117 \times 10^{-6}) t}{(0.05)^2} \right] \quad (2)$$

The value of  $t$  can be calculated as 4.5 s.

Stainless steel:

Substitution of the values into Eq. (1) gives

$$\frac{100 - 40}{100 - 20} = 2 \sum_{n=0}^{\infty} \frac{(-1)^n}{\left(n + \frac{1}{2}\right) \pi} \exp \left[ - \left( n + \frac{1}{2} \right)^2 \frac{\pi^2 (3.91 \times 10^{-6}) t}{(0.05)^2} \right] \quad (3)$$

The value of  $t$  can be calculated as 136 s.

**Comment:** For an unsteady-state conduction problem, the ratio of the rate of accumulation to the rate of conduction is equal to the Fourier number. Let subscripts  $c$  and  $s$  represent copper and stainless steel, respectively. Then, it is possible to equate the Fourier numbers, i.e.,

$$\left( \frac{\alpha t}{L_{ch}^2} \right)_c = \left( \frac{\alpha t}{L_{ch}^2} \right)_s \quad (4)$$

Since  $L_{ch}$  is the same for both cases, Eq. (4) simplifies to

$$\begin{aligned} t_s &= t_c \left( \frac{\alpha_c}{\alpha_s} \right) \\ &= 4.5 \left( \frac{117 \times 10^{-6}}{3.91 \times 10^{-6}} \right) = 135 \text{ s} \end{aligned}$$

which is almost equal to the exact value.

10.2.1.1 Macroscopic equation

Integration of the governing equation, Eq. (10.2-7), over the volume of the system gives

$$\int_{-L}^L \int_0^W \int_0^H \rho \hat{C}_P \frac{\partial T}{\partial t} dx dy dz = \int_{-L}^L \int_0^W \int_0^H k \frac{\partial^2 T}{\partial z^2} dx dy dz \quad (10.2-33)$$

Evaluation of the integrations yields

$$\underbrace{\frac{d}{dt} \left[ \int_{-L}^L \int_0^W \int_0^H \rho \hat{C}_P (T - T_{ref}) dx dy dz \right]}_{\text{Rate of accumulation of energy}} = \underbrace{2WH \left( k \frac{\partial T}{\partial z} \Big|_{z=L} \right)}_{\text{Rate of energy entering from surfaces at } z = \pm L} \quad (10.2-34)$$

Note that Eq. (10.2-34) is the macroscopic energy balance by considering the rectangular slab as a system. The rate of energy entering into the slab,  $\dot{Q}$ , can be calculated from Eq. (10.2-34) as

$$\begin{aligned} \dot{Q} &= 2WH \left( k \frac{\partial T}{\partial z} \Big|_{z=L} \right) \\ &= - \frac{2WHk(T_1 - T_o)}{L} \frac{\partial \theta}{\partial \xi} \Big|_{\xi=1} \end{aligned} \quad (10.2-35)$$

Substitution of Eq. (10.2-32) into Eq. (10.2-35) gives

$$\dot{Q} = \frac{4WHk(T_1 - T_o)}{L} \sum_{n=0}^{\infty} \exp \left[ - \frac{(2n+1)^2 \pi^2 \tau}{4} \right] \quad (10.2-36)$$

The amount of heat transferred can be calculated from

$$Q = \int_0^t \dot{Q} dt = \frac{L^2}{\alpha} \int_0^\tau \dot{Q} d\tau \quad (10.2-37)$$

Substitution of Eq. (10.2-36) into Eq. (10.2-37) yields

$$\frac{Q}{Q_\infty} = 1 - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp \left[ - \frac{(2n+1)^2 \pi^2 \tau}{4} \right] \quad (10.2-38)$$

where  $Q_\infty$  is the amount of heat transferred to the slab when it reaches steady-state, i.e.,

$$Q_\infty = \underbrace{2LWH\rho}_{\text{Mass of the slab}} \hat{C}_P (T_1 - T_o) \quad (10.2-39)$$

## 10.2.1.2 Solution for short times

Let  $s$  be the distance measured from the surface of the slab, i.e.,

$$s = L - z \quad (10.2-40)$$

so that Eq. (10.2-7) reduces to

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial s^2} \quad (10.2-41)$$

At small values of time, the heat does not penetrate very far into the slab. Under these circumstances, it is possible to consider the slab as a semi-infinite medium in the  $s$ -direction. The initial and boundary conditions associated with Eq. (10.2-41) become

$$\begin{aligned} \text{at } t = 0 & \quad T = T_o \\ \text{at } s = 0 & \quad T = T_1 \\ \text{at } s = \infty & \quad T = T_o \end{aligned} \quad (10.2-42)$$

Introduction of the dimensionless temperature

$$\phi = \frac{T - T_o}{T_1 - T_o} \quad (10.2-43)$$

reduces Eqs. (10.2-41) and (10.2-42) to

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial s^2} \quad (10.2-44)$$

$$\begin{aligned} \text{at } t = 0 & \quad \phi = 0 \\ \text{at } s = 0 & \quad \phi = 1 \\ \text{at } s = \infty & \quad \phi = 0 \end{aligned} \quad (10.2-45)$$

Since there is no length scale in the problem, this parabolic partial differential equation can be solved by the similarity solution as explained in Section B.6.2 in Appendix B. The solution is sought in the form

$$\phi = f(\eta) \quad (10.2-46)$$

where

$$\eta = \frac{s}{\sqrt{4\alpha t}} \quad (10.2-47)$$

The chain rule of differentiation gives

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= \frac{df}{d\eta} \frac{\partial \eta}{\partial t} \\ &= -\frac{1}{2} \frac{\eta}{t} \frac{df}{d\eta} \end{aligned} \quad (10.2-48)$$

$$\begin{aligned}\frac{\partial^2 \phi}{\partial s^2} &= \frac{d^2 f}{d\eta^2} \left( \frac{\partial \eta}{\partial s} \right)^2 + \frac{df}{d\eta} \frac{\partial^2 \eta}{\partial s^2} \\ &= \frac{1}{4\alpha t} \frac{d^2 f}{d\eta^2}\end{aligned}\quad (10.2-49)$$

Substitution of Eqs. (10.2-48) and (10.2-49) into Eq. (10.2-44) gives

$$\frac{d^2 f}{d\eta^2} + 2\eta \frac{df}{d\eta} = 0 \quad (10.2-50)$$

The boundary conditions associated with Eq. (10.2-50) are

$$\begin{aligned}\text{at } \eta = 0 & \quad f = 1 \\ \text{at } \eta = \infty & \quad f = 0\end{aligned}\quad (10.2-51)$$

The integrating factor for Eq. (10.2-50) is  $\exp(\eta^2)$ . Multiplication of Eq. (10.2-50) by the integrating factor yields

$$\frac{d}{d\eta} \left( e^{\eta^2} \frac{df}{d\eta} \right) = 0 \quad (10.2-52)$$

which implies that

$$\frac{df}{d\eta} = C_1 e^{-\eta^2} \quad (10.2-53)$$

Integration of Eq. (10.2-53) gives

$$f = C_1 \int_0^\eta e^{-u^2} du + C_2 \quad (10.2-54)$$

where  $u$  is a dummy variable of integration. Application of the boundary condition at  $\eta = 0$  gives  $C_2 = 1$ . On the other hand, application of the boundary condition at  $\eta = 1$  gives

$$C_1 = -\frac{1}{\int_0^\infty e^{-u^2} du} = -\frac{2}{\sqrt{\pi}} \quad (10.2-55)$$

Therefore, the solution becomes

$$f = 1 - \frac{2}{\sqrt{\pi}} \int_0^\eta e^{-u^2} du = 1 - \text{erf}(\eta) \quad (10.2-56)$$

or,

$$\frac{T - T_o}{T_1 - T_o} = 1 - \text{erf} \left( \frac{s}{\sqrt{4\alpha t}} \right) \quad (10.2-57)$$

where  $\text{erf}(x)$  is the error function defined by

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du \quad (10.2-58)$$

Further simplification of Eq. (10.2-57) gives

$$\frac{T_1 - T}{T_1 - T_o} = \operatorname{erf} \left( \frac{s}{\sqrt{4\alpha t}} \right) \quad (10.2-59)$$

The rate of heat transfer into the semi-infinite slab of cross-sectional area  $A$  is

$$\begin{aligned} \dot{Q} &= A \left( -k \frac{\partial T}{\partial s} \Big|_{s=0} \right) \\ &= \frac{Ak(T_1 - T_o)}{\sqrt{\pi\alpha t}} \end{aligned} \quad (10.2-60)$$

The amount of heat transferred is

$$\begin{aligned} Q &= \int_0^t \dot{Q} dt \\ &= \frac{2Ak(T_1 - T_o)\sqrt{t}}{\sqrt{\pi\alpha}} \end{aligned} \quad (10.2-61)$$

**Example 10.2** *One of the surfaces of a thick wall is exposed to gases at 350°C. If the initial wall temperature is uniform at 20°C, determine the time required for a point 5 cm below the surface to reach 280°C. The thermal diffusivity of the wall is  $4 \times 10^{-7} \text{ m}^2/\text{s}$ .*

### Solution

#### Assumption

1. *The Biot number is large enough to neglect the external resistance to heat transfer so that the surface temperature of the wall is almost equal to the gas temperature.*
2. *Since the wall thickness is large, it may be considered as a semi-infinite medium.*

#### Analysis

The left-side of Eq. (10.2-59) is

$$\frac{T_1 - T}{T_1 - T_o} = \frac{350 - 280}{350 - 20} = 0.212 \quad (1)$$

Therefore,

$$\operatorname{erf} \left( \frac{s}{\sqrt{4\alpha t}} \right) = 0.212 \quad \Rightarrow \quad \frac{s}{\sqrt{4\alpha t}} = 0.19 \quad (2)$$

The time required is

$$\begin{aligned} t &= \frac{1}{4\alpha} \left( \frac{s}{0.19} \right)^2 \\ &= \frac{1}{4(4 \times 10^{-7})} \left( \frac{0.05}{0.19} \right)^2 = 43,283 \text{ s} \simeq 12 \text{ h} \end{aligned} \quad (3)$$

**Comment:** Note that when  $s/\sqrt{4\alpha t} = 2$ , Eq. (10.2-59) becomes

$$\frac{T_1 - T}{T_1 - T_o} = \text{erf}(2) = 0.995$$

indicating that  $T \simeq T_o$ . Therefore, the penetration distance for heat,  $\delta_t$ , is given by

$$\delta_t = 4\sqrt{\alpha t}$$

In this particular example, the penetration distance after 12 hours is

$$\delta_t = 4\sqrt{(4 \times 10^{-7})(12)(3600)} = 0.53 \text{ m}$$

## 10.2.2 Heating of a Rectangular Slab: Revisited

In Section 10.2.1, the temperatures of the surfaces at  $z = \pm L$  are assumed constant at  $T_1$ . This boundary condition is only applicable when the external resistance to heat transfer is negligible, i.e.,  $\text{Bi}_H > 40$ . In practice, however, it is not the surface temperature but the temperature of the medium surrounding the slab,  $T_\infty$ , that is generally constant and the external resistance to heat transfer should be taken into consideration. The governing equation for temperature is given by Eq. (10.2-7). The initial and the boundary conditions are given by

$$\text{at } t = 0 \quad T = T_o \quad \text{for all } z \quad (10.2-62)$$

$$\text{at } z = 0 \quad \frac{\partial T}{\partial z} = 0 \quad t > 0 \quad (10.2-63)$$

$$\text{at } z = L \quad k \frac{\partial T}{\partial z} = \langle h \rangle (T_\infty - T) \quad t > 0 \quad (10.2-64)$$

Introduction of the dimensionless quantities

$$\theta = \frac{T_\infty - T}{T_\infty - T_o} \quad (10.2-65)$$

$$\xi = \frac{z}{L} \quad (10.2-66)$$

$$\tau = \frac{\alpha t}{L^2} \quad (10.2-67)$$

$$\text{Bi}_H = \frac{\langle h \rangle L}{k} \quad (10.2-68)$$

reduces Eqs. (10.2-7), (10.2-62), (10.2-63) and (10.2-64) to

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} \quad (10.2-69)$$

$$\text{at } \tau = 0 \quad \theta = 1 \quad (10.2-70)$$

$$\text{at } \xi = 0 \quad \frac{\partial \theta}{\partial \xi} = 0 \quad (10.2-71)$$

$$\text{at } \xi = 1 \quad -\frac{\partial \theta}{\partial \xi} = \text{Bi}_H \theta \quad (10.2-72)$$

The use of the method of separation of variables in which the solution is sought in the form

$$\theta(\tau, \xi) = F(\tau) G(\xi) \quad (10.2-73)$$

reduces the differential equation, Eq. (10.2-69) to

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2 G}{d\xi^2} = -\lambda^2 \quad (10.2-74)$$

Equation (10.2-74) results in two ordinary differential equations:

$$\frac{dF}{d\tau} + \lambda^2 F = 0 \quad \Rightarrow \quad F(\tau) = e^{-\lambda^2 \tau} \quad (10.2-75)$$

$$\frac{d^2 G}{d\xi^2} + \lambda^2 G = 0 \quad \Rightarrow \quad G(\xi) = A \sin(\lambda \xi) + B \cos(\lambda \xi) \quad (10.2-76)$$

Therefore, the solution becomes

$$\theta = e^{-\lambda^2 \tau} [A \sin(\lambda \xi) + B \cos(\lambda \xi)] \quad (10.2-77)$$

The application of Eq. (10.2-71) indicates that  $A = 0$ . Application of the boundary condition defined by Eq. (10.2-72) gives

$$B \lambda e^{-\lambda^2 \tau} \sin \lambda = \text{Bi}_H B e^{-\lambda^2 \tau} \cos \lambda \quad (10.2-78)$$

Solving for  $\lambda$  yields

$$\lambda_n \tan \lambda_n = \text{Bi}_H \quad (10.2-79)$$

The first five roots of Eq. (10.2-79) are given as a function of  $\text{Bi}_H$  in Table 10.3.

The general solution is the summation of all possible solutions, i.e.,

$$\theta = \sum_{n=1}^{\infty} C_n e^{-\lambda_n^2 \tau} \cos(\lambda_n \xi) \quad (10.2-80)$$

**Table 10.3** The roots of Eq. (10.2-79).

$Bi_H$	$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$	$\lambda_5$
0	0.000	3.142	6.283	9.425	12.566
0.1	0.311	3.173	6.299	9.435	12.574
0.5	0.653	3.292	6.362	9.477	12.606
1.0	0.860	3.426	6.437	9.529	12.645
2.0	1.077	3.644	6.578	9.630	12.722
10.0	1.429	4.306	7.228	10.200	13.214

The unknown coefficients  $C_n$  can be determined by using the initial condition given by Eq. (10.2-70). The result is

$$\begin{aligned}
 C_n &= \frac{\int_0^1 \cos(\lambda_n \xi) d\xi}{\int_0^1 \cos^2(\lambda_n \xi) d\xi} \\
 &= \frac{2 \sin \lambda_n}{\lambda_n + \sin \lambda_n \cos \lambda_n}
 \end{aligned} \tag{10.2-81}$$

Therefore, the solution becomes

$$\theta = 2 \sum_{n=1}^{\infty} \frac{\sin \lambda_n}{\lambda_n + \sin \lambda_n \cos \lambda_n} e^{-\lambda_n^2 \tau} \cos(\lambda_n \xi) \tag{10.2-82}$$

When  $\tau \geq 0.2$ , the series solution given by Eq. (10.2-82) can be approximated by the first term of the series.

The rate of energy entering into the slab,  $\dot{Q}$ , is given by

$$\begin{aligned}
 \dot{Q} &= 2WH \left( k \frac{\partial T}{\partial z} \Big|_{z=L} \right) \\
 &= - \frac{2WHk(T_{\infty} - T_o)}{L} \frac{\partial \theta}{\partial \xi} \Big|_{\xi=1}
 \end{aligned} \tag{10.2-83}$$

Substitution of Eq. (10.2-82) into Eq. (10.2-83) gives

$$\dot{Q} = \frac{4WHk(T_{\infty} - T_o)}{L} \sum_{n=1}^{\infty} \frac{\lambda_n \sin^2 \lambda_n}{\lambda_n + \sin \lambda_n \cos \lambda_n} \exp(-\lambda_n^2 \tau) \tag{10.2-84}$$

The amount of heat transferred can be calculated from

$$Q = \int_0^t \dot{Q} dt = \frac{L^2}{\alpha} \int_0^{\tau} \dot{Q} d\tau \tag{10.2-85}$$

Substitution of Eq. (10.2-84) into Eq. (10.2-85) yields

$$\frac{Q}{Q_o} = \sum_{n=0}^{\infty} \frac{2}{\lambda_n} \frac{\sin^2 \lambda_n}{\lambda_n + \sin \lambda_n \cos \lambda_n} [1 - \exp(-\lambda_n^2 \tau)] \quad (10.2-86)$$

where  $Q_o$  is the amount of heat transferred to the slab when the driving force is constant and equal to its greatest (or, initial) value, i.e.,

$$Q_o = 2LWH \rho \hat{C}_P (T_{\infty} - T_o) \quad (10.2-87)$$

**Example 10.3** A cake baked at 175°C for half an hour is taken out of the oven and inverted on a rack to cool. The kitchen temperature is 20°C and the average heat transfer coefficient is 12 W/m<sup>2</sup>.K. If the thickness of the cake is 6 cm, estimate the time it takes for the center to reach 40°C. Take  $k = 0.18$  W/m.K and  $\alpha = 1.2 \times 10^{-7}$  m<sup>2</sup>/s for the cake.

### Solution

The Biot number is

$$\begin{aligned} \text{Bi}_H &= \frac{\langle h \rangle L}{k} \\ &= \frac{(12)(0.03)}{(0.18)} = 2 \end{aligned} \quad (1)$$

From Table 10.2  $\lambda_1 = 1.077$ . Considering only the first term of the series in Eq. (10.2-82), the temperature at the center,  $T_c$ , is

$$\frac{T_{\infty} - T_c}{T_{\infty} - T_o} = \frac{2 \sin \lambda_1}{\lambda_1 + \sin \lambda_1 \cos \lambda_1} \exp(-\lambda_1^2 \tau) \quad (2)$$

Substitution of the values into Eq. (2) gives

$$\frac{20 - 40}{20 - 175} = \frac{2 \sin 61.7}{1.077 + \sin 61.7 \cos 61.7} \exp[-(1.077)^2 \tau] \quad (3)$$

in which 1.077 rad = 61.7°. Solving for  $\tau$  yields

$$\tau = 1.907 \quad (4)$$

Therefore, the time is

$$\begin{aligned} t &= \frac{\tau L^2}{\alpha} \\ &= \frac{(1.907)(0.03)^2}{1.2 \times 10^{-7}} = 14,303 \text{ s} \simeq 4 \text{ h} \end{aligned}$$

**Comment:** The actual cooling time is obviously less than 4 h as a result of the heat loss from the edges as well as the heat transfer to the rack by conduction.

### 10.2.3 Heating of a Spherical Particle

A spherical particle of radius  $R$  is initially at a uniform temperature of  $T_o$ . At  $t = 0$  it is exposed to a fluid of temperature  $T_\infty$  ( $T_\infty > T_o$ ). It is required to determine the amount of heat transferred to the spherical particle.

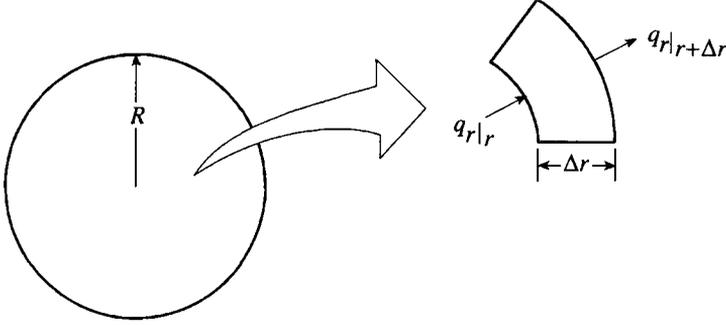


Figure 10.3 Heating of a spherical particle.

Since the heat transfer takes place in the  $r$ -direction, Table C.6 in Appendix C indicates that the only non-zero energy flux component is  $e_r$  and it is given by

$$e_r = q_r = -k \frac{\partial T}{\partial r} \quad (10.2-88)$$

For a spherical differential volume of thickness  $\Delta r$ , as shown in Figure 10.3, Eq. (10.2-1) is expressed as

$$q_r|_r 4\pi r^2 - q_r|_{r+\Delta r} 4\pi (r + \Delta r)^2 = \frac{\partial}{\partial t} \left[ 4\pi r^2 \Delta r \rho \hat{C}_P (T - T_{ref}) \right] \quad (10.2-89)$$

Dividing Eq. (10.2-89) by  $4\pi \Delta r$  and letting  $\Delta r \rightarrow 0$  gives

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = \frac{1}{r^2} \lim_{\Delta r \rightarrow 0} \frac{(r^2 q_r)|_r - (r^2 q_r)|_{r+\Delta r}}{\Delta r} \quad (10.2-90)$$

or,

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = -\frac{1}{r^2} \frac{\partial (r^2 q_r)}{\partial r} \quad (10.2-91)$$

Substitution of Eq. (10.2-88) into Eq. (10.2-91) gives the governing differential equation for temperature as

$$\boxed{\rho \hat{C}_P \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right)} \quad (10.2-92)$$

The initial and the boundary conditions associated with Eq. (10.2-92) are

$$\text{at } t = 0 \quad T = T_o \quad (10.2-93)$$

$$\text{at } r = 0 \quad \frac{\partial T}{\partial r} = 0 \quad (10.2-94)$$

$$\text{at } r = R \quad k \frac{\partial T}{\partial r} = \langle h \rangle (T_\infty - T) \quad (10.2-95)$$

Introduction of the dimensionless quantities

$$\theta = \frac{T_\infty - T}{T_\infty - T_o} \quad (10.2-96)$$

$$\tau = \frac{\alpha t}{R^2} \quad (10.2-97)$$

$$\xi = \frac{r}{R} \quad (10.2-98)$$

$$\text{Bi}_H = \frac{\langle h \rangle R}{k} \quad (10.2-99)$$

reduces Eqs. (10.2-92)-(10.2-95) to

$$\frac{\partial \theta}{\partial \tau} = \frac{1}{\xi^2} \frac{\partial}{\partial \xi} \left( \xi^2 \frac{\partial \theta}{\partial \xi} \right) \quad (10.2-100)$$

$$\text{at } \tau = 0 \quad \theta = 1 \quad (10.2-101)$$

$$\text{at } \xi = 0 \quad \frac{\partial \theta}{\partial \xi} = 0 \quad (10.2-102)$$

$$\text{at } \xi = 1 \quad -\frac{\partial \theta}{\partial \xi} = \text{Bi}_H \theta \quad (10.2-103)$$

### 10.2.2.1 Solution for $0.1 < \text{Bi}_H < 40$

Note that the transformation

$$\theta = \frac{u}{\xi} \quad (10.2-104)$$

converts the spherical geometry into the rectangular geometry. Substitution of Eq. (10.2-104) into Eq. (10.2-100) leads to

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} \quad (10.2-105)$$

which is identical with Eq. (10.2-69). Therefore, the solution is

$$u = e^{-\lambda^2 \tau} [A \sin(\lambda \xi) + B \cos(\lambda \xi)] \quad (10.2-106)$$

or,

$$\theta = e^{-\lambda^2 \tau} \left[ A \frac{\sin(\lambda \xi)}{\xi} + B \frac{\cos(\lambda \xi)}{\xi} \right] \quad (10.2-107)$$

The boundary condition defined by Eq. (10.2-102) indicates that  $B = 0$ . Application of Eq. (10.2-103) yields

$$A e^{-\lambda^2 \tau} (\sin \lambda - \lambda \cos \lambda) = \text{Bi}_H A e^{-\lambda^2 \tau} \sin \lambda \quad (10.2-108)$$

Solving for  $\lambda$  gives

$$\lambda_n \cot \lambda_n = 1 - \text{Bi}_H \quad (10.2-109)$$

The first five roots of Eq. (10.2-109) are given as a function of  $\text{Bi}_H$  in Table 10.4.

**Table 10.4** The roots of Eq. (10.2-109).

$\text{Bi}_H$	$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$	$\lambda_5$
0	0.000	4.493	7.725	10.904	14.066
0.1	0.542	4.516	7.738	10.913	14.073
0.5	1.166	4.604	7.790	10.950	14.102
1.0	1.571	4.712	7.854	10.996	14.137
2.0	2.029	4.913	7.979	11.086	14.207
10.0	2.836	5.717	8.659	11.653	14.687

The complete solution is

$$\theta = \sum_{n=1}^{\infty} C_n e^{-\lambda_n^2 \tau} \frac{\sin(\lambda_n \xi)}{\xi} \quad (10.2-110)$$

The unknown coefficients  $C_n$  can be determined from Eq. (10.2-101). The result is

$$\begin{aligned} C_n &= \frac{\int_0^1 \xi \sin(\lambda_n \xi) d\xi}{\int_0^1 \sin^2(\lambda_n \xi) d\xi} \\ &= \frac{2}{\lambda_n} \left( \frac{\sin \lambda_n - \lambda_n \cos \lambda_n}{\lambda_n - \sin \lambda_n \cos \lambda_n} \right) \end{aligned} \quad (10.2-111)$$

Therefore, the solution becomes

$$\theta = 2 \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \left( \frac{\sin \lambda_n - \lambda_n \cos \lambda_n}{\lambda_n - \sin \lambda_n \cos \lambda_n} \right) e^{-\lambda_n^2 \tau} \frac{\sin(\lambda_n \xi)}{\xi} \quad (10.2-112)$$

The rate of energy entering into the sphere,  $\dot{Q}$ , is given by

$$\begin{aligned} \dot{Q} &= 4\pi R^2 \left( k \frac{\partial T}{\partial r} \Big|_{r=R} \right) \\ &= -4\pi R k (T_\infty - T_o) \frac{\partial \theta}{\partial \xi} \Big|_{\xi=1} \end{aligned} \tag{10.2-113}$$

Substitution of Eq. (10.2-112) into Eq. (10.2-113) results in

$$\dot{Q} = 8\pi R k (T_\infty - T_o) \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \frac{(\sin \lambda_n - \lambda_n \cos \lambda_n)^2}{(\lambda_n - \sin \lambda_n \cos \lambda_n)} \exp(-\lambda_n^2 \tau) \tag{10.2-114}$$

The amount of heat transferred can be calculated from

$$Q = \int_0^t \dot{Q} dt = \frac{L^2}{\alpha} \int_0^\tau \dot{Q} d\tau \tag{10.2-115}$$

Substitution of Eq. (10.2-114) into Eq. (10.2-115) yields

$$\frac{Q}{Q_o} = \sum_{n=0}^{\infty} \frac{6}{\lambda_n^3} \frac{(\sin \lambda_n - \lambda_n \cos \lambda_n)^2}{(\lambda_n - \sin \lambda_n \cos \lambda_n)} [1 - \exp(-\lambda_n^2 \tau)] \tag{10.2-116}$$

where  $Q_o$  is the amount of heat transferred to the sphere when the driving force is constant and equal to its greatest (or, initial) value, i.e.,

$$Q_o = \frac{4}{3}\pi R^3 \rho \hat{C}_P (T_\infty - T_o) \tag{10.2-117}$$

**Example 10.4** *Due to an unexpected cold spell, air temperature drops down to  $-3^\circ\text{C}$  accompanied by a wind blowing at a velocity of 3 m/s in Florida. Farmers have to take precautions in order to avoid frost in their orange orchards. If frost formation starts when the surface temperature of the orange reaches  $0^\circ\text{C}$ , use your engineering judgement to estimate the time the farmers have to take precautions. Assume the oranges are spherical in shape with a diameter of 10 cm and at an initial uniform temperature of  $10^\circ\text{C}$ . The thermal conductivity and the thermal diffusivity of an orange are  $0.51 \text{ W/m}\cdot\text{K}$  and  $1.25 \times 10^{-7} \text{ m}^2/\text{s}$ , respectively.*

**Solution**

**Physical properties**

Initially the film temperature is  $(-3 + 10)/2 = 3.5^\circ\text{C}$ .

$$\text{For air at } 3.5^\circ\text{C (276.5 K)} : \begin{cases} \nu = 13.61 \times 10^{-6} \text{ m}^2/\text{s} \\ k = 24.37 \times 10^{-3} \text{ W/m}\cdot\text{K} \\ \text{Pr} = 0.716 \end{cases}$$

**Analysis**

It is first necessary to calculate the average heat transfer coefficient. The Reynolds number is

$$\begin{aligned} \text{Re}_P &= \frac{D_P v_\infty}{\nu} \\ &= \frac{(10 \times 10^{-2})(3)}{13.61 \times 10^{-6}} = 22,043 \end{aligned} \quad (1)$$

The use of the Ranz-Marshall correlation, Eq. (4.3-29), gives

$$\begin{aligned} \text{Nu} &= 2 + 0.6 \text{Re}_P^{1/2} \text{Pr}^{1/3} \\ &= 2 + 0.6 (22,043)^{1/2} (0.716)^{1/3} \\ &= 81.7 \end{aligned} \quad (2)$$

The average heat transfer coefficient is

$$\begin{aligned} \langle h \rangle &= \text{Nu} \left( \frac{k}{D_P} \right) \\ &= (81.7) \left( \frac{24.37 \times 10^{-3}}{10 \times 10^{-2}} \right) = 19.9 \text{ W/m}^2 \cdot \text{K} \end{aligned} \quad (3)$$

The Biot number is

$$\begin{aligned} \text{Bi}_H &= \frac{\langle h \rangle R}{k} \\ &= \frac{(19.9)(5 \times 10^{-2})}{0.51} = 1.95 \end{aligned} \quad (4)$$

From Eq. (10.2-109), the first root is  $\lambda_1 = 2.012$ . Considering only the first term of the series in Eq. (10.2-112) gives

$$\theta = \frac{T_\infty - T}{T_\infty - T_o} = \frac{2}{\lambda_1} \left( \frac{\sin \lambda_1 - \lambda_1 \cos \lambda_1}{\lambda_1 - \sin \lambda_1 \cos \lambda_1} \right) e^{-\lambda_1^2 \tau} \frac{\sin(\lambda_1 \xi)}{\xi} \quad (5)$$

The time required for the surface of the orange, i.e.,  $\xi = 1$ , to reach  $0^\circ\text{C}$  is

$$\frac{-3 - 0}{-3 - 10} = \frac{2}{2.012} \left( \frac{\sin 115.3 - 2.012 \cos 115.3}{2.012 - \sin 115.3 \cos 115.3} \right) e^{-(2.012)^2 \tau} \sin 115.3 \quad (6)$$

in which  $2.012 \text{ rad} = 115.3^\circ$ . Solving for  $\tau$  yields

$$\tau = 0.26 \quad (7)$$

Therefore, the time is

$$\begin{aligned} t &= \frac{\tau R^2}{\alpha} \\ &= \frac{(0.26)(5 \times 10^{-2})^2}{1.25 \times 10^{-7}} = 5200 \text{ s} \simeq 1 \text{ h } 27 \text{ min} \end{aligned}$$

**Example 10.5** A 2-kg spherical rump roast is placed into a 175°C oven. How long does it take for the center to reach 80°C if the initial temperature is 5°C? The average heat transfer coefficient in the oven is 15 W/m<sup>2</sup>.K and the physical properties of meat are given as:  $\rho = 1076 \text{ kg/m}^3$ ,  $k = 0.514 \text{ W/m.K}$ ,  $\hat{C}_P = 3.431 \text{ kJ/kg.K}$ .

**Solution**

The diameter of the roast is

$$\begin{aligned} D &= \left( \frac{6M}{\pi\rho} \right)^{1/3} \\ &= \left[ \frac{6(2)}{\pi(1076)} \right]^{1/3} = 0.153 \text{ m} \end{aligned} \quad (1)$$

The Biot number is

$$\begin{aligned} \text{Bi}_H &= \frac{(h)R}{k} \\ &= \frac{(15)(0.153/2)}{0.514} = 2.23 \end{aligned} \quad (2)$$

From Eq. (10.2-109), the first root is  $\lambda_1 = 2.101$ . Considering only the first term of the series in Eq. (10.2-112) gives

$$\theta = \frac{T_\infty - T}{T_\infty - T_o} = \frac{2}{\lambda_1} \left( \frac{\sin \lambda_1 - \lambda_1 \cos \lambda_1}{\lambda_1 - \sin \lambda_1 \cos \lambda_1} \right) e^{-\lambda_1^2 \tau} \frac{\sin(\lambda_1 \xi)}{\xi} \quad (3)$$

Since

$$\lim_{\xi \rightarrow 0} \frac{\sin(\lambda_1 \xi)}{\xi} = \lambda_1 \quad (4)$$

the temperature at the center,  $T_c$ , is given by

$$\frac{T_\infty - T_c}{T_\infty - T_o} = 2 \left( \frac{\sin \lambda_1 - \lambda_1 \cos \lambda_1}{\lambda_1 - \sin \lambda_1 \cos \lambda_1} \right) e^{-\lambda_1^2 \tau} \quad (5)$$

Substitution of the values into Eq. (5) gives

$$\frac{175 - 80}{175 - 5} = 2 \left( \frac{\sin 120.4 - 2.101 \cos 120.4}{2.101 - \sin 120.4 \cos 120.4} \right) e^{-(2.101)^2 \tau} \quad (6)$$

in which 2.101 rad = 120.4°. Solving for  $\tau$  yields

$$\tau = 0.226 \quad (7)$$

Therefore, the time is

$$\begin{aligned} t &= \frac{\tau R^2}{\alpha} \\ &= \frac{(0.226)(0.153/2)^2}{0.514 / [(1076)(3431)]} = 9500 \text{ s} \simeq 2.64 \text{ h} \end{aligned} \quad (8)$$

**Example 10.6<sup>3</sup>** A hen's egg of mass 50 grams requires 5 minutes to hard boil. How long will it take to hard boil an ostrich's egg of mass 3 kg?

**Solution**

For an unsteady-state conduction problem, the ratio of the rate of accumulation to the rate of conduction is equal to the Fourier number. Let subscripts *h* and *o* represent hen and ostrich, respectively. Then, it is possible to equate the Fourier numbers as we did in Example 10.1:

$$\left(\frac{\alpha t}{L_{ch}^2}\right)_h = \left(\frac{\alpha t}{L_{ch}^2}\right)_o \quad (1)$$

If both eggs are chemically similar, then  $\alpha_h = \alpha_o$ . Since volume and hence mass, *M*, is proportional to  $L_{ch}^3$ , Eq. (1) reduces to

$$t_o = t_h \left(\frac{M_o}{M_h}\right)^{2/3} \quad (2)$$

Substitution of the numerical values into Eq. (2) gives the time required to hard boil ostrich's egg as

$$t_o = (5) \left(\frac{3000}{50}\right)^{2/3} = 76.6 \text{ min} \quad (3)$$

**10.2.2.2 Solution for  $Bi_H < 0.1$**

When  $Bi_H < 0.1$ , internal resistance to heat transfer is negligible. Considering the sphere as a system, the inventory rate equation for thermal energy can be written as

$$\text{Rate of energy in} = \text{Rate of energy accumulation} \quad (10.2-118)$$

or,

$$4\pi R^2 \langle h \rangle (T_\infty - T) = \frac{d}{dt} \left[ \frac{4}{3} \pi R^3 \rho \hat{C}_P (T - T_{ref}) \right] \quad (10.2-119)$$

Rearrangement of Eq. (10.2-119) gives

$$\int_{T_o}^T \frac{dT}{T_\infty - T} = \frac{3 \langle h \rangle}{\rho \hat{C}_P R} \int_0^t dt \quad (10.2-120)$$

Evaluation of the integrations leads to

$$\boxed{T_\infty - T = (T_\infty - T_o) \exp\left(-\frac{3 \langle h \rangle t}{\rho \hat{C}_P R}\right)} \quad (10.2-121)$$

<sup>3</sup>This problem is taken from Konak (1994).

The amount of heat transferred to the sphere can be calculated as

$$Q = 4\pi R^2 \langle h \rangle \int_0^t (T_\infty - T) dt \tag{10.2-122}$$

Substitution of Eq. (10.2-121) into Eq. (10.2-122) gives

$$Q = \frac{4}{3} \pi R^3 \rho \hat{C}_P (T_\infty - T_o) \left[ 1 - \exp\left(-\frac{3 \langle h \rangle t}{\rho \hat{C}_P R}\right) \right] \tag{10.2-123}$$

or,

$$\boxed{\frac{Q}{Q_o} = 1 - \exp(-3 \text{Bi}_H \tau)} \tag{10.2-124}$$

The exact values of  $Q/Q_o$  obtained from Eq. (10.2-86) are compared with the approximate results obtained from Eq. (10.2-124) for different values of  $\text{Bi}_H$  in Table 10.5. As expected, when  $\text{Bi}_H = 0.1$ , the approximate values are almost equal to the exact ones. For  $\text{Bi}_H > 0.1$ , the use of Eq. (10.2-124) overestimates the exact values.

**Table 10.5** Comparison of  $Q/Q_o$  values obtained from Eqs. (10.2-86) and (10.2-124).

$Q/Q_o$								
$\tau$	$\text{Bi}_H = 0.1$		$\tau$	$\text{Bi}_H = 1$		$\tau$	$\text{Bi}_H = 10$	
	Exact	Approx.		Exact	Approx.		Exact	Approx.
0	0.000	0.000	0	0.000	0.000	0	0.000	0.000
1	0.255	0.259	0.1	0.229	0.259	0.01	0.157	0.259
2	0.444	0.451	0.2	0.398	0.451	0.02	0.259	0.451
3	0.586	0.593	0.3	0.530	0.593	0.03	0.337	0.593
4	0.691	0.699	0.4	0.633	0.699	0.04	0.402	0.699
5	0.770	0.777	0.5	0.713	0.777	0.05	0.457	0.777
6	0.828	0.835	0.6	0.776	0.835	0.06	0.505	0.835
7	0.872	0.878	0.7	0.825	0.878	0.07	0.548	0.878
8	0.905	0.909	0.8	0.863	0.909	0.08	0.586	0.909
9	0.929	0.933	0.9	0.893	0.933	0.09	0.620	0.933
10	0.947	0.950	1.0	0.916	0.950	0.10	0.650	0.950

### 10.3 MASS TRANSPORT

The conservation statement for species  $\mathcal{A}$  is expressed as

$$\left( \begin{array}{c} \text{Rate of} \\ \text{species } \mathcal{A} \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{species } \mathcal{A} \text{ out} \end{array} \right) = \left( \begin{array}{c} \text{Rate of species } \mathcal{A} \\ \text{accumulation} \end{array} \right) \tag{10.3-1}$$

As in Section 8.4, our analysis will be restricted to the application of Eq. (10.3-1) to diffusion in solids and stationary liquids. The solutions of almost all imaginable diffusion problems in different coordinate systems with various initial and boundary conditions are given by Crank (1956). As will be shown later, conduction and diffusion problems become analogous in dimensionless form. Therefore, solutions given by Carslaw and Jaeger (1959) can also be used for diffusion problems.

The Biot number is given by Eq. (7.1-14) as

$$\text{Bi} = \frac{(\text{Difference in driving force})_{\text{solid}}}{(\text{Difference in driving force})_{\text{fluid}}} \quad (10.3-2)$$

In the case of mass transfer, when  $\text{Bi}_M \ll 1$  the internal resistance to mass transfer is negligible and the concentration distribution is considered uniform within the solid phase. When  $\text{Bi}_M \gg 1$ , the external resistance to mass transfer is considered negligible and the concentration in the fluid at the solid surface is almost the same as in the bulk fluid.

### 10.3.1 Mass Transfer Into a Rectangular Slab

Consider a rectangular slab of thickness  $2L$  as shown in Figure 10.4. Initially the concentration of species  $\mathcal{A}$  within the slab is uniform at a value of  $c_{A_0}$ . At  $t = 0$  the surfaces at  $z = \pm L$  are kept at a concentration of  $c_{A_1}$ . To calculate the amount of species  $\mathcal{A}$  transferred into the slab, it is first necessary to determine the concentration distribution of species  $\mathcal{A}$  within the slab as a function of position and time.

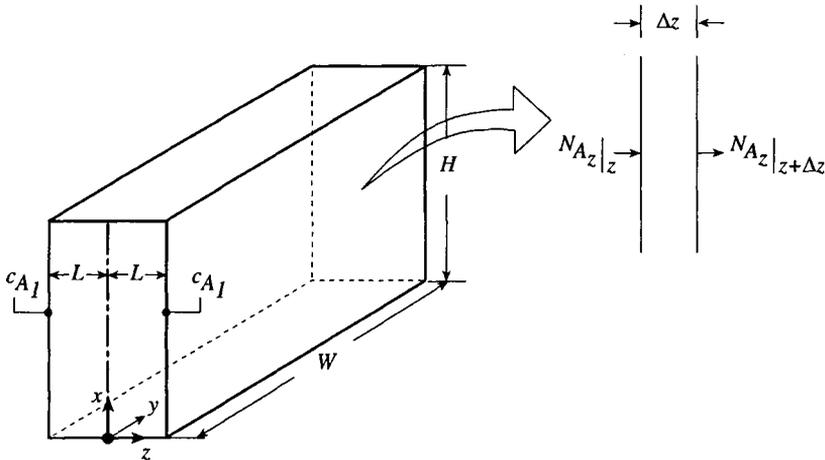


Figure 10.4 Mass transfer into a rectangular slab.

If  $2L/H \ll 1$  and  $2L/W \ll 1$ , then it is possible to assume that the diffusion is one-dimensional and postulate that  $c_A = c_A(t, z)$ . In that case, Table C.7 in Appendix C indicates that the only non-zero molar flux component is  $N_{A_z}$  and it is given by

$$N_{A_z} = J_{A_z}^* = -\mathcal{D}_{AB} \frac{dc_A}{dz} \quad (10.3-3)$$

For a rectangular differential volume element of thickness  $\Delta z$ , as shown in Figure 10.4, Eq. (10.3-1) is expressed as

$$N_{A_z}|_z WH - N_{A_z}|_{z+\Delta z} WH = \frac{\partial}{\partial t} (WH \Delta z c_A) \quad (10.3-4)$$

Dividing Eq. (10.3-4) by  $WH \Delta z$  and letting  $\Delta z \rightarrow 0$  gives

$$\frac{\partial c_A}{\partial t} = \lim_{\Delta z \rightarrow 0} \frac{N_{A_z}|_z - N_{A_z}|_{z+\Delta z}}{\Delta z} \quad (10.3-5)$$

or,

$$\frac{\partial c_A}{\partial t} = -\frac{\partial N_{A_z}}{\partial z} \quad (10.3-6)$$

Substitution of Eq. (10.3-3) into Eq. (10.3-6) gives the governing equation for concentration of species  $A$  as

$$\boxed{\frac{\partial c_A}{\partial t} = \mathcal{D}_{AB} \frac{\partial^2 c_A}{\partial z^2}} \quad (10.3-7)$$

in which the diffusion coefficient is considered constant. The initial and the boundary conditions associated with Eq. (10.3-7) are

$$\begin{array}{lll} \text{at } t = 0 & c_A = c_{A_0} & \text{for all } z \\ \text{at } z = L & c_A = c_{A_1} & t > 0 \\ \text{at } z = -L & c_A = c_{A_1} & t > 0 \end{array} \quad (10.3-8)$$

Note that  $z = 0$  represents a plane of symmetry across which there is no net flux, i.e.,  $\partial c_A / \partial z = 0$ . Therefore, it is also possible to express the initial and boundary conditions as

$$\begin{array}{lll} \text{at } t = 0 & c_A = c_{A_0} & \text{for all } z \\ \text{at } z = 0 & \frac{\partial c_A}{\partial z} = 0 & t > 0 \\ \text{at } z = L & c_A = c_{A_1} & t > 0 \end{array} \quad (10.3-9)$$

The boundary condition at  $z = 0$  can also be interpreted as an impermeable surface. As a result, Eqs. (10.3-7) and (10.3-9) also represent the following problem statement: "Initially the concentration of species  $A$  within a slab of thickness  $L$  is uniform at a value of  $c_{A_0}$ . While one of the surfaces is impermeable to species  $A$ , the other side is kept at a constant concentration of  $c_{A_1}$  with  $c_{A_1} > c_{A_0}$  for  $t > 0$ ."

The physical significance and the order of magnitude of the terms in Eq. (10.3-7) are given in Table 10.6.

**Table 10.6** The physical significance and the order of magnitude of the terms in Eq. (10.3-7).

Term	Physical Significance	Order of Magnitude
$\mathcal{D}_{AB} \frac{\partial^2 c_A}{\partial z^2}$	Rate of diffusion	$\frac{\mathcal{D}_{AB} (c_{A_1} - c_{A_o})}{L^2}$
$\frac{\partial c_A}{\partial t}$	Rate of accumulation of mass $\mathcal{A}$	$\frac{c_{A_1} - c_{A_o}}{t}$

Therefore, the ratio of the rate of diffusion to the rate of accumulation of mass  $\mathcal{A}$  is given by

$$\frac{\text{Rate of diffusion}}{\text{Rate of mass } \mathcal{A} \text{ accumulation}} = \frac{\mathcal{D}_{AB} (c_{A_1} - c_{A_o})/L^2}{(c_{A_1} - c_{A_o})/t} = \frac{\mathcal{D}_{AB} t}{L^2} \tag{10.3-10}$$

which is completely analogous to the *Fourier number*, Fo.

Introduction of the dimensionless quantities

$$\theta = \frac{c_{A_1} - c_A}{c_{A_1} - c_{A_o}} \tag{10.3-11}$$

$$\xi = \frac{z}{L} \tag{10.3-12}$$

$$\tau = \frac{\mathcal{D}_{AB} t}{L^2} \tag{10.3-13}$$

reduces Eqs. (10.3-7) and (10.3-8) to

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} \tag{10.3-14}$$

$$\begin{aligned} \text{at } \tau = 0 & \quad \theta = 1 \\ \text{at } \xi = 1 & \quad \theta = 0 \\ \text{at } \xi = -1 & \quad \theta = 0 \end{aligned} \tag{10.3-15}$$

Note that Eqs. (10.3-14) and (10.3-15) are identical with Eqs. (10.2-14) and (10.2-15). Therefore, the solution given by Eq. (10.2-32) is also valid for this case, i.e.,

$$\theta = 2 \sum_{n=0}^{\infty} \frac{(-1)^n}{(n + \frac{1}{2}) \pi} e^{-(n + \frac{1}{2})^2 \pi^2 \tau} \cos \left[ \left( n + \frac{1}{2} \right) \pi \xi \right] \tag{10.3-16}$$

**Example 10.7** A 1 mm thick membrane in the form of a flat sheet is immersed in a well-stirred 0.15 M solution of species A. If species A has the diffusion coefficient of  $0.65 \times 10^{-9} \text{ m}^2/\text{s}$  and the partition coefficient of 0.4, determine the concentration distribution as a function of position and time.

### Solution

Using Eq. (10.3-16), the concentration distribution is given as

$$\frac{c_A}{0.06} = 1 - 2 \sum_{n=0}^{\infty} \frac{(-1)^n}{\left(n + \frac{1}{2}\right) \pi} \exp \left[ - \left(n + \frac{1}{2}\right)^2 \frac{\pi^2 (0.65 \times 10^{-9})}{(0.5 \times 10^{-3})^2} t \right] \cos \left[ \left(n + \frac{1}{2}\right) \pi \xi \right]$$

The variation of  $c_A$  as a function of the dimensionless distance,  $\xi$ , at various values of time is given in the table below. Note that  $\xi = 0$  and  $\xi = 1$  represent the center and the surface of the sheet, respectively.

$\xi$	$c_A \times 10^2 \text{ M}$			
	$t = 1 \text{ min}$	$t = 2 \text{ min}$	$t = 5 \text{ min}$	$t = 10 \text{ min}$
0	0.881	2.465	4.885	5.837
0.1	0.936	2.510	4.889	5.839
0.2	1.103	2.637	4.940	5.845
0.3	1.381	2.848	5.007	5.855
0.4	1.770	3.137	5.098	5.868
0.5	2.268	3.497	5.212	5.885
0.6	2.869	3.918	5.345	5.904
0.7	3.561	4.391	5.494	5.926
0.8	4.329	4.905	5.656	5.950
0.9	5.151	5.445	5.826	5.975
1.0	6.000	6.000	6.000	6.000

#### 10.3.1.1 Macroscopic equation

Integration of the governing equation, Eq. (10.3-7), over the volume of the system gives

$$\int_{-L}^L \int_0^W \int_0^H \frac{\partial c_A}{\partial t} dx dy dz = \int_{-L}^L \int_0^W \int_0^H D_{AB} \frac{\partial^2 c_A}{\partial z^2} dx dy dz \quad (10.3-17)$$

Evaluation of the integrations yields

$$\underbrace{\frac{d}{dt} \left[ \int_{-L}^L \int_0^W \int_0^H c_A dx dy dz \right]}_{\text{Rate of accumulation of species A}} = \underbrace{2WH \left( D_{AB} \frac{\partial c_A}{\partial z} \Big|_{z=L} \right)}_{\text{Rate of species A entering from surfaces at } z = \pm L} \quad (10.3-18)$$

Note that Eq. (10.3-18) is the macroscopic mass balance for species  $\mathcal{A}$  by considering the rectangular slab as a system.

The molar rate of species  $\mathcal{A}$  entering into the slab,  $\dot{n}_A$ , can be calculated from Eq. (10.3-18) as

$$\begin{aligned} \dot{n}_A &= 2WH \left( \mathcal{D}_{AB} \frac{\partial c_A}{\partial z} \Big|_{z=L} \right) \\ &= - \frac{2WH\mathcal{D}_{AB}(c_{A_1} - c_{A_o})}{L} \frac{\partial \theta}{\partial \xi} \Big|_{\xi=1} \end{aligned} \tag{10.3-19}$$

Substitution of Eq. (10.3-16) into Eq. (10.3-19) gives

$$\dot{n}_A = \frac{4WH\mathcal{D}_{AB}(c_{A_1} - c_{A_o})}{L} \sum_{n=0}^{\infty} \exp \left[ - \frac{(2n+1)^2 \pi^2 \tau}{4} \right] \tag{10.3-20}$$

The number of moles of species  $\mathcal{A}$  transferred can be calculated from

$$n_A = \int_0^t \dot{n}_A dt = \frac{L^2}{\mathcal{D}_{AB}} \int_0^\tau \dot{n}_A d\tau \tag{10.3-21}$$

Substitution of Eq. (10.3-20) into Eq. (10.3-21) yields

$$\frac{M_A}{M_{A_\infty}} = 1 - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp \left[ - \frac{(2n+1)^2 \pi^2 \tau}{4} \right] \tag{10.3-22}$$

where  $M_A$  is the mass of species transferred into the slab and  $M_{A_\infty}$  is the maximum amount of species  $\mathcal{A}$  transferred into the slab, i.e.,

$$M_{A_\infty} = 2LWH(c_{A_1} - c_{A_o})\mathcal{M}_A \tag{10.3-23}$$

### 10.3.1.2 Solution for short times

Let  $s$  be the distance measured from the surface of the slab, i.e.,

$$s = L - z \tag{10.3-24}$$

so that Eq. (10.3-7) reduces to

$$\frac{\partial c_A}{\partial t} = \mathcal{D}_{AB} \frac{\partial^2 c_A}{\partial s^2} \tag{10.3-25}$$

At small values of time, species  $\mathcal{A}$  does not penetrate very far into the slab. Under these circumstances, it is possible to consider the slab as a semi-infinite medium in the  $s$ -direction. The initial and the boundary conditions associated with Eq. (10.3-25) become

$$\begin{aligned} \text{at } t = 0 & \quad c_A = c_{A_o} \\ \text{at } s = 0 & \quad c_A = c_{A_1} \\ \text{at } s = \infty & \quad c_A = c_{A_o} \end{aligned} \tag{10.3-26}$$

Introduction of the dimensionless concentration

$$\phi = \frac{c_A - c_{A_o}}{c_{A_1} - c_{A_o}} \quad (10.3-27)$$

reduces Eqs. (10.3-25) and (10.3-26) to

$$\frac{\partial \phi}{\partial t} = \mathcal{D}_{AB} \frac{\partial^2 \phi}{\partial s^2} \quad (10.3-28)$$

$$\begin{aligned} \text{at } t = 0 & \quad \phi = 0 \\ \text{at } s = 0 & \quad \phi = 1 \\ \text{at } s = \infty & \quad \phi = 0 \end{aligned} \quad (10.3-29)$$

Note that Eqs. (10.3-28) and (10.3-29) are identical with Eqs. (10.2-44) and (10.2-45) with the exception that  $\alpha$  is replaced by  $\mathcal{D}_{AB}$ . Therefore, the solution is given by Eq. (10.2-56), i.e.,

$$\boxed{\frac{c_A - c_{A_o}}{c_{A_1} - c_{A_o}} = 1 - \operatorname{erf}\left(\frac{s}{\sqrt{4\mathcal{D}_{AB}t}}\right)} \quad (10.3-30)$$

The molar rate of transfer of species  $\mathcal{A}$  into the semi-infinite slab of cross-sectional area  $A$  is

$$\begin{aligned} \dot{n}_A &= A \left( -\mathcal{D}_{AB} \frac{\partial c_A}{\partial s} \Big|_{s=0} \right) \\ &= A(c_{A_1} - c_{A_o}) \sqrt{\frac{\mathcal{D}_{AB}}{\pi t}} \end{aligned} \quad (10.3-31)$$

The number of moles of species  $\mathcal{A}$  transferred is

$$\begin{aligned} n_A &= \int_0^t \dot{n}_A dt \\ &= 2A(c_{A_1} - c_{A_o}) \sqrt{\frac{\mathcal{D}_{AB}t}{\pi}} \end{aligned} \quad (10.3-32)$$

The maximum amount of species  $\mathcal{A}$  transferred to the slab is

$$M_{A_\infty} = AL(c_{A_1} - c_{A_o})\mathcal{M}_A \quad (10.3-33)$$

Hence, the ratio of the uptake of species  $\mathcal{A}$  relative to the maximum is given by

$$\boxed{\frac{M_A}{M_{A_\infty}} = \frac{2}{\sqrt{\pi}} \sqrt{\frac{\mathcal{D}_{AB}t}{L^2}}} \quad (10.3-34)$$

The values of  $M_A/M_{A_\infty}$  calculated from Eqs. (10.3-22) and (10.3-34) are compared in Table 10.7. Note that the values obtained from the short time solution are almost equal to the exact values up to  $\sqrt{\mathcal{D}_{AB}t}/L^2 = 0.6$ .

**Table 10.7** Comparison of the exact fractional uptake values with a short time solution.

$\sqrt{\frac{D_{AB}t}{L^2}}$	$M_A/M_{A\infty}$	
	Exact Eq. (10.3-22)	Approx. Eq. (10.3-34)
0.1	0.113	0.113
0.2	0.226	0.226
0.3	0.339	0.339
0.4	0.451	0.451
0.5	0.562	0.564
0.6	0.667	0.677
0.7	0.758	0.790
0.8	0.833	0.903
0.9	0.890	1.016
1.0	0.931	1.128

**Example 10.8** For a semi-infinite medium, penetration distances for the momentum and heat transfer are estimated as

$$\delta = 4\sqrt{\nu t}$$

$$\delta_t = 4\sqrt{\alpha t}$$

Develop an analogous equation for the mass transfer.

### Solution

When  $s/\sqrt{4D_{AB}t} = 2$ , Eq. (10.3-30) becomes

$$\frac{c_A - c_{A_o}}{c_{A_1} - c_{A_o}} = 1 - \operatorname{erf}(2) = 0.005$$

indicating that  $c_A \simeq c_{A_o}$ . Therefore, the penetration distance for mass transfer,  $\delta_c$ , is given by

$$\delta_c = 4\sqrt{D_{AB}t}$$

### 10.3.2 Gas Absorption Into a Spherical Droplet

Consider a liquid droplet ( $\mathcal{B}$ ) of radius  $R$  surrounded by gas  $\mathcal{A}$  as shown in Figure 10.5. We are interested in the rate of absorption of species  $\mathcal{A}$  into the liquid. The problem will be analyzed with the following assumptions:

1. Convective flux is negligible with respect to the molecular flux, i.e.,  $v_z^* \simeq 0$ .
2. The total concentration is constant.

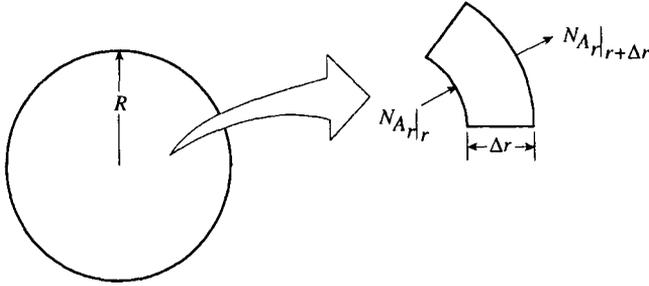


Figure 10.5 Gas absorption into a droplet.

Since  $c_A = c_A(r)$ , Table C.9 in Appendix C indicates that the only non-zero molar flux component is  $N_{A_r}$  and it is given by

$$N_{A_r} = J_{A_r}^* = -\mathcal{D}_{AB} \frac{dc_A}{dr} \tag{10.3-35}$$

For a spherical differential volume element of thickness  $\Delta r$ , as shown in Figure 10.5, Eq. (10.3-1) is expressed in the form

$$N_{A_r}|_r 4\pi r^2 - N_{A_r}|_{r+\Delta r} 4\pi (r + \Delta r)^2 = \frac{\partial}{\partial t} [4\pi r^2 \Delta r (c_A - c_{A_o})] \tag{10.3-36}$$

Dividing Eq. (20.3-36) by  $4\pi\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\frac{\partial c_A}{\partial t} = \frac{1}{r^2} \lim_{\Delta r \rightarrow 0} \frac{(r^2 N_{A_r})|_r - (r^2 N_{A_r})|_{r+\Delta r}}{\Delta r} \tag{10.3-37}$$

or,

$$\frac{\partial c_A}{\partial t} = -\frac{1}{r^2} \frac{\partial (r^2 N_{A_r})}{\partial r} \tag{10.3-38}$$

Substitution of Eq. (10.3-35) into Eq. (10.3-38) gives the governing differential equation for the concentration of species  $A$  as

$$\boxed{\frac{\partial c_A}{\partial t} = \frac{\mathcal{D}_{AB}}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_A}{\partial r} \right)} \tag{10.3-39}$$

The initial and the boundary conditions associated with Eq. (10.3-39) are

$$\text{at } t = 0 \quad c_A = c_{A_o} \tag{10.3-40}$$

$$\text{at } r = 0 \quad \frac{\partial c_A}{\partial r} = 0 \tag{10.3-41}$$

$$\text{at } r = R \quad c_A = c_A^* \tag{10.3-42}$$

where  $c_A^*$  is the equilibrium solubility of species  $A$  in liquid  $B$ .

Introduction of the dimensionless quantities

$$\theta = \frac{c_A^* - c_A}{c_A^* - c_{A_0}} \quad (10.3-43)$$

$$\xi = \frac{z}{L} \quad (10.3-44)$$

$$\tau = \frac{D_{AB} t}{R^2} \quad (10.3-45)$$

reduces Eqs. (10.3-39)-(10.3-42) to

$$\frac{\partial \theta}{\partial \tau} = \frac{1}{\xi^2} \frac{\partial}{\partial \xi} \left( \xi^2 \frac{\partial \theta}{\partial \xi} \right) \quad (10.3-46)$$

$$\text{at } \tau = 0 \quad \theta = 1 \quad (10.3-47)$$

$$\text{at } \xi = 0 \quad \frac{\partial \theta}{\partial \xi} = 0 \quad (10.3-48)$$

$$\text{at } \xi = 1 \quad \theta = 0 \quad (10.3-49)$$

The transformation

$$\theta = \frac{u}{\xi} \quad (10.3-50)$$

converts the spherical geometry into the rectangular geometry. Substitution of Eq. (10.3-50) into Eq. (10.3-46) leads to

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} \quad (10.3-51)$$

which is identical with Eq. (10.2-69). Therefore, the solution is

$$u = e^{-\lambda^2 \tau} [A \sin(\lambda \xi) + B \cos(\lambda \xi)] \quad (10.3-52)$$

or,

$$\theta = e^{-\lambda^2 \tau} \left[ A \frac{\sin(\lambda \xi)}{\xi} + B \frac{\cos(\lambda \xi)}{\xi} \right] \quad (10.3-53)$$

The boundary condition defined by Eq. (10.3-48) indicates that  $B = 0$ . Application of Eq. (10.3-49) yields

$$\sin \lambda = 0 \quad \Rightarrow \quad \lambda_n = n\pi \quad n = 1, 2, 3, \dots \quad (10.3-54)$$

Therefore, the general solution is

$$\theta = \sum_{n=1}^{\infty} C_n e^{-n^2 \pi^2 \tau} \frac{\sin(n\pi \xi)}{\xi} \quad (10.3-55)$$

The unknown coefficients  $C_n$  can be determined from the initial condition defined by Eq. (10.3-47). The result is

$$\begin{aligned} C_n &= \frac{\int_0^1 \xi \sin(n\pi\xi) d\xi}{\int_0^1 \sin^2(n\pi\xi) d\xi} \\ &= -\frac{2 \cos(n\pi)}{n\pi} = -\frac{2(-1)^n}{n\pi} \end{aligned} \quad (10.3-56)$$

Hence, the solution becomes

$$\theta = -\frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} e^{-n^2\pi^2\tau} \frac{\sin(n\pi\xi)}{\xi} \quad (10.3-57)$$

or,

$$\frac{c_A^* - c_A}{c_A^* - c_{A_0}} = -\frac{2R}{\pi\tau} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \exp\left(-\frac{n^2\pi^2\mathcal{D}_{AB}t}{R^2}\right) \sin\left(\frac{n\pi r}{R}\right) \quad (10.3-58)$$

The molar rate of absorption of species  $\mathcal{A}$  is given by

$$\begin{aligned} \dot{n}_A &= 4\pi R^2 \left( \mathcal{D}_{AB} \frac{\partial c_A}{\partial r} \Big|_{r=R} \right) \\ &= -4\pi R \mathcal{D}_{AB} (c_A^* - c_{A_0}) \frac{\partial \theta}{\partial \xi} \Big|_{\xi=1} \end{aligned} \quad (10.3-59)$$

Substitution of Eq. (10.3-57) into Eq. (10.3-59) results in

$$\dot{n}_A = 8\pi R \mathcal{D}_{AB} (c_A^* - c_{A_0}) \sum_{n=1}^{\infty} \exp(-n^2\pi^2\tau) \quad (10.3-60)$$

The moles of species  $\mathcal{A}$  absorbed can be calculated from

$$n_A = \int_0^t \dot{n}_A dt = \frac{R^2}{\mathcal{D}_{AB}} \int_0^\tau \dot{n}_A d\tau \quad (10.3-61)$$

Substitution of Eq. (10.3-60) into Eq. (10.3-61) yields

$$n_A = \frac{8R^3(c_A^* - c_{A_0})}{\pi} \sum_{n=1}^{\infty} \frac{1}{n^2} \left(1 - e^{-n^2\pi^2\tau}\right) \quad (10.3-62)$$

The maximum amount of species  $\mathcal{A}$  absorbed by the droplet is given by

$$M_{A\infty} = \frac{4}{3}\pi R^3(c_A^* - c_{A_o})\mathcal{M}_A \quad (10.3-63)$$

Therefore, the mass of species  $\mathcal{A}$  absorbed by the droplet relative to the maximum is

$$\frac{M_A}{M_{A\infty}} = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp(-n^2\pi^2\tau) \quad (10.3-64)$$

## NOTATION

$A$	area, $\text{m}^2$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ}/\text{kg}\cdot\text{K}$
$c_i$	concentration of species $i$ , $\text{kmol}/\text{m}^3$
$D_P$	particle diameter, $\text{m}$
$D_{AB}$	diffusion coefficient for system $\mathcal{A}\text{-}\mathcal{B}$ , $\text{m}^2/\text{s}$
$e$	total energy flux, $\text{W}/\text{m}^2$
$F_D$	drag force, $\text{N}$
$h$	heat transfer coefficient, $\text{W}/\text{m}^2\cdot\text{K}$
$J^*$	molecular molar flux, $\text{kmol}/\text{m}^2\cdot\text{s}$
$k_c$	mass transfer coefficient, $\text{m}/\text{s}$
$L$	length, $\text{m}$
$M$	mass, $\text{kg}$
$\dot{m}$	mass flow rate, $\text{kg}/\text{s}$
$\mathcal{M}$	molecular weight, $\text{kg}/\text{kmol}$
$N$	total molar flux, $\text{kmol}/\text{m}^2\cdot\text{s}$
$\dot{n}$	molar flow rate, $\text{kmol}/\text{s}$
$\dot{Q}$	heat transfer rate, $\text{W}$
$Q$	volumetric flow rate, $\text{m}^3/\text{s}$
$q$	heat flux, $\text{W}/\text{m}^2$
$R$	radius, $\text{m}$
$T$	temperature, $^{\circ}\text{C}$ or $\text{K}$
$t$	time, $\text{s}$
$V$	velocity of the plate in Couette flow, $\text{m}/\text{s}$ ; volume, $\text{m}^3$
$v$	velocity, $\text{m}/\text{s}$
$W$	width, $\text{m}$
$\alpha$	thermal diffusivity, $\text{m}^2/\text{s}$
$\delta$	penetration distance for momentum, $\text{m}$
$\delta_c$	penetration distance for mass, $\text{m}$

$\delta_t$	penetration distance for heat, m
$\mu$	viscosity, kg/m.s
$\nu$	kinematic viscosity, m <sup>2</sup> /s
$\rho$	density, kg/m <sup>3</sup>
$\pi$	total momentum flux, N/m <sup>2</sup>
$\tau$	dimensionless time
$\tau_{ij}$	shear stress (flux of $j$ – momentum in the $i$ – direction, N/m <sup>2</sup> )

**Bracket**

$\langle a \rangle$	average value of $a$
---------------------	----------------------

**Subscripts**

$A, B$	species in binary systems
$c$	center
$ch$	characteristic
$ref$	reference

**Dimensionless Numbers**

$Bi_H$	Biot number for heat transfer
$Bi_M$	Biot number for mass transfer
$Fo$	Fourier number
$Nu$	Nusselt number
$Pr$	Prandtl number
$Re$	Reynolds number

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## PROBLEMS

**10.1** A spherical material of 15 cm in radius is initially at a uniform temperature of 60 °C. It is placed in a room where the temperature is 23 °C. Estimate the average heat transfer coefficient if it takes 42 min for the center temperature to reach 30 °C. Take  $k = 0.12 \text{ W/m.K}$  and  $\alpha = 2.7 \times 10^{-6} \text{ m}^2/\text{s}$ .

(Answer: 6.5 W/m<sup>2</sup>.K)

**10.2** The fuel oil pipe that supplies the heating system of a house is laid 1 m below the ground. Around a temperature of 2 °C the viscosity of the fuel oil increases to a point that pumping becomes almost impossible. When the air temperature drops to -15 °C, how long does it take to have problems in the heating system? Assume that the initial ground temperature is 10 °C and the physical properties are:  $k = 0.38 \text{ W/m.K}$  and  $\alpha = 4 \times 10^{-7} \text{ m}^2/\text{s}$

(Answer: 351.3h)

**10.3** Two semi-infinite solids  $A$  and  $B$ , initially at  $T_{A_0}$  and  $T_{B_0}$  with  $T_{A_0} > T_{B_0}$ , are suddenly brought into contact at  $t = 0$ . The contact resistance between the metals is negligible.

a) Equating the heat fluxes at the interface, show that the interface temperature,  $T_i$ , is given by

$$\frac{T_i - T_{B_0}}{T_{A_0} - T_{B_0}} = \frac{\sqrt{\alpha_B} k_A}{\sqrt{\alpha_B} k_A + \sqrt{\alpha_A} k_B}$$

b) Consider two slabs made of copper and wood which are at a temperature of 80 °C. You want to check if they are hot by touching them with your finger. Explain why you think the copper slab feels hotter. The physical properties are given as follows:

	$k$ W/m.K	$\alpha$ m <sup>2</sup> /s
Skin	0.3	$1.5 \times 10^{-7}$
Copper	401	$117 \times 10^{-6}$
Wood	0.15	$1.2 \times 10^{-7}$

10.4 In Section 10.3.1-2, the number of moles of species  $A$  transferred into the semi-infinite medium,  $n_A$ , is determined by integrating the molar transfer rate over time, i.e., Eq. (10.3-32). It is also possible to determine  $n_A$  from

$$n_A = A \int_0^\infty (c_A - c_{A_o}) ds$$

Show that the substitution of Eq. (10.3-30) into the above equation leads to Eq. (10.3-32).

10.5 A polymer sheet with the dimensions of  $2 \times 50 \times 50$  mm is exposed to chloroform vapor at  $20^\circ\text{C}$  and 5 mmHg. The weight of the polymer sheet is recorded with the help of a sensitive electrobalance and the following data are obtained:

Time (h)	Weight of polymer sheet (g)
0	6.0000
54	6.0600
$\infty$	6.1200

Assuming that the mass transport of chloroform in the polymer sheet is described by a Fickian type diffusion process, estimate the diffusion coefficient of chloroform in the polymer sheet.

(Answer:  $1.01 \times 10^{-12} \text{ m}^2/\text{s}$ )

10.6 Consider an unsteady-state diffusion of species  $A$  through a plane slab with the following initial and boundary conditions:

$$\frac{\partial c_A}{\partial t} = D_{AB} \frac{\partial^2 c_A}{\partial z^2} \quad (1)$$

$$\text{at } t = 0 \quad c_A = 0 \quad (2)$$

$$\text{at } z = 0 \quad c_A = c_{A_o} \quad (3)$$

$$\text{at } z = L \quad c_A = 0 \quad (4)$$

a) In terms of the dimensionless quantities

$$\theta = \frac{c_{A_o} - c_A}{c_{A_o}} \quad (5)$$

$$\xi = \frac{z}{L} \quad (6)$$

$$\tau = \frac{D_{AB} t}{L^2} \quad (7)$$

show that Eqs. (1)-(4) become

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} \quad (8)$$

$$\text{at } \tau = 0 \quad \theta = 1 \quad (9)$$

$$\text{at } \xi = 0 \quad \theta = 0 \quad (10)$$

$$\text{at } \xi = 1 \quad \theta = 1 \quad (11)$$

b) Note that the boundary condition at  $\xi = 1$  is not homogeneous and, as a result, the method of separation of variables cannot be applied. To circumvent this problem, propose a solution in the form

$$\theta(\tau, \xi) = \theta_\infty(\xi) - \theta_t(\tau, \xi) \quad (12)$$

in which  $\theta_\infty(\xi)$  is the steady-state solution, i.e.,

$$\frac{d^2 \theta_\infty}{d\xi^2} = 0 \quad (13)$$

with the following boundary conditions

$$\text{at } \xi = 0 \quad \theta_\infty = 0 \quad (14)$$

$$\text{at } \xi = 1 \quad \theta_\infty = 1 \quad (15)$$

Show that the steady-state solution is

$$\theta_\infty = \xi \quad (16)$$

On the other hand, the transient contribution  $\theta_t(\tau, \xi)$  satisfies Eq. (8), i.e.,

$$\frac{\partial \theta_t}{\partial \tau} = \frac{\partial^2 \theta_t}{\partial \xi^2} \quad (17)$$

with the following initial and boundary conditions

$$\text{at } \tau = 0 \quad \theta_t = \xi - 1 \quad (18)$$

$$\text{at } \xi = 0 \quad \theta_t = 0 \quad (19)$$

$$\text{at } \xi = 1 \quad \theta_t = 0 \quad (20)$$

c) Use the method of separation of variables and show that the solution of Eq. (17) is given as

$$\theta_t = -\frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} e^{-n^2 \pi^2 \tau} \sin(n\pi\xi) \quad (21)$$

d) Show that the concentration distribution is given by

$$\frac{c_A}{c_{A_0}} = 1 - \xi - \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} e^{-n^2 \pi^2 \tau} \sin(n\pi\xi) \quad (22)$$

# Chapter 11

## Unsteady-State Microscopic Balances With Generation

This chapter briefly considers the cases in which all the terms in the inventory rate equation are non-zero. The resulting governing equations for velocity, temperature and concentration are obviously partial differential equations. Nonhomogeneity introduced either by the governing equation itself or by the boundary conditions further complicates the problem.

### 11.1 UNSTEADY LAMINAR FLOW IN A TUBE

A horizontal tube of radius  $R$  is filled with a stationary incompressible Newtonian fluid as shown in Figure 11.1. At time  $t = 0$ , a constant pressure gradient is imposed and the fluid begins to flow. It is required to determine the development of velocity profile as a function of position and time.

Postulating  $v_z = v_z(t, r)$  and  $v_r = v_\theta = 0$ , Table C.2 in Appendix C indicates that the only non-zero shear stress component is  $\tau_{rz}$  and the components of the total momentum flux are given by

$$\pi_{rz} = \tau_{rz} + (\rho v_z) v_r = \tau_{rz} = -\mu \frac{\partial v_z}{\partial r} \quad (11.1-1)$$

$$\pi_{\theta z} = \tau_{\theta z} + (\rho v_z) v_\theta \quad (11.1-2)$$

$$\pi_{zz} = \tau_{zz} + (\rho v_z) v_z \quad (11.1-3)$$

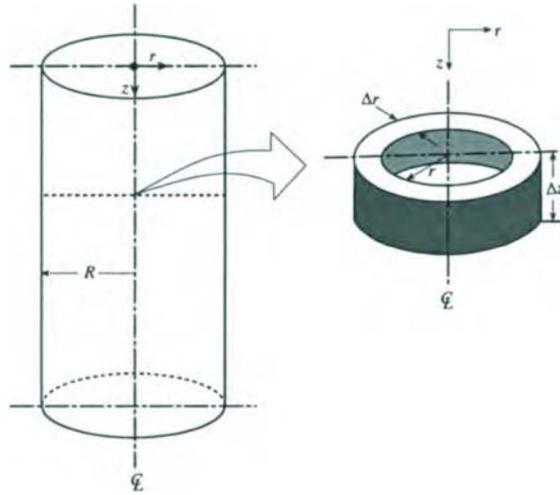


Figure 11.1 Unsteady-state flow in a circular pipe.

The conservation statement for momentum is expressed as

$$\left( \begin{array}{c} \text{Rate of} \\ \text{momentum in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{momentum out} \end{array} \right) + \left( \begin{array}{c} \text{Forces acting} \\ \text{on a system} \end{array} \right) = \left( \begin{array}{c} \text{Rate of momentum} \\ \text{accumulation} \end{array} \right) \quad (11.1-4)$$

The pressure in the pipe depends on  $z$ . Therefore, it is necessary to consider only the  $z$ -component of the equation of motion. For a cylindrical differential volume element of thickness  $\Delta r$  and length  $\Delta z$ , as shown in Figure 11.1, Eq. (11.1-4) is expressed as

$$\begin{aligned} & (\pi_{zz}|_z 2\pi r \Delta r + \pi_{rz}|_r 2\pi r \Delta z) - [\pi_{zz}|_{z+\Delta z} 2\pi r \Delta r + \pi_{rz}|_{r+\Delta r} 2\pi(r + \Delta r) \Delta z] \\ & + (P|_z - P|_{z+\Delta z}) 2\pi r \Delta r + 2\pi r \Delta r \Delta z \rho g = \frac{\partial}{\partial t} (2\pi r \Delta r \Delta z \rho v_z) \end{aligned} \quad (11.1-5)$$

Dividing Eq. (11.1-5) by  $2\pi \Delta r \Delta z$  and taking the limit as  $\Delta r \rightarrow 0$  and  $\Delta z \rightarrow 0$  gives

$$\begin{aligned} \rho \frac{\partial v_z}{\partial t} = \lim_{\Delta z \rightarrow 0} \left( \frac{P|_z - P|_{z+\Delta z}}{\Delta z} \right) + \frac{1}{r} \lim_{\Delta r \rightarrow 0} \frac{(r\pi_{rz})|_r - (r\pi_{rz})|_{r+\Delta r}}{\Delta r} \\ + \lim_{\Delta z \rightarrow 0} \left( \frac{\pi_{zz}|_z - \pi_{zz}|_{z+\Delta z}}{\Delta z} \right) + \rho g \end{aligned} \quad (11.1-6)$$

or,

$$\rho \frac{\partial v_z}{\partial t} = - \frac{dP}{dz} - \frac{1}{r} \frac{\partial(r\pi_{rz})}{\partial r} - \frac{\partial \pi_{zz}}{\partial z} + \rho g \quad (11.1-7)$$

Substitution of Eqs. (11.1-1) and (11.1-3) into Eq. (11.1-7) and noting that  $\partial v_z / \partial z = 0$  gives

$$\rho \frac{\partial v_z}{\partial t} = -\frac{dP}{dz} + \frac{\mu}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right) + \rho g \quad (11.1-8)$$

The modified pressure is defined by

$$\mathcal{P} = P - \rho g z \quad (11.1-9)$$

so that

$$\frac{d\mathcal{P}}{dz} = \frac{dP}{dz} - \rho g \quad (11.1-10)$$

Substitution of Eq. (11.1-10) into Eq. (11.1-8) yields

$$\underbrace{\rho \frac{\partial v_z}{\partial t} - \frac{\mu}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right)}_{f(t,r)} = \underbrace{-\frac{d\mathcal{P}}{dz}}_{f(z)} \quad (11.1-11)$$

Note that while the right-side of Eq. (11.1-11) is a function of  $z$  only, the left-side is dependent on  $r$  and  $t$ . This is possible if and only if both sides of Eq. (11.1-11) are equal to a constant, say  $\lambda$ . Hence,

$$-\frac{d\mathcal{P}}{dz} = \lambda \quad \Rightarrow \quad \lambda = \frac{\mathcal{P}_o - \mathcal{P}_L}{L} \quad (11.1-12)$$

where  $\mathcal{P}_o$  and  $\mathcal{P}_L$  are the values of  $\mathcal{P}$  at  $z = 0$  and  $z = L$ , respectively. Substitution of Eq. (11.1-12) into Eq. (11.1-11) gives the governing equation for velocity as

$$\boxed{\rho \frac{\partial v_z}{\partial t} = \frac{\mathcal{P}_o - \mathcal{P}_L}{L} + \frac{\mu}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right)} \quad (11.1-13)$$

The initial and the boundary conditions associated with Eq. (11.1-13) are

$$\text{at } t = 0 \quad v_z = 0 \quad \text{for all } r \quad (11.1-14)$$

$$\text{at } r = 0 \quad \frac{\partial v_z}{\partial r} = 0 \quad \text{for } t \geq 0 \quad (11.1-15)$$

$$\text{at } r = R \quad v_z = 0 \quad \text{for } t \geq 0 \quad (11.1-16)$$

### 11.1.1 Exact Solution

Introduction of the following dimensionless quantities

$$\theta = \frac{4\mu v_z}{\left( \frac{\mathcal{P}_o - \mathcal{P}_L}{L} \right) R^2} \quad (11.1-17)$$

$$\xi = \frac{r}{R} \quad (11.1-18)$$

$$\tau = \frac{\mu t}{\rho R^2} \quad (11.1-19)$$

reduces Eq. (11.1-13)-(11.1-16) to the form

$$\frac{\partial \theta}{\partial \tau} = 4 + \frac{1}{\xi} \frac{\partial}{\partial \xi} \left( \xi \frac{\partial \theta}{\partial \xi} \right) \quad (11.1-20)$$

$$\text{at } \tau = 0 \quad \theta = 0 \quad (11.1-21)$$

$$\text{at } \xi = 0 \quad \frac{\partial \theta}{\partial \xi} = 0 \quad (11.1-22)$$

$$\text{at } \xi = 1 \quad \theta = 0 \quad (11.1-23)$$

Since Eq. (11.1-20) is not homogeneous, the solution is proposed in the form

$$\theta(\tau, \xi) = \theta_{\infty}(\xi) - \theta_t(\tau, \xi) \quad (11.1-24)$$

in which  $\theta_{\infty}$  is the steady-state solution, i.e.,

$$0 = 4 + \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{d\theta_{\infty}}{d\xi} \right) \quad (11.1-25)$$

with the following boundary conditions

$$\text{at } \xi = 0 \quad \frac{d\theta_{\infty}}{d\xi} = 0 \quad (11.1-26)$$

$$\text{at } \xi = 1 \quad \theta_{\infty} = 0 \quad (11.1-27)$$

Integration of Eq. (11.1-25) gives

$$\xi \frac{d\theta_{\infty}}{d\xi} = -2\xi^2 + C_1 \quad (11.1-28)$$

The use of Eq. (11.1-26) gives  $C_1 = 0$ . Integration of Eq. (11.1-28) once more and the application of the boundary condition defined by Eq. (11.1-27) gives the steady-state solution as

$$\theta_{\infty} = 1 - \xi^2 \quad (11.1-29)$$

which is identical with Eq. (9.1-79).

The use of Eq. (11.1-29) in Eq. (11.1-24) gives

$$\theta(\tau, \xi) = 1 - \xi^2 - \theta_t(\tau, \xi) \quad (11.1-30)$$

Substitution of Eq. (11.1-30) into Eqs. (11.1-20)-(11.1-23) leads to the following governing equation for the transient problem together with the initial and the boundary conditions

$$\frac{\partial \theta_t}{\partial \tau} = \frac{1}{\xi} \frac{\partial}{\partial \xi} \left( \xi \frac{\partial \theta_t}{\partial \xi} \right) \quad (11.1-31)$$

$$\text{at } \tau = 0 \quad \theta_t = 1 - \xi^2 \quad (11.1-32)$$

$$\text{at } \xi = 0 \quad \frac{\partial \theta_t}{\partial \xi} = 0 \quad (11.1-33)$$

$$\text{at } \xi = 1 \quad \theta_t = 0 \quad (11.1-34)$$

which can be solved by the method of separation of variables.

Representing the solution as a product of two functions of the form

$$\theta_t(\tau, \xi) = F(\tau) G(\xi) \quad (11.1-35)$$

reduces Eq. (11.1-31) to

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G\xi} \frac{d}{d\xi} \left( \xi \frac{dG}{d\xi} \right) \quad (11.1-36)$$

While the left side of Eq. (11.1-36) is a function of  $\tau$  only, the right side is dependent only on  $\xi$ . This is possible if both sides of Eq. (11.1-36) are equal to a constant, say  $-\lambda^2$ , i.e.,

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G\xi} \frac{d}{d\xi} \left( \xi \frac{dG}{d\xi} \right) = -\lambda^2 \quad (11.1-37)$$

Equation (11.1-37) results in two ordinary differential equations. The equation for  $F$  is given by

$$\frac{dF}{d\tau} + \lambda^2 F = 0 \quad (11.1-38)$$

The solution of Eq. (11.1-38) is

$$F(\tau) = e^{-\lambda^2 \tau} \quad (11.1-39)$$

On the other hand, the equation for  $G$  is

$$\frac{d}{d\xi} \left( \xi \frac{dG}{d\xi} \right) + \lambda^2 \xi G = 0 \quad (11.1-40)$$

and it is subject to the boundary conditions

$$\text{at } \xi = 0 \quad \frac{dG}{d\xi} = 0 \quad (11.1-41)$$

$$\text{at } \xi = 1 \quad G = 0 \quad (11.1-42)$$

Note that Eq. (11.1-40) is a Sturm-Liouville equation with a weight function of  $\xi$ . The solution of Eq. (11.1-40) is given in terms of the Bessel functions as

$$G(\xi) = A J_o(\lambda\xi) + B Y_o(\lambda\xi) \quad (11.1-43)$$

where  $A$  and  $B$  are constants. Since  $Y_o(0) = -\infty$ ,  $B = 0$ . Application of the Eq. (11.1-42) gives

$$J_o(\lambda) = 0 \quad \Rightarrow \quad \lambda = \lambda_1, \lambda_2, \dots \quad (11.1-44)$$

Therefore, the transient solution is

$$\theta_t = \sum_{n=1}^{\infty} C_n e^{-\lambda_n^2 \tau} J_o(\lambda_n \xi) \quad (11.1-45)$$

The unknown coefficients  $C_n$  can be determined by using the initial condition given by Eq. (11.1-32). The result is

$$1 - \xi^2 = \sum_{n=1}^{\infty} C_n J_o(\lambda_n \xi) \quad (11.1-46)$$

Since the eigenfunctions are orthogonal to each other with respect to the weight function  $w(\xi) = \xi$ , multiplication of Eq. (11.1-46) by  $\xi J_o(\lambda_m \xi)$  and integration from  $\xi = 0$  to  $\xi = 1$  gives

$$\int_0^1 (1 - \xi^2) \xi J_o(\lambda_m \xi) d\xi = \sum_{n=1}^{\infty} C_n \int_0^1 \xi J_o(\lambda_n \xi) J_o(\lambda_m \xi) d\xi \quad (11.1-47)$$

Note that the integral on the right-side of Eq. (11.1-47) is zero when  $n \neq m$  and nonzero when  $n = m$ . Therefore, when  $n = m$  the summation drops out and Eq. (11.1-47) reduces to the form

$$\int_0^1 (1 - \xi^2) \xi J_o(\lambda_n \xi) d\xi = C_n \int_0^1 \xi [J_o(\lambda_n \xi)]^2 d\xi \quad (11.1-48)$$

Evaluation of the integrals gives

$$C_n = \frac{8}{\lambda_n^3 J_1(\lambda_n)} \quad (11.1-49)$$

The transient solution takes the form

$$\theta_t = 8 \sum_{n=1}^{\infty} \frac{1}{\lambda_n^3 J_1(\lambda_n)} e^{-\lambda_n^2 \tau} J_o(\lambda_n \xi) \quad (11.1-50)$$

Substitution of the steady-state and the transient solutions, Eqs. (11.1-29) and (11.1-50), into Eq. (11.1-24) gives the solution as

$$\theta = 1 - \xi^2 - 8 \sum_{n=1}^{\infty} \frac{1}{\lambda_n^3 J_1(\lambda_n)} e^{-\lambda_n^2 \tau} J_o(\lambda_n \xi) \quad (11.1-51)$$

The volumetric flow rate can be determined by integrating the velocity distribution over the cross-sectional area of the tube, i.e.,

$$\begin{aligned} Q &= \int_0^{2\pi} \int_0^R v_z r dr d\theta \\ &= \frac{\pi(\mathcal{P}_o - \mathcal{P}_L)R^4}{2\mu L} \end{aligned} \quad (11.1-52)$$

Substitution of Eq. (11.1-51) into Eq. (11.1-52) gives

$$Q = \frac{\pi(\mathcal{P}_o - \mathcal{P}_L)R^4}{8\mu L} \left[ 1 - \sum_{n=1}^{\infty} \frac{32}{\lambda_n^4} \exp(-\lambda_n^2 \tau) \right] \quad (11.1-53)$$

Note that when  $\tau \rightarrow \infty$ ,  $Q \rightarrow \pi(\mathcal{P}_o - \mathcal{P}_L)R^4/8\mu L$  which is identical with Eq. (9.1-83).

### 11.1.2 Approximate Solution by the Area Averaging Technique<sup>1</sup>

It should be kept in mind that the purpose of obtaining the velocity distribution is to get a relationship between the volumetric flow rate and the pressure drop in order to estimate the power required to pump the fluid.

The area averaging technique enables one to calculate the average velocity, and hence the volumetric flow rate, without determining the velocity distribution. Multiplication of Eq. (11.1-13) by  $r dr d\theta$  and integration over the cross-sectional area of the pipe gives

$$\rho \int_0^{2\pi} \int_0^R \frac{\partial v_z}{\partial t} r dr d\theta = \int_0^{2\pi} \int_0^R \left( \frac{\mathcal{P}_o - \mathcal{P}_L}{L} \right) r dr d\theta + \int_0^{2\pi} \int_0^R \frac{\mu}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right) r dr d\theta \quad (11.1-54)$$

The term on the left side of Eq. (11.1-54) can be rearranged in the form

$$\rho \int_0^{2\pi} \int_0^R \frac{\partial v_z}{\partial t} r dr d\theta = \rho \left( \underbrace{\frac{d}{dt} \int_0^{2\pi} \int_0^R v_z r dr d\theta}_{\pi R^2 \langle v_z \rangle} \right) = \rho \pi R^2 \frac{d \langle v_z \rangle}{dt} \quad (11.1-55)$$

Therefore, Eq. (11.1-54) becomes

$$\rho \pi R^2 \frac{d \langle v_z \rangle}{dt} = \pi R^2 \left( \frac{\mathcal{P}_o - \mathcal{P}_L}{L} \right) + 2\pi \mu R \left. \frac{\partial v_z}{\partial r} \right|_{r=R} \quad (11.1-56)$$

Note that the area averaging technique transforms a partial differential equation to an ordinary differential equation. However, one has to pay the price for this simplification. That is, to proceed further, it is necessary to express the velocity gradient at the wall,  $(\partial v_z / \partial r)_{r=R}$ , in terms of the average velocity,  $\langle v_z \rangle$ . If it is

<sup>1</sup>This development is taken from Slattery (1972).

assumed that the velocity gradient at the wall is approximately equal to that for the steady-state case, from Eqs. (9.1-79) and (9.1-84)

$$\left. \frac{\partial v_z}{\partial r} \right|_{r=R} = -\frac{4\langle v_z \rangle}{R} \quad (11.1-57)$$

Substitution of Eq. (11.1-57) into Eq. (11.1-56) yields the following linear ordinary differential equation

$$\frac{d\langle v_z \rangle}{dt} + \frac{8\mu}{\rho R^2} \langle v_z \rangle = \frac{1}{\rho} \left( \frac{\mathcal{P}_o - \mathcal{P}_L}{L} \right) \quad (11.1-58)$$

The initial condition associated with Eq. (11.1-58) is

$$\text{at } t = 0 \quad \langle v_z \rangle = 0 \quad (11.1-59)$$

The integrating factor is

$$\text{Integrating factor} = \exp\left(\frac{8\mu t}{\rho R^2}\right) \quad (11.1-60)$$

Multiplication of Eq. (11.1-58) by the integrating factor gives

$$\frac{d}{dt} \left[ \langle v_z \rangle \exp\left(\frac{8\mu t}{\rho R^2}\right) \right] = \frac{1}{\rho} \left( \frac{\mathcal{P}_o - \mathcal{P}_L}{L} \right) \exp\left(\frac{8\mu t}{\rho R^2}\right) \quad (11.1-61)$$

Integration of Eq. (11.1-61) leads to

$$\langle v_z \rangle = \frac{R^2(\mathcal{P}_o - \mathcal{P}_L)}{8\mu L} \left[ 1 - \exp\left(\frac{8\mu t}{\rho R^2}\right) \right] \quad (11.1-62)$$

Therefore, the volumetric flow rate is

$$\boxed{Q = \frac{\pi(\mathcal{P}_o - \mathcal{P}_L)R^4}{8\mu L} \left[ 1 - \exp\left(\frac{8\mu t}{\rho R^2}\right) \right]} \quad (11.1-63)$$

Slattery (1972) compared Eq. (11.1-63) with the exact solution, Eq. (11.1-53), and concluded that the error introduced is less than 20% when  $\mu t / (\rho R^2) > 0.05$ .

## 11.2 UNSTEADY CONDUCTION WITH HEAT GENERATION

Consider a slab of thickness  $L$  with a uniform initial temperature of  $T_o$ . At  $t = 0$  heat starts to generate within the slab at a uniform rate of  $\mathfrak{R}$  and to avoid the excessive heating of the slab, the surfaces at  $z = 0$  and  $z = L$  are maintained at  $T_1$ ,

$T_1 < T_o$  as shown in Figure 11.2. We are interested in obtaining the temperature distribution within the slab.

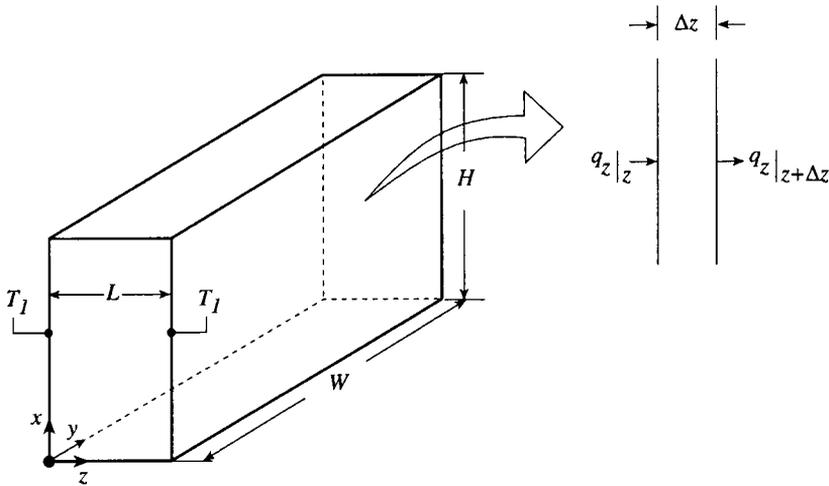


Figure 11.2 Unsteady-state conduction with generation.

If  $L/H \ll 1$  and  $L/W \ll 1$ , then it is possible to assume that the conduction is one-dimensional and postulate that  $T = T(t, z)$ . In that case, Table C.4 in Appendix C indicates that the only non-zero energy flux component is  $e_z$  and it is given by

$$e_z = q_z = -k \frac{\partial T}{\partial z} \quad (11.2-1)$$

The conservation statement for energy is expressed as

$$\left( \begin{array}{c} \text{Rate of} \\ \text{energy in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{energy in} \end{array} \right) + \left( \begin{array}{c} \text{Rate of energy} \\ \text{generation} \end{array} \right) = \left( \begin{array}{c} \text{Rate of energy} \\ \text{accumulation} \end{array} \right) \quad (11.2-2)$$

For a differential volume element of thickness  $\Delta z$ , as shown in Figure 11.2, Eq. (11.2-2) is expressed as

$$q_z|_z A - q_z|_{z+\Delta z} A + A \Delta z \mathfrak{R} = \frac{\partial}{\partial t} \left[ A \Delta z \rho \hat{C}_P (T - T_{ref}) \right] \quad (11.2-3)$$

Dividing Eq. (11.2-3) by  $A \Delta z$  and taking the limit  $\Delta z \rightarrow 0$  gives

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = \lim_{\Delta z \rightarrow 0} \frac{q_z|_z - q_z|_{z+\Delta z}}{\Delta z} + \mathfrak{R} \quad (11.2-4)$$

or,

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = - \frac{\partial q_z}{\partial z} + \mathfrak{R} \quad (11.2-5)$$

Substitution of Eq. (11.2-1) into Eq. (11.2-5) gives the governing equation for temperature as

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} + \mathfrak{R} \quad (11.2-6)$$

All physical properties are assumed to be independent of temperature in the development of Eq. (11.2-6). The initial and boundary conditions associated with Eq. (11.2-6) are

$$\text{at } t = 0 \quad T = T_o \quad (11.2-7)$$

$$\text{at } z = 0 \quad T = T_1 \quad (11.2-8)$$

$$\text{at } z = L \quad T = T_1 \quad (11.2-9)$$

Introduction of the dimensionless quantities

$$\theta = \frac{T - T_1}{T_o - T_1} \quad (11.2-10)$$

$$\xi = \frac{z}{L} \quad (11.2-11)$$

$$\tau = \frac{\alpha t}{L^2} \quad (11.2-12)$$

reduces Eqs. (11.2-6)-(11.2-9) to

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} + \Omega \quad (11.2-13)$$

$$\text{at } \tau = 0 \quad \theta = 1 \quad (11.2-14)$$

$$\text{at } \xi = 0 \quad \theta = 0 \quad (11.2-15)$$

$$\text{at } \xi = 1 \quad \theta = 0 \quad (11.2-16)$$

where

$$\Omega = \frac{\mathfrak{R}L^2}{k(T_o - T_1)} \quad (11.2-17)$$

Since Eq. (11.2-13) is not homogeneous, the solution is proposed in the form

$$\theta(\tau, \xi) = \theta_\infty(\xi) - \theta_i(\tau, \xi) \quad (11.2-18)$$

in which  $\theta_\infty$  is the steady-state solution, i.e.,

$$\frac{d^2 \theta_\infty}{d\xi^2} + \Omega = 0 \quad (11.2-19)$$

with the following boundary conditions

$$\text{at } \xi = 0 \quad \theta_\infty = 0 \quad (11.2-20)$$

$$\text{at } \xi = 1 \quad \theta_\infty = 0 \quad (11.2-21)$$

The solution of Eq. (11.2-19) is

$$\theta_\infty = \frac{\Omega}{2} (\xi - \xi^2) \quad (11.2-22)$$

The use of Eq. (11.2-22) in Eq. (11.2-18) gives

$$\theta(\tau, \xi) = \frac{\Omega}{2} (\xi - \xi^2) - \theta_t(\tau, \xi) \quad (11.2-23)$$

Substitution of Eq. (11.2-23) into Eqs. (11.2-13)-(11.2-16) leads to the following governing equation for the transient problem together with the initial and the boundary conditions

$$\frac{\partial \theta_t}{\partial \tau} = \frac{\partial^2 \theta_t}{\partial \xi^2} \quad (11.2-24)$$

$$\text{at } \tau = 0 \quad \theta_t = \frac{\Omega}{2} (\xi - \xi^2) - 1 \quad (11.2-25)$$

$$\text{at } \xi = 0 \quad \theta_t = 0 \quad (11.2-26)$$

$$\text{at } \xi = 1 \quad \theta_t = 0 \quad (11.2-27)$$

which can be solved by the method of separation of variables.

Representing the solution as a product of two functions of the form

$$\theta_t(\tau, \xi) = F(\tau) G(\xi) \quad (11.2-28)$$

reduces Eq. (11.2-24) to

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G\xi} \frac{d}{d\xi} \left( \xi \frac{dG}{d\xi} \right) \quad (11.2-29)$$

While the left side of Eq. (11.2-29) is a function of  $\tau$  only, the right side is dependent only on  $\xi$ . This is possible if both sides of Eq. (11.2-29) are equal to a constant, say  $-\lambda^2$ , i.e.,

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2 G}{d\xi^2} = -\lambda^2 \quad (11.2-30)$$

Equation (11.2-30) results in two ordinary differential equations. The equation for  $F$  is given by

$$\frac{dF}{d\tau} + \lambda^2 F = 0 \quad \Rightarrow \quad F(\tau) = e^{-\lambda^2 \tau} \quad (11.2-31)$$

On the other hand, the equation for  $G$  is

$$\frac{d^2 G}{d\xi^2} + \lambda^2 G = 0 \quad (11.2-32)$$

and it is subject to the boundary conditions

$$\text{at } \xi = 0 \quad G = 0 \quad (11.2-33)$$

$$\text{at } \xi = 1 \quad G = 0 \quad (11.2-34)$$

Equation (11.2-32) is a Sturm-Liouville equation with a weight function of unity. The solution of Eq. (11.2-32) is

$$G(\xi) = A \sin(\lambda\xi) + B \cos(\lambda\xi) \quad (11.2-35)$$

where  $A$  and  $B$  are constants. From Eq. (11.2-33),  $B = 0$ . Application of the boundary condition defined by Eq. (11.2-34) gives

$$A \sin \lambda = 0 \quad (11.2-36)$$

For a nontrivial solution, the eigenvalues are given by

$$\sin \lambda = 0 \quad \Rightarrow \quad \lambda_n = n\pi \quad n = 1, 2, \dots \quad (11.2-37)$$

Therefore, the general solution is

$$\theta_t = \sum_{n=1}^{\infty} C_n e^{-n^2\pi^2\tau} \sin(n\pi\xi) \quad (11.2-38)$$

The unknown coefficients  $C_n$  can be determined by using the initial condition, Eq. (11.2-25), with the result

$$\begin{aligned} C_n &= \frac{\int_0^1 \left[ \frac{\Omega}{2} (\xi - \xi^2) - 1 \right] \sin(n\pi\xi) d\xi}{\int_0^1 \sin^2(n\pi\xi) d\xi} \\ &= \frac{2[(-1)^n - 1]}{n\pi} \left( 1 - \frac{\Omega}{n^2\pi^2} \right) \end{aligned} \quad (11.2-39)$$

Note that

$$C_n = \begin{cases} -\frac{4}{n\pi} \left( 1 - \frac{\Omega}{n^2\pi^2} \right) & n = 1, 3, 5, \dots \\ 0 & n = 2, 4, 6, \dots \end{cases} \quad (11.2-40)$$

Therefore, the transient solution is given by

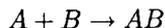
$$\theta_t = -\frac{4}{\pi} \sum_{n=1,3,5}^{\infty} \frac{1}{n} \left( 1 - \frac{\Omega}{n^2\pi^2} \right) e^{-n^2\pi^2\tau} \sin(n\pi\xi) \quad (11.2-41)$$

Substitution of the steady-state and the transient solutions, Eqs. (11.2-22) and (11.2-41), into Eq. (11.2-18) gives the solution as

$$\theta = \frac{\Omega}{2} (\xi - \xi^2) + \frac{4}{\pi} \sum_{n=1,3,5}^{\infty} \frac{1}{n} \left( 1 - \frac{\Omega}{n^2\pi^2} \right) e^{-n^2\pi^2\tau} \sin(n\pi\xi) \quad (11.2-42)$$

## 11.3 GAS ABSORPTION INTO A LIQUID DROPLET WITH REACTION

A liquid droplet ( $B$ ) of radius  $R$  is initially  $A$ -free. At  $t = 0$  it is surrounded by gas  $A$  as shown in Figure 11.3. As species  $A$  diffuses into  $B$ , it undergoes an irreversible chemical reaction with  $B$  to form  $AB$ , i.e.,



The rate of reaction is expressed by

$$r = k c_A$$

We are interested in the rate of absorption of species  $A$  into the liquid during the unsteady-state period. The problem will be analyzed with the following assumptions:

1. Convective flux is negligible with respect to the molecular flux, i.e.,  $v_z^* \approx 0$ .
2. The total concentration is constant.
3. Pseudo-binary behavior.

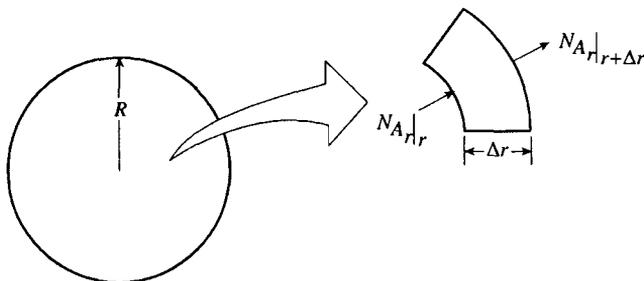


Figure 11.2 Unsteady-state absorption with chemical reaction.

Since  $c_A = c_A(t, r)$ , Table C.9 in Appendix C indicates that the only non-zero molar flux component is  $N_{A,r}$  and it is given by

$$N_{A,r} = J_{A,r}^* = -D_{AB} \frac{\partial c_A}{\partial r} \quad (11.3-1)$$

The conservation statement for species  $A$  is expressed as

$$\left( \begin{array}{c} \text{Rate of} \\ \text{species } A \text{ in} \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{species } A \text{ in} \end{array} \right) + \left( \begin{array}{c} \text{Rate of species } A \\ \text{generation} \end{array} \right) = \left( \begin{array}{c} \text{Rate of species } A \\ \text{accumulation} \end{array} \right) \quad (11.3-2)$$

For a spherical differential volume element of thickness  $\Delta r$ , as shown in Figure 11.3, Eq. (11.3-2) is expressed in the form

$$N_{A_r}|_r 4\pi r^2 - N_{A_r}|_{r+\Delta r} 4\pi(r+\Delta r)^2 - (k c_A)4\pi r^2 \Delta r = \frac{\partial}{\partial t} (4\pi r^2 \Delta r c_A) \quad (11.3-3)$$

Dividing Eq. (11.3-3) by  $4\pi\Delta r$  and taking the limit as  $\Delta r \rightarrow 0$  gives

$$\frac{\partial c_A}{\partial t} = \frac{1}{r^2} \lim_{\Delta r \rightarrow 0} \frac{(r^2 N_{A_r})|_r - (r^2 N_{A_r})|_{r+\Delta r}}{\Delta r} - k c_A \quad (11.3-4)$$

or,

$$\frac{\partial c_A}{\partial t} = -\frac{1}{r^2} \frac{\partial(r^2 N_{A_r})}{\partial r} - k c_A \quad (11.3-5)$$

Substitution of Eq. (11.3-1) into Eq. (11.3-5) gives the governing differential equation for the concentration of species  $A$  as

$$\boxed{\frac{\partial c_A}{\partial t} = \frac{D_{AB}}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_A}{\partial r} \right) - k c_A} \quad (11.3-6)$$

The initial and the boundary conditions associated with Eq. (11.3-6) are

$$\text{at } t = 0 \quad c_A = 0 \quad (11.3-7)$$

$$\text{at } r = 0 \quad \frac{\partial c_A}{\partial r} = 0 \quad (11.3-8)$$

$$\text{at } r = R \quad c_A = c_A^* \quad (11.3-9)$$

where  $c_A^*$  is the equilibrium solubility of species  $A$  in liquid  $B$ .

Danckwerts (1951) showed that the partial differential equation of the form

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - kc \quad (11.3-10)$$

with the following initial and the boundary conditions

$$\text{at } t = 0 \quad c = 0 \quad (11.3-11)$$

$$\text{at } r = 0 \quad \frac{\partial c}{\partial r} = 0 \quad (11.3-12)$$

$$\text{at } r = R \quad c_A = c_A^* \quad (11.3-13)$$

has the solution

$$c = k \int_0^t \phi(\eta, x) e^{-k\eta} d\eta + \phi(t, x) e^{-kt} \quad (11.3-14)$$

where  $\phi(t, x)$  is the solution of Eq. (11.3-10) without the chemical reaction, i.e.,

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2} \quad (11.3-15)$$

and is subject to the same initial and boundary conditions given by Eqs. (11.3-11)-(11.3-13). Note that  $\eta$  is a dummy variable of the integration in Eq. (11.3-14).

The solution of Eq. (11.3-6) without the chemical reaction is given by Eq. (10.3-58), i.e.,

$$\frac{c_A}{c_A^*} = 1 + \frac{2R}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \exp\left(-\frac{n^2\pi^2\mathcal{D}_{AB}t}{R^2}\right) \sin\left(\frac{n\pi r}{R}\right) \quad (11.3-16)$$

Substitution of Eq. (11.3-16) into Eq. (11.3-14) gives

$$\begin{aligned} \frac{c_A}{c_A^*} = k \int_0^t \left[ 1 + \frac{2R}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \exp\left(-\frac{n^2\pi^2\mathcal{D}_{AB}\eta}{R^2}\right) \sin\left(\frac{n\pi r}{R}\right) \right] e^{-k\eta} d\eta \\ + \left[ 1 + \frac{2R}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \exp\left(-\frac{n^2\pi^2\mathcal{D}_{AB}t}{R^2}\right) \sin\left(\frac{n\pi r}{R}\right) \right] e^{-kt} \end{aligned} \quad (11.3-17)$$

Carrying out the integration gives the solution as

$$\boxed{\frac{c_A}{c_A^*} = 1 + \frac{2R}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^n}{n(1+\chi)} \sin\left(\frac{n\pi r}{R}\right) [1 + \chi e^{-(1+\chi)kt}]} \quad (11.3-18)$$

where

$$\chi = \frac{n^2\pi^2\mathcal{D}_{AB}}{kR^2} \quad (11.3-19)$$

The molar rate of absorption of species  $\mathcal{A}$  is given by

$$\dot{n}_A = 4\pi R^2 \left( \mathcal{D}_{AB} \frac{\partial c_A}{\partial r} \Big|_{r=R} \right) \quad (11.2-20)$$

Substitution of Eq. (11.3-18) into Eq. (11.3-20) results in

$$\boxed{\dot{n}_A = 8\pi R \mathcal{D}_{AB} c_A^* \sum_{n=1}^{\infty} \frac{1}{1+\chi} [1 + \chi e^{-(1+\chi)kt}]} \quad (11.3-21)$$

The moles of species  $\mathcal{A}$  absorbed can be calculated from

$$n_A = \int_0^t \dot{n}_A dt \quad (11.3-22)$$

Substitution of Eq. (11.3-21) into Eq. (11.3-22) yields

$$\boxed{n_A = 8\pi R \mathcal{D}_{AB} c_A^* \sum_{n=1}^{\infty} \frac{t}{1+\chi} \left\{ 1 + \frac{[1 - e^{-(1+\chi)kt}]}{(1+\chi^{-1})kt} \right\}} \quad (11.3-23)$$

**Example 11.1** Show that the solution given by Eq. (11.3-14) satisfies Eq. (11.3-10).

**Solution**

Differentiation of Eq. (11.3-14) with respect to  $t$  by using Leibnitz's rule gives

$$\begin{aligned}\frac{\partial c}{\partial t} &= k \phi(t, x) e^{-kt} - k \phi(t, x) e^{-kt} + \frac{\partial \phi}{\partial t} e^{-kt} \\ &= \frac{\partial \phi}{\partial t} e^{-kt}\end{aligned}\quad (1)$$

Differentiation of Eq. (11.3-14) twice with respect to  $x$  yields

$$\frac{\partial^2 c}{\partial x^2} = k \int_0^t \frac{\partial^2 \phi(\eta, x)}{\partial x^2} e^{-k\eta} d\eta + \frac{\partial^2 \phi(t, x)}{\partial x^2} e^{-kt} \quad (2)$$

The use of Eq. (11.2-15) in Eq. (2) leads to

$$\mathcal{D} \frac{\partial^2 c}{\partial x^2} = k \int_0^t \frac{\partial \phi(\eta, x)}{\partial \eta} e^{-k\eta} d\eta + \frac{\partial \phi(t, x)}{\partial t} e^{-kt} \quad (3)$$

Substitution of Eq. (1) into Eq. (3) yields

$$\mathcal{D} \frac{\partial^2 c}{\partial x^2} = k \int_0^t \frac{\partial c}{\partial \eta} d\eta + \frac{\partial c}{\partial t} \quad (4)$$

or,

$$\mathcal{D} \frac{\partial^2 c}{\partial x^2} = k c + \frac{\partial c}{\partial t} \quad (5)$$

which is identical with Eq. (11.3-10).

**NOTATION**

$A$	area, $\text{m}^2$
$\hat{C}_P$	heat capacity at constant pressure, $\text{kJ/kg}\cdot\text{K}$
$c_i$	concentration of species $i$ , $\text{kmol/m}^3$
$\mathcal{D}_{AB}$	diffusion coefficient for system $A$ - $B$ , $\text{m}^2/\text{s}$
$e$	total energy flux, $\text{W/m}^2$
$J^*$	molecular molar flux, $\text{kmol/m}^2\cdot\text{s}$
$L$	length, $\text{m}$
$\dot{m}$	mass flow rate, $\text{kg/s}$
$\mathcal{M}$	molecular weight, $\text{kg/kmol}$
$N$	total molar flux, $\text{kmol/m}^2\cdot\text{s}$

$n$	number of moles, kmol
$\dot{n}$	molar flow rate, kmol/s
$\dot{Q}$	heat transfer rate, W
$Q$	volumetric flow rate, m <sup>3</sup> /s
$q$	heat flux, W/m <sup>2</sup>
$R$	radius, m
$\mathfrak{R}$	rate of generation (momentum, energy, mass) per unit volume
$T$	temperature, °C or K
$t$	time, s
$V$	volume, m <sup>3</sup>
$v$	velocity, m/s
$\alpha$	thermal diffusivity, m <sup>2</sup> /s
$\mu$	viscosity, kg/m.s
$\nu$	kinematic viscosity, m <sup>2</sup> /s
$\rho$	density, kg/m <sup>3</sup>
$\pi$	total momentum flux, N/m <sup>2</sup>
$\tau_{ij}$	shear stress (flux of $j$ – momentum in the $i$ – direction), N/m <sup>2</sup>

**Bracket**

$\langle a \rangle$  average value of  $a$

**Subscripts**

$A, B$  species in binary systems  
 $i$  species in multicomponent systems

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# Appendix A

## Mathematical Preliminaries

### A.1 THE CYLINDRICAL AND SPHERICAL COORDINATE SYSTEMS

For cylindrical coordinates, the variables  $(r, \theta, z)$  are related to the rectangular coordinates  $(x, y, z)$  as follows:

$$x = r \cos \theta \quad r = \sqrt{x^2 + y^2} \quad (\text{A.1-1})$$

$$y = r \sin \theta \quad \theta = \arctan(y/x) \quad (\text{A.1-2})$$

$$z = z \quad z = z \quad (\text{A.1-3})$$

The ranges of the variables  $(r, \theta, z)$  are

$$0 \leq r \leq \infty \quad 0 \leq \theta \leq 2\pi \quad -\infty \leq z \leq \infty$$

For spherical coordinates the variables  $(r, \theta, \phi)$  are related to the rectangular coordinates  $(x, y, z)$  as follows:

$$x = r \sin \theta \cos \phi \quad r = \sqrt{x^2 + y^2 + z^2} \quad (\text{A.1-4})$$

$$y = r \sin \theta \sin \phi \quad \theta = \arctan\left(\sqrt{x^2 + y^2}/z\right) \quad (\text{A.1-5})$$

$$z = r \cos \theta \quad \phi = \arctan(y/x) \quad (\text{A.1-6})$$

The ranges of the variables  $(r, \theta, \phi)$  are

$$0 \leq r \leq \infty \quad 0 \leq \theta \leq \pi \quad 0 \leq \phi \leq 2\pi$$

The cylindrical and the spherical coordinate systems are shown in Figure A.1. The differential volumes in these coordinate systems are given by

$$dV = \begin{cases} r \, dr \, d\theta \, dz & \text{cylindrical} \\ r^2 \sin \theta \, dr \, d\theta \, d\phi & \text{spherical} \end{cases} \quad (\text{A.1-7})$$

The application of Eq. (1.3-1) to determine the rate of a quantity requires the integration of the flux of a quantity over a differential area. The differential areas in the cylindrical and spherical coordinate systems are given as follows:

$$dA_{cylindrical} = \begin{cases} R d\theta dz & \text{flux is in the } r - \text{direction} \\ dr dz & \text{flux is in the } \theta - \text{direction} \\ r dr d\theta & \text{flux is in the } z - \text{direction} \end{cases} \quad (\text{A.1-8})$$

$$dA_{spherical} = \begin{cases} R^2 \sin \theta d\theta d\phi & \text{flux is in the } r - \text{direction} \\ r \sin \theta dr d\phi & \text{flux is in the } \theta - \text{direction} \\ r dr d\theta & \text{flux is in the } \phi - \text{direction} \end{cases} \quad (\text{A.1-9})$$

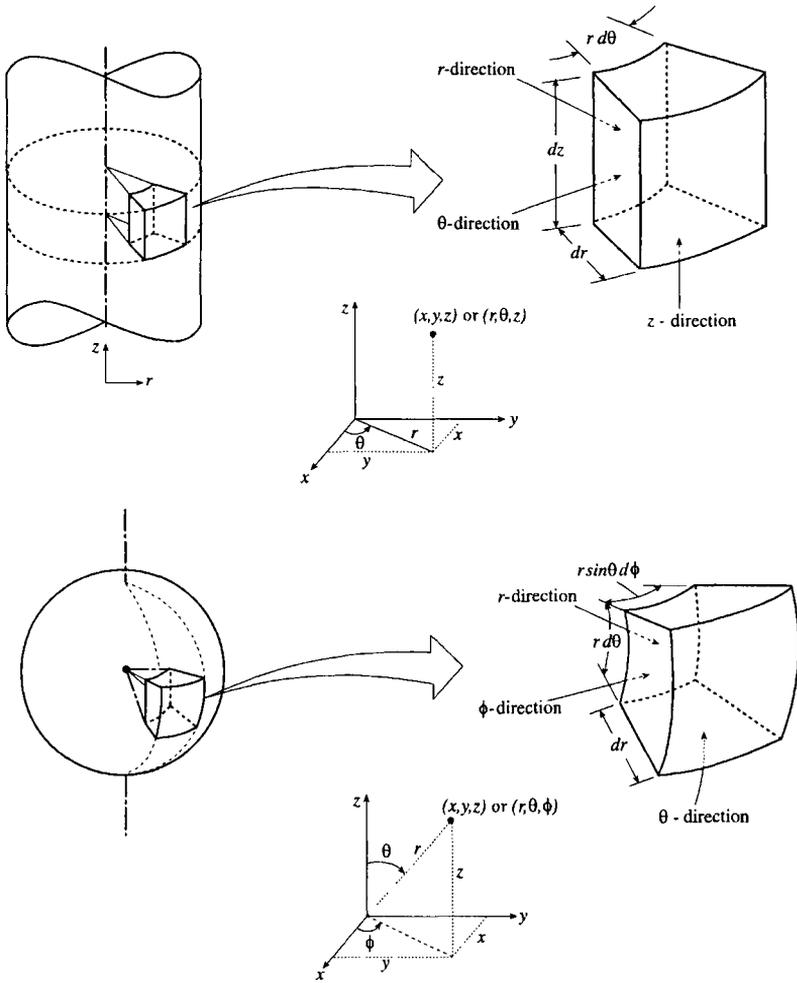


Figure A.1 The cylindrical and spherical coordinate systems.

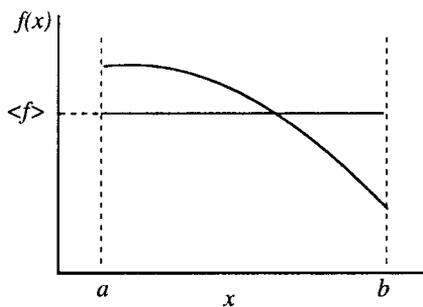
## A.2 MEAN VALUE THEOREM

If  $f(x)$  is continuous in the interval  $a \leq x \leq b$ , then the value of the integration of  $f(x)$  over an interval  $x = a$  to  $x = b$  is

$$I = \int_a^b f(x) dx = \langle f \rangle \int_a^b dx = \langle f \rangle (b - a) \quad (\text{A.2-1})$$

where  $\langle f \rangle$  is the average value of  $f$  in the interval  $a \leq x \leq b$ .

In Figure A.2 note that  $\int_a^b f(x) dx$  is the area under the curve between  $a$  and  $b$ . On the other hand,  $\langle f \rangle (b - a)$  is the area under the rectangle of height  $\langle f \rangle$  and width  $(b - a)$ . The average value of  $f$ ,  $\langle f \rangle$ , is defined such that these two areas are equal to each other.



**Figure A.2** The mean value of the function  $f(x)$ .

It is possible to extend the definition of mean value to two- and three-dimensional cases as

$$\langle f \rangle = \frac{\iint_A f(x, y) dx dy}{\iint_A dx dy} \quad \text{and} \quad \langle f \rangle = \frac{\iiint_V f(x, y, z) dx dy dz}{\iiint_V dx dy dz} \quad (\text{A.2-2})$$

## PROBLEMS

**A.1** Two rooms have the same average temperature,  $\langle T \rangle$ , defined by

$$\langle T \rangle = \frac{\iiint_V T(x, y, z) dx dy dz}{\iiint_V dx dy dz}$$

However, while one of the rooms is very comfortable, the other is very uncomfortable. With the mean value theorem in mind, how would you explain the difference in comfort levels of the two rooms? What design alterations would you suggest to make the room that is uncomfortable comfortable?

**A.2** Wind speed is measured by anemometers placed at an altitude of 10 m from the ground. Buckler (1969) carried out series of experiments to determine the effect of height above ground level on wind speed and proposed the following equation for the winter months

$$v = v_{10} \left( \frac{z}{10} \right)^{0.21}$$

where  $z$  is the vertical distance measured from the ground in meter and  $v_{10}$  is the measured wind speed.

Estimate the average wind speed encountered by a person of height 1.7 m at the ground level if the wind speed measured by an anemometer 10 m above the ground is 30 km/h.

(Answer: 17.1 km/h)

### A.3 SLOPES ON LOG-LOG AND SEMI-LOG GRAPH PAPERS

A mathematical transformation that converts the logarithm of a number to a length in the  $x$ -direction is given by

$$\ell_x = L_x \log x \tag{A.3-1}$$

where  $\ell_x$  is the distance in the  $x$ -direction and  $L_x$  is the cycle length for the  $x$ -coordinate. Therefore, if the cycle length is taken as 10 cm, the distances in the  $x$ -direction for various values of  $x$  are given in Table A.1.

**Table A.1** Distances in the  $x$ -direction for a logarithmic  $x$ -axis.

$x$	$\ell_x$
1	0
2	3.01
3	4.77
4	6.02
5	6.99
6	7.78
7	8.45
8	9.03
9	9.54
10	10.00

The slope of a straight line,  $m$ , on a log – log graph paper is

$$m = \frac{\log y_2 - \log y_1}{\log x_2 - \log x_1} = \left( \frac{\ell_{y_2} - \ell_{y_1}}{\ell_{x_2} - \ell_{x_1}} \right) \frac{L_x}{L_y} \tag{A.3-2}$$

On the other hand, the slope of a straight line,  $m$ , on a semi– log graph paper ( $y$ -axis is logarithmic) is

$$m = \frac{\log y_2 - \log y_1}{x_2 - x_1} = \left( \frac{\ell_{y_2} - \ell_{y_1}}{x_2 - x_1} \right) \frac{1}{L_y} \tag{A.3-3}$$

## A.4 LEIBNITZ'S RULE FOR DIFFERENTIATION OF INTEGRALS

Let  $f(x, t)$  be continuous and have a continuous derivative  $\partial f/\partial t$  in a domain of the  $xt$  plane which includes the rectangle  $a \leq x \leq b, t_1 \leq t \leq t_2$ . Then for  $t_1 \leq t \leq t_2$

$$\frac{d}{dt} \int_a^b f(x, t) dx = \int_a^b \frac{\partial f}{\partial t} dx \tag{A.4-1}$$

In other words, differentiation and integration can be interchanged if the limits of the integration are fixed.

On the other hand, if the limits of the integral in Eq. (A.4-1) are dependent on time, then

$$\frac{d}{dt} \int_{a(t)}^{b(t)} f(x, t) dx = \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t} dx + f[b(t), t] \frac{db}{dt} - f[a(t), t] \frac{da}{dt} \tag{A.4-2}$$

If  $f = f(x)$  only, then Eq. (A.4-2) reduces to

$$\frac{d}{dt} \int_{a(t)}^{b(t)} f(x) dx = f[b(t)] \frac{db}{dt} - f[a(t)] \frac{da}{dt} \tag{A.4-3}$$

## A.5 NUMERICAL DIFFERENTIATION OF EXPERIMENTAL DATA

The determination of a rate requires the differentiation of the original experimental data. As explained by De Nevers (1966), given a table of  $x - y$  data, the value of  $dy/dx$  can be calculated by:

1. Plotting the data on graph paper, drawing a smooth curve through the points with the help of a French curve, and then drawing a tangent to this curve.
2. Fitting the entire set of data with an empirical equation, such as a polynomial, and then differentiating the empirical equation.

3. Fitting short sections of the data by arbitrary functions.
4. Using the difference table method, i.e., plotting the differences and smoothing the differences graphically.

De Nevers also points out the fact that although the value of  $dy/dx$  obtained by any of the above four methods is approximately equal, the value of  $d^2y/dx^2$  is extremely sensitive to the method used.

In the case of the graphical method, there are infinite number of ways of drawing the curve through the data points. As a result, the slope of the tangent will be affected by the mechanics of drawing the curved line and the tangent.

The availability of computer programs makes the second and the third methods highly attractive. However, since the choice of the functional form of the equation is highly arbitrary, the final result is almost as subjective and biased as the use of a French curve.

Two methods, namely, Douglass-Avakian (1933) and Whitaker-Pigford (1960) methods, are worth mentioning among the third approach. Both of these methods require the values of the independent variable,  $x$ , be *equally* spaced by an amount  $\Delta x$ .

### A.5.1 Douglass-Avakian Method

In this method, the value of  $dy/dx$  is determined by fitting a fourth-degree polynomial to seven consecutive data points, with the point in question as the mid-point, by least squares. If the mid-point is designated by  $x_c$ , then the value of  $dy/dx$  at this particular location is given by

$$\frac{dy}{dx} = \frac{397(\sum Xy) - 49(\sum X^3y)}{1512 \Delta x} \quad (\text{A.5-1})$$

where

$$X = \frac{x - x_c}{\Delta x} \quad (\text{A.5-2})$$

### A.5.2 Whitaker-Pigford Method

In this case, a parabola is fitted to five consecutive data points, with the point in question as the mid-point, by least squares. The value of  $dy/dx$  at  $x_c$  is given by

$$\frac{dy}{dx} = \frac{\sum Xy}{10 \Delta x} \quad (\text{A.5-3})$$

where  $X$  is defined by Eq. (A.5-2).

**Example A.1** Given the enthalpy of steam at  $P = 0.01$  MPa as a function of temperature as follows, determine the heat capacity at constant pressure at  $500^\circ\text{C}$ .

$T$ (°C)	$\hat{H}$ (J/g)
100	2687.5
200	2879.5
300	3076.5
400	3279.6
500	3489.1
600	3705.4
700	3928.7
800	4159.0
900	4396.4
1000	4640.0
1100	4891.2

### Solution

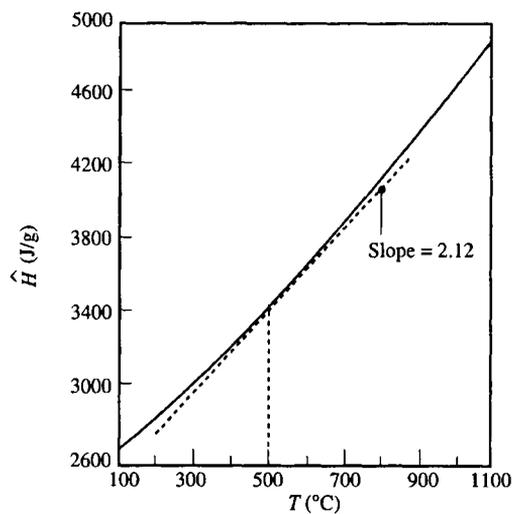
The heat capacity at constant pressure,  $\hat{C}_P$ , is defined as

$$\hat{C}_P = \left( \frac{\partial \hat{H}}{\partial T} \right)_P$$

Therefore, determination of  $\hat{C}_P$  requires numerical differentiation of the  $\hat{H}$  versus  $T$  data.

### Graphical method

The plot of  $\hat{H}$  versus  $T$  is given in the figure shown below. The slope of the tangent to the curve at  $T = 500^\circ\text{C}$  gives  $\hat{C}_P = 2.12 \text{ J/g}\cdot\text{K}$ .



**Dougllass-Avakian method**

The required values to use Eq. (A.5-1) are given in the table shown below:

$x = T$	$y = \hat{H}$	$X$	$Xy$	$X^3y$
200	2879.5	-3	-8638.5	-77746.5
300	3076.5	-2	-6153	-24612
400	3279.6	-1	-3279.6	-3279.6
500	3489.1	0	0	0
600	3705.4	1	3705.4	3705.4
700	3928.7	2	7857.4	31429.6
800	4159.0	3	12477	112293
		$\Sigma = 5968.7$		$\Sigma = 41789.9$

Therefore, the heat capacity at constant pressure at 500°C is given by

$$\begin{aligned}\hat{C}_P &= \frac{397(\Sigma Xy) - 49(\Sigma X^3y)}{1512 \Delta x} \\ &= \frac{(397)(5968.7) - (49)(41,789.9)}{(1512)(100)} = 2.13 \text{ J/g} \cdot \text{K}\end{aligned}$$

**Whitaker-Pigford method**

By taking  $X = T$  and  $y = \hat{H}$ , the parameters in Eq. (A.5-3) are given in the following table:

$X = T$	$y = \hat{H}$	$X$	$Xy$
300	3076.5	-2	-6153
400	3279.6	-1	-3279.6
500	3489.1	0	0
600	3705.4	1	3705.4
700	3928.7	2	7857.4
			$\Sigma = 2130.2$

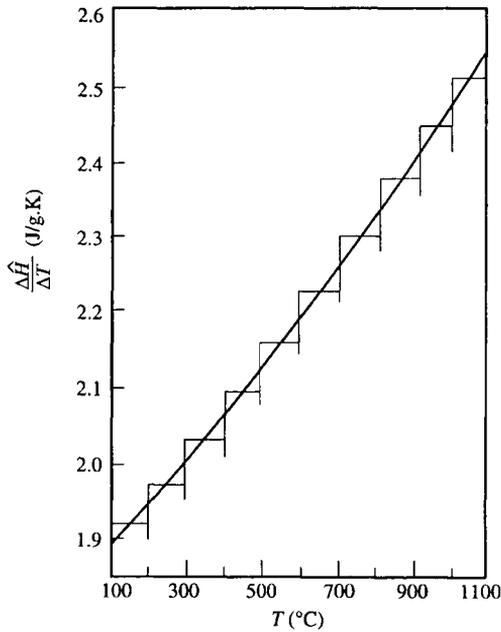
Therefore, the use of Eq. (A.5-3) gives the heat capacity at constant pressure as

$$\begin{aligned}\hat{C}_P &= \frac{\Sigma Xy}{10 \Delta x} \\ &= \frac{2130.2}{(10)(100)} = 2.13 \text{ J/g} \cdot \text{K}\end{aligned}$$

**The difference table method**

The use of the difference table method is explained by Churchill (1974) in detail. To smooth the data by using this method, the divided differences  $\Delta\hat{H}/\Delta T$  shown in the table below are plotted versus temperature in the figure.

$T$	$\hat{H}$	$\Delta T$	$\Delta \hat{H}$	$\Delta \hat{H} / \Delta T$
100	2687.5			
		100	192	1.92
200	2879.5			
		100	197	1.97
300	3076.5			
		100	203.1	2.031
400	3279.6			
		100	209.5	2.095
500	3489.1			
		100	216.3	2.163
600	3705.4			
		100	223.3	2.233
700	3928.7			
		100	230.3	2.303
800	4159.0			
		100	237.4	2.374
900	4396.4			
		100	243.6	2.436
1000	4640.0			
		100	251.2	2.512
1100	4891.2			



Each line represents the average value of  $d\hat{H}/dT$  over the specified temperature range. The smooth curve should be drawn so as to equalize the area under the group of bars. From the figure, the heat capacity at constant pressure at 500°C is 2.15 J/g.K.

## A.6 REGRESSION AND CORRELATION

To predict the mechanism of a process, we often need to know the relationship of one process variable to another, i.e., how the reactor yield depends on pressure. A relationship between the two variables  $x$  and  $y$ , measured over a range of values, can be obtained by proposing linear relationships first, because they are the simplest. The analyses we use for this are *correlation*, which indicates whether there is indeed a linear relationship, and *regression*, which finds the equation of a straight line that best fits the observed  $x - y$  data.

### A.6.1 Simple Linear Regression

The equation describing a straight line is

$$y = ax + b \quad (\text{A.6-1})$$

where  $a$  denotes the slope of the line and  $b$  denotes the  $y$ -axis intercept. Most of the time the variables  $x$  and  $y$  do not have a linear relationship. However, transformation of the variables may result in a linear relationship. Some examples of transformation are given in Table A.2. Thus, linear regression can be applied even to nonlinear data.

**Table A.2** Transformation of nonlinear equations to linear forms.

Nonlinear Form	Linear Form	Linear Form
$y = \frac{ax}{b + cx}$	$\frac{x}{y} = \frac{c}{a}x + \frac{b}{a}$	$\frac{x}{y}$ vs $x$ is linear
	$\frac{1}{y} = \frac{b}{a} \frac{1}{x} + \frac{c}{a}$	$\frac{1}{y}$ vs $\frac{1}{x}$ is linear
$y = ax^n$	$\log y = n \log x + \log a$	$\log y$ vs $\log x$ is linear

### A.6.2 Sum of Squared Deviations

Suppose we have a set of observations  $x_1, x_2, x_3, \dots, x_n$ . The sum of the squares of their deviations from some mean value,  $x_m$ , is

$$S = \sum_{i=1}^N (x_i - x_m)^2 \quad (\text{A.6-2})$$

Now suppose we wish to minimize  $S$  with respect to the mean value  $x_m$ , i.e.,

$$\frac{\partial S}{\partial x_m} = 0 = \sum_{i=1}^N -2(x_i - x_m) = 2 \left( Nx_m - \sum_{i=1}^N x_i \right) \quad (\text{A.6-3})$$

or,

$$x_m = \frac{1}{N} \sum_i x_i = \bar{x} \quad (\text{A.6-4})$$

Therefore, the mean value which minimizes the sum of the squares of the deviations is the arithmetic mean,  $\bar{x}$ .

### A.6.3 The Method of Least Squares

The parameters  $a$  and  $b$  in Eq. (A.6-1) are estimated by the method of least squares. These values have to be chosen such that the sum of the squares of the deviations

$$S = \sum_{i=1}^N [y_i - (ax_i + b)]^2 \quad (\text{A.6-5})$$

is minimum. This is accomplished by differentiating the function  $S$  with respect to  $a$  and  $b$ , and setting these derivatives equal to zero:

$$\frac{\partial S}{\partial a} = 0 = -2 \sum_i (y_i - ax_i - b) x_i \quad (\text{A.6-6})$$

$$\frac{\partial S}{\partial b} = 0 = -2 \sum_i (y_i - ax_i - b) \quad (\text{A.6-7})$$

Equations (A.6-6) and (A.6-7) can be simplified as

$$a \sum_i x_i^2 + b \sum_i x_i = \sum_i x_i y_i \quad (\text{A.6-8})$$

$$a \sum_i x_i + Nb = \sum_i y_i \quad (\text{A.6-9})$$

Simultaneous solution of Eqs. (A.6-8) and (A.6-9) gives

$$a = \frac{N (\sum_i x_i y_i) - (\sum_i x_i) (\sum_i y_i)}{N (\sum_i x_i^2) - (\sum_i x_i)^2} \quad (\text{A.6-10})$$

$$b = \frac{(\sum_i y_i) (\sum_i x_i^2) - (\sum_i x_i) (\sum_i x_i y_i)}{N (\sum_i x_i^2) - (\sum_i x_i)^2} \quad (\text{A.6-11})$$

**Example A.2** *Experimental measurements of the density of benzene vapor at 563 K are given as follows:*

$P$ (atm)	$\tilde{V}$ (cm <sup>3</sup> /mol)
30.64	1164
31.60	1067
32.60	1013
33.89	956
35.17	900
36.63	842
38.39	771
40.04	707
41.79	646
43.59	591
45.48	506
47.07	443
48.07	386

Assume that the data obey the virial equation of state, i.e.,

$$Z = \frac{P\tilde{V}}{\mathcal{R}T} = 1 + \frac{B}{\tilde{V}} + \frac{C}{\tilde{V}^2}$$

and determine the virial coefficients  $B$  and  $C$ .

### Solution

The equation of state can be rearranged as

$$\left(\frac{P\tilde{V}}{\mathcal{R}T} - 1\right)\tilde{V} = B + \frac{C}{\tilde{V}}$$

Note that this equation has the form

$$y = B + Cx$$

where

$$y = \left(\frac{P\tilde{V}}{\mathcal{R}T} - 1\right)\tilde{V} \quad \text{and} \quad x = \frac{1}{\tilde{V}}$$

Taking  $\mathcal{R} = 82.06 \text{ cm}^3 \cdot \text{atm} / \text{mol} \cdot \text{K}$ , the required values are calculated as follows:

$y_i$	$x_i \times 10^3$	$x_i y_i$	$x_i^2 \times 10^6$
-265.4	0.859	-0.2280	0.738
-288.3	0.937	-0.2702	0.878
-288.9	0.987	-0.2852	0.975
-285.6	1.046	-0.2987	1.094
-283.4	1.111	-0.3149	1.235
-279.9	1.188	-0.3324	1.411
-277	1.297	-0.3593	1.682
-273.8	1.414	-0.3873	2.001
-268.5	1.548	-0.4157	2.396
-261.4	1.692	-0.4424	2.863
-254	1.976	-0.5019	3.906
-243.1	2.257	-0.5487	5.096
-231	2.591	-0.5984	6.712
$\sum y_i = -3500.3 \quad \sum x_i = 0.0189 \quad \sum x_i y_i = -4.9831 \quad \sum x_i^2 = 30.99 \times 10^{-6}$			

The values of  $B$  and  $C$  are

$$B = \frac{(\sum_i y_i)(\sum_i x_i^2) - (\sum_i x_i)(\sum_i x_i y_i)}{N(\sum_i x_i^2) - (\sum_i x_i)^2}$$

$$= \frac{(-3500.3)(30.99 \times 10^{-6}) - (0.0189)(-4.9831)}{(13)(30.99 \times 10^{-6}) - (0.0189)^2} = -313 \text{ cm}^3/\text{mol}$$

$$C = \frac{N(\sum_i x_i y_i) - (\sum_i x_i)(\sum_i y_i)}{N(\sum_i x_i^2) - (\sum_i x_i)^2}$$

$$= \frac{(13)(-4.9831) - (0.0189)(-3500.3)}{(13)(30.99 \times 10^{-6}) - (0.0189)^2} = 30,122 \text{ (cm}^3/\text{mol)}^2$$

The method of least squares can also be applied to higher order polynomials. For example, consider a second-order polynomial

$$y = ax^2 + bx + c \quad (\text{A.6-12})$$

To find the constants  $a$ ,  $b$ , and  $c$ , the sum of the squared deviations

$$S = \sum_{i=1}^N [y_i - (ax_i^2 + bx_i + c)]^2 \quad (\text{A.6-13})$$

must be minimum. Hence,

$$\frac{\partial S}{\partial a} = \frac{\partial S}{\partial b} = \frac{\partial S}{\partial c} = 0 \quad (\text{A.6-14})$$

Partial differentiation of Eq. (A.6-13) gives

$$a \sum_i x_i^4 + b \sum_i x_i^3 + c \sum_i x_i^2 = \sum_i x_i^2 y_i \quad (\text{A.6-15})$$

$$a \sum_i x_i^3 + b \sum_i x_i^2 + c \sum_i x_i = \sum_i x_i y_i \quad (\text{A.6-16})$$

$$a \sum_i x_i^2 + b \sum_i x_i + c N = \sum_i y_i \quad (\text{A.6-17})$$

These equations may then be solved for the constants  $a$ ,  $b$ , and  $c$ .

If the equation is of the form

$$y = a x^n + b \quad (\text{A.6-18})$$

then the parameters  $a$ ,  $b$ , and  $n$  can be determined as follows:

1. Least squares values of  $a$  and  $b$  can be found for a series of chosen values of  $n$ .
2. The sum of the squares of the deviations can then be calculated and plotted versus  $n$  to find the minimum and, hence, the best value of  $n$ . The corresponding values of  $a$  and  $b$  are readily found by plotting the calculated values versus  $n$  and interpolating.

Alternatively, Eq. (A.6-18) might first be arranged as

$$\log(y - b) = n \log x + \log a \quad (\text{A.6-19})$$

and least squares values of  $n$  and  $\log a$  are determined for a series of chosen values of  $b$ , etc.

**Example A.3<sup>1</sup>** *It is proposed to correlate the data for forced convection heat transfer to a sphere in terms of the equation*

$$\text{Nu} = 2 + a \text{Re}^n$$

*The following values were obtained from McAdams (1954) for heat transfer from air to spheres by forced convection:*

Re	Nu
10	2.8
100	6.3
1000	19.0

<sup>1</sup>This problem is taken from Churchill (1974).

**Solution**

The equation can be rearranged as

$$\log(Nu - 2) = n \log Re + \log a$$

Note that this equation has the form

$$y = nx + b$$

where

$$y = \log(Nu - 2) \quad x = \log Re \quad b = \log a$$

$y_i$	$x_i$	$x_i y_i$	$x_i^2$
-0.09691	1	-0.09691	1
0.63347	2	1.26694	4
1.23045	3	3.69135	9
$\sum y_i = 1.76701$	$\sum x_i = 6$	$\sum x_i y_i = 4.86138$	$\sum x_i^2 = 14$

The values of  $n$  and  $b$  are

$$n = \frac{(3)(4.86138) - (6)(1.76701)}{(3)(14) - (6)^2} = 0.66368$$

$$b = \frac{(14)(1.76701) - (6)(4.86138)}{(3)(14) - (6)^2} = -0.73835 \Rightarrow a = 0.1827$$

**A.6.4 Correlation Coefficient**

If two variables,  $x$  and  $y$ , are related in such a way that the points of a scatter plot tend to fall in a straight line, then we say that there is an association between the variables and that they are linearly correlated. The most common measure of the strength of the association between the variables is the *Pearson correlation coefficient*,  $r$ . It is defined by

$$r = \frac{\sum x_i y_i - \frac{\sum x_i \sum y_i}{n}}{\sqrt{\left(\sum x_i^2 - \frac{(\sum x_i)^2}{n}\right) \left(\sum y_i^2 - \frac{(\sum y_i)^2}{n}\right)}} \tag{A.6-20}$$

The value of  $r$  can range from  $-1$  to  $+1$ . A value of  $-1$  means a *perfect negative correlation*. Perfect negative correlation implies that  $y = ax + b$  where  $a < 0$ . *Perfect positive correlation* ( $r = +1$ ) implies that  $y = ax + b$  where  $a > 0$ . When  $r = 0$ , the variables are uncorrelated. This, however, does not imply that the variables are unrelated. It simply indicates that if a relationship exists, then it is not linear.

## A.7 THE ROOT OF AN EQUATION

In engineering problems, we frequently encounter with equations of the form

$$f(x) = 0 \quad (\text{A.7-1})$$

and want to determine the values of  $x$  satisfying Eq. (A.7-1). These values are called the *roots* of  $f(x)$  and may be real or imaginary. Since imaginary roots appear as complex conjugates, the number of imaginary roots must always be even.

The function  $f(x)$  may be a polynomial in  $x$  or, it may be a transcendental equation involving trigonometric and/or logarithmic terms.

### A.7.1 Roots of a Polynomial

If  $f(x)$  is a polynomial, then *Descartes' rule of sign* determines the maximum number of real roots:

- The maximum number of real positive roots is equal to the number of sign changes in  $f(x) = 0$ .
- The maximum number of real negative roots is equal to the number of sign changes in  $f(-x) = 0$ .

In applying the sign rule, zero coefficients are regarded as positive.

#### A.7.1.1 Quadratic equation

The roots of a quadratic equation

$$ax^2 + bx + c = 0 \quad (\text{A.7-2})$$

are given as

$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (\text{A.7-3})$$

If  $a, b, c$  are real and if  $\Delta = b^2 - 4ac$  is the discriminant, then

- $\Delta > 0$ ; the roots are real and unequal,
- $\Delta = 0$ ; the roots are real and equal,
- $\Delta < 0$ ; the roots are complex conjugate.

**A.7.1.2 Cubic equation**

Consider the cubic equation

$$x^3 + px^2 + qx + r = 0 \quad (\text{A.7-4})$$

Let us define the terms  $M$  and  $N$  as

$$M = \frac{3q - p^2}{9} \quad (\text{A.7-5})$$

$$N = \frac{9pq - 27r - 2p^3}{54} \quad (\text{A.7-6})$$

If  $p, q, r$  are real and if  $\Delta = M^3 + N^2$  is the discriminant, then

- $\Delta > 0$ ; one root is real and two complex conjugate,
- $\Delta = 0$ ; all roots are real and at least two are equal,
- $\Delta < 0$ ; all roots are real and unequal.

**Case (i) Solutions for  $\Delta \geq 0$** 

In this case the roots are given by

$$x_1 = S + T - \frac{1}{3}p \quad (\text{A.7-7})$$

$$x_2 = -\frac{1}{2}(S + T) - \frac{1}{3}p + \frac{1}{2}i\sqrt{3}(S - T) \quad (\text{A.7-8})$$

$$x_3 = -\frac{1}{2}(S + T) - \frac{1}{3}p - \frac{1}{2}i\sqrt{3}(S - T) \quad (\text{A.7-9})$$

where

$$S = \sqrt[3]{N + \sqrt{\Delta}} \quad (\text{A.7-10})$$

$$T = \sqrt[3]{N - \sqrt{\Delta}} \quad (\text{A.7-11})$$

**Case (ii) Solutions for  $\Delta < 0$** 

The roots are given by

$$x_1 = \pm 2\sqrt{-M} \cos\left(\frac{\theta}{3}\right) - \frac{1}{3}p \quad (\text{A.7-12})$$

$$x_2 = \pm 2\sqrt{-M} \cos\left(\frac{\theta}{3} + 120^\circ\right) - \frac{1}{3}p \quad (\text{A.7-13})$$

$$x_3 = \pm 2\sqrt{-M} \cos\left(\frac{\theta}{3} + 240^\circ\right) - \frac{1}{3}p \quad (\text{A.7-14})$$

where

$$\theta = \arccos \sqrt{\frac{N^2}{(-M)^3}} \quad (\theta \text{ is in degrees}) \quad (\text{A.7-15})$$

In Eqs. (A.7-12)-(A.7-14) the upper sign applies if  $N$  is positive, the lower sign applies if  $N$  is negative.

**Example A.4** *Cubic equations of state are frequently used in thermodynamics to describe the PVT behavior of liquids and vapors. These equations are expressed in the form*

$$P = \frac{\mathcal{R}T}{\tilde{V} - b} - \frac{a(T)}{\tilde{V}^\alpha + \beta \tilde{V} + \gamma} \quad (\text{A.7-16})$$

where the terms  $\alpha$ ,  $\beta$ ,  $\gamma$ , and  $a(T)$  for different types of equations of state are given by

Eqn. of State	$\alpha$	$\beta$	$\gamma$	$a(T)$
van der Waals	2	0	0	$a$
Redlich-Kwong	2	$b$	0	$a/\sqrt{T}$
Peng-Robinson	2	$2b$	$-b^2$	$a(T)$

When Eq. (A.7-16) has three real roots, the largest and the smallest roots correspond to the molar volumes of the vapor and liquid phases, respectively. The intermediate root has no physical meaning.

Predict the density of saturated methanol vapor at 10.84 atm and 140°C using the van der Waals equation of state. The coefficients  $a$  and  $b$  are given as

$$\begin{aligned} a &= 9.3424 \text{ m}^6 \cdot \text{atm} / \text{kmol}^2 \\ b &= 0.0658 \text{ m}^3 / \text{kmol} \end{aligned}$$

The experimental value of the density of saturated methanol vapor is 0.01216 g/cm<sup>3</sup>.

### Solution

For the van der Waals equation of state, Eq. (A.7-16) takes the form

$$\tilde{V}^3 - \left( b + \frac{\mathcal{R}T}{P} \right) \tilde{V}^2 + \frac{a}{P} \tilde{V} - \frac{ab}{P} = 0 \quad (1)$$

Substitution of the values of  $a$ ,  $b$ ,  $R$ , and  $P$  into Eq. (1) gives

$$\tilde{V}^3 - 3.1923 \tilde{V}^2 + 0.8618 \tilde{V} - 0.0567 = 0 \quad (2)$$

Application of the sign rule indicates that the maximum number of real positive roots is equal to three. The terms  $M$  and  $N$  are

$$\begin{aligned} M &= \frac{3q - p^2}{9} \\ &= \frac{(3)(0.8618) - (3.1923)^2}{9} = -0.845 \end{aligned} \quad (3)$$

$$\begin{aligned} N &= \frac{9pq - 27r - 2p^3}{54} \\ &= \frac{(9)(-3.1923)(0.8618) - (27)(-0.0567) + (2)(3.1923)^3}{54} \\ &= 0.775 \end{aligned} \quad (4)$$

The discriminant,  $\Delta$ , is

$$\begin{aligned} \Delta &= M^3 + N^2 \\ &= (-0.845)^3 + (0.775)^2 = -0.003 \end{aligned} \quad (5)$$

Therefore, all the roots of Eq. (2) are real and unequal. Before calculating the roots by using Eqs. (A.7-12)-(A.7-14),  $\theta$  must be determined. From Eq. (A.7-15)

$$\begin{aligned} \theta &= \arccos \sqrt{\frac{N^2}{(-M)^3}} \\ &= \arccos \sqrt{\frac{(0.775)^2}{(0.845)^3}} = 3.85^\circ \end{aligned} \quad (6)$$

Hence, the roots are

$$\tilde{V}_1 = (2)\sqrt{0.845} \cos\left(\frac{3.85}{3}\right) + \frac{3.1923}{3} = 2.902 \quad (7)$$

$$\tilde{V}_2 = (2)\sqrt{0.845} \cos\left(\frac{3.85}{3} + 120\right) + \frac{3.1923}{3} = 0.109 \quad (8)$$

$$\tilde{V}_3 = (2)\sqrt{0.845} \cos\left(\frac{3.85}{3} + 240\right) + \frac{3.1923}{3} = 0.181 \quad (9)$$

The molar volume of saturated vapor,  $\tilde{V}_g$ , corresponds to the largest root, i.e.,  $2.902 \text{ m}^3/\text{kmol}$ . Since, the molecular weight,  $M$ , of methanol is 32, the density of saturated vapor,  $\rho_g$ , is given by

$$\begin{aligned} \rho_g &= \frac{\mathcal{M}}{\tilde{V}_g} \\ &= \frac{(32)}{(2.902)(1 \times 10^3)} = 0.01103 \text{ g/cm}^3 \end{aligned} \quad (10)$$

## A.7.2 Numerical Methods

Numerical methods should be used when the equations to be solved are complex and do not have direct analytical solutions. Various numerical methods have been developed for solving Eq. (A.7-1). Some of the most convenient techniques to solve the chemical engineering problems are summarized by Serghides (1982), Gjumbir and Olujic (1984), and Tao (1988). The *Newton-Raphson method* and the *Secant method* are the two most widely used techniques and will be explained below.

One of the most important problems in the application of numerical techniques is *convergence*. It can be promoted by finding a good starting value and/or a suitable transformation of the variable, or the equation.

When using numerical methods, it is always important to use the engineering common sense. The following advice of Tao (1989) should always be remembered in the application of numerical techniques:

- To err is digital, to catch the error is divine.
- An ounce of theory is worth 100 lb of computer output.
- Numerical methods are like political candidates; they'll tell you anything you want to hear.

### A.7.2.1 Newton-Raphson method

Expansion of the function  $f(x)$  by Taylor series around an estimate  $x_k$  gives

$$f(x) = f(x_k) + (x - x_k) \left. \frac{df}{dx} \right|_{x_k} + \frac{(x - x_k)^2}{2!} \left. \frac{d^2 f}{dx^2} \right|_{x_k} + \dots \quad (\text{A.7-17})$$

If we neglect the derivatives higher than the first order and let  $x = x_{k+1}$  be the value of  $x$  that makes  $f(x) = 0$ , then Eq. (A.7-17) becomes

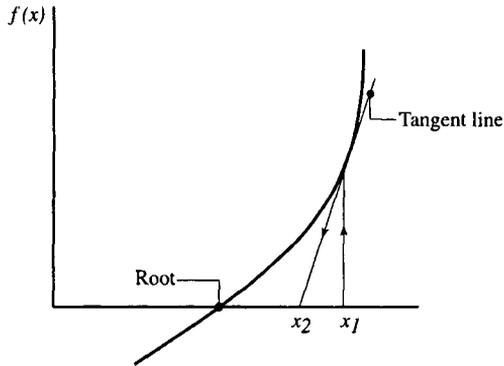
$$x_{k+1} = x_k - \frac{f(x_k)}{\left. \frac{df}{dx} \right|_{x_k}} \quad (\text{A.7-18})$$

The convergence is achieved when  $|x_{k+1} - x_k| < \varepsilon$ , where  $\varepsilon$  is a small number determined by the desired accuracy.

The Newton-Raphson method proceeds as shown in Figure A.3. Note that the method breaks down if  $(df/dx)_{x_k} = 0$  at some point.

### A.7.2.2 Secant method

Application of the Newton-Raphson method, Eq. (A.7-18), requires the evaluation of the first derivative of the function. Unfortunately, this is not always easily found. The secant method, on the other hand, requires only the evaluation of the function.



**Figure A.3** The Newton-Raphson method.

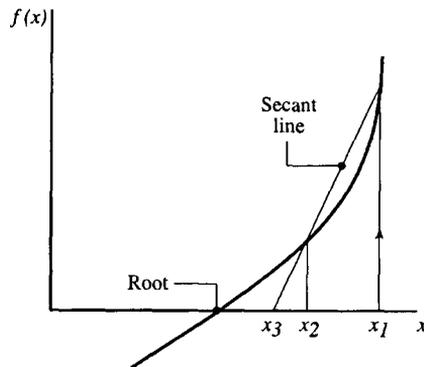
To evaluate the derivative in Eq. (A.7-18), linear interpolation between two points,  $x_k$  and  $x_{k-1}$ , on the function is applied in the form

$$\left. \frac{df}{dx} \right|_{x_k} = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \quad (\text{A.7-19})$$

Substitution of Eq. (A.7-19) into Eq. (A.7-18) gives

$$x_{k+1} = x_k - \left[ \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} \right] f(x_k) \quad (\text{A.7-20})$$

Note that the secant method requires two initial guesses. The secant method is illustrated in Figure A.4.



**Figure A.4** The Secant method.

## PROBLEMS

**A.3** Caffeine is extracted from coffee grains by means of a crossflow extractor. The standard error of the exit concentration versus time curve was found as  $\sigma = 1.31$ , where standard deviation,  $\sigma^2$ , is given as

$$\sigma^2 = \frac{2}{\text{Pe}} + \frac{2}{\text{Pe}^2} (1 - e^{-\text{Pe}})$$

Solve this equation and determine the Peclet number,  $\text{Pe}$ , which is a measure of axial dispersion in the extractor.

(Answer: 1.72)

**A.4** The roof of a building absorbs energy at a rate of 225 kW due to solar radiation. The roof loses energy by radiation and convection. The loss of energy flux as a result of convection from the roof to the surrounding air at 25°C is expressed as

$$q = 2.5 (T - T_\infty)^{1.25}$$

where  $T$  and  $T_\infty$  are the temperatures of roof and air in degrees Kelvin, respectively, and  $q$  is in  $\text{W}/\text{m}^2$ . Calculate the steady-state temperature of the roof if it has the dimensions of 10 m  $\times$  30 m and its emissivity is 0.9.

(Answer: 352 K)

## A.8 METHODS OF INTEGRATION

Analytical evaluation of a definite integral

$$I = \int_a^b f(x) dx \tag{A.8-1}$$

is possible only for limited cases. When analytical evaluation is impossible, then the following techniques can be used to estimate the value of the integral.

### A.8.1 Mean Value Theorem

As stated in Section A.2, if  $f(x)$  is continuous in the interval  $a \leq x \leq b$ , then the value of  $I$  is

$$I = \int_a^b f(x) dx = \langle f \rangle (b - a) \tag{A.8-2}$$

where  $\langle f \rangle$  is the average value of  $f$  in the interval  $a \leq x \leq b$ .

If  $f(x)$  is a monotonic function, then the value of  $I$  is bounded by  $I_{\min}$  and  $I_{\max}$  such that

$$f(x) = \begin{cases} \text{Monotonically increasing function} & \begin{cases} I_{\min} = f(a)(b-a) \\ I_{\max} = f(b)(b-a) \end{cases} \\ \text{Monotonically decreasing function} & \begin{cases} I_{\min} = f(b)(b-a) \\ I_{\max} = f(a)(b-a) \end{cases} \end{cases} \quad (\text{A.8-3})$$

In some cases, only part of the integrand may be approximated to permit analytical integration, i.e.,

$$I = \int_a^b f(x)g(x) dx = \begin{cases} \langle f \rangle \int_a^b g(x) dx \\ \langle g \rangle \int_a^b f(x) dx \end{cases} \quad (\text{A.8-4})$$

**Example A.5** Evaluate the integral

$$I = \int_0^{10} x^2 \sqrt{0.1x + 2} dx$$

**Solution**

Analytical evaluation of the integral is possible and the result is

$$\begin{aligned} I &= \int_0^{10} x^2 \sqrt{0.1x + 2} dx \\ &= \frac{2(0.15x^2 - 2.4x + 32)}{0.105} \sqrt{(0.1x + 2)^3} \Big|_{x=0}^{x=10} = 552.4 \end{aligned}$$

The same integral can be evaluated approximately as follows: Note that the integrand is the product of two terms and the integral can be written as

$$I = \int_a^b f(x)g(x) dx \quad (1)$$

where

$$f(x) = x^2 \quad \text{and} \quad g(x) = \sqrt{0.1x + 2} \quad (2)$$

The value of  $g(x)$  is 1.732 and 1.414 at  $x = 10$  and  $x = 0$ , respectively. Since the value of  $g(x)$  does not change drastically over the interval  $0 \leq x \leq 10$ , Eq. (1) can be expressed in the form

$$I = \langle g \rangle \int_0^{10} f(x) dx \quad (3)$$

As a rough approximation, the average value of the function  $g$ ,  $\langle g \rangle$ , can be taken as the arithmetic average, i.e.,

$$\langle g \rangle = \frac{1.732 + 1.414}{2} = 1.573 \quad (4)$$

Therefore, Eq. (3) becomes

$$I = 1.573 \int_0^{10} x^2 dx = \frac{1.573}{3} x^3 \Big|_{x=0}^{x=10} = 524.3 \quad (5)$$

with a percent error of approximately 5%.

## A.8.2 Graphical Integration

In order to evaluate the integral given by Eq. (A.8-1) graphically, first  $f(x)$  is plotted as a function of  $x$ . Then, the area under this curve in the interval  $[a, b]$  is determined.

## A.8.3 Numerical Integration or Quadrature

Numerical integration or *quadrature*<sup>2</sup> is an alternative to graphical and analytical integration. In this method, the integrand is replaced with a polynomial and this polynomial is integrated to give a summation:

$$I = \int_a^b f(x) dx = \int_c^d F(u) du = \sum_{i=0}^n w_i F(u_i) \quad (\text{A.8-5})$$

Numerical integration is preferred for the following cases:

- The function  $f(x)$  is not known but the values of  $f(x)$  is known at equally spaced discrete points.
- The function  $f(x)$  is known, but too difficult to integrate analytically.

### A.8.3.1 Numerical integration with equally spaced base points

Consider Figure A.5 in which  $f(x)$  is known only at 5 equally spaced base points. The two most frequently used numerical integration methods for this case are the *trapezoidal rule* and the *Simpson's rule*.

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<sup>2</sup>The word *quadrature* is used for *approximate integration*.

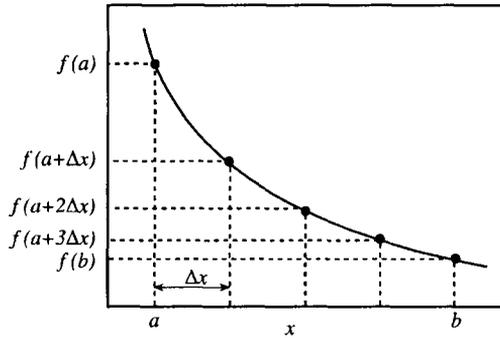


Figure A.5 Values of the function  $f(x)$  at five equally spaced points.

**Trapezoidal rule**

In this method, the required area under the solid curve is approximated by the area under the dotted straight line (the shaded trapezoid) as shown in Figure A.6.

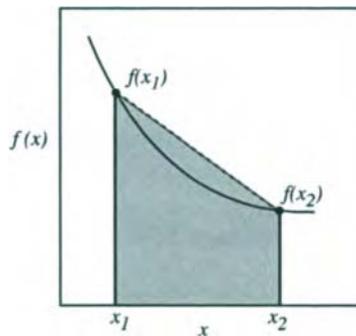


Figure A.6 The trapezoidal rule.

The area of the trapezoid is then

$$\text{Area} = \frac{[f(x_1) + f(x_2)](x_2 - x_1)}{2} \tag{A.8-6}$$

If this procedure is repeated at 4 equally spaced intervals given in Figure A.5, the value of the integral is

$$I = \int_a^b f(x) dx = \frac{[f(a) + f(a + \Delta x)] \Delta x}{2} + \frac{[f(a + \Delta x) + f(a + 2\Delta x)] \Delta x}{2} + \frac{[f(a + 2\Delta x) + f(a + 3\Delta x)] \Delta x}{2} + \frac{[f(a + 3\Delta x) + f(b)] \Delta x}{2} \tag{A.8-7}$$

or,

$$\begin{aligned}
 I &= \int_a^b f(x) dx \\
 &= \Delta x \left[ \frac{f(a)}{2} + f(a + \Delta x) + f(a + 2\Delta x) + f(a + 3\Delta x) + \frac{f(b)}{2} \right] \quad (\text{A.8-8})
 \end{aligned}$$

This result can be generalized as

$$\begin{aligned}
 I &= \int_a^b f(x) dx \\
 &= \frac{\Delta x}{2} \left[ f(a) + 2 \sum_{i=1}^{n-2} f(a + i\Delta x) + f(b) \right] \quad (\text{A.8-9})
 \end{aligned}$$

where

$$n = 1 + \frac{b - a}{\Delta x} \quad (\text{A.8-10})$$

### Simpson's rule

The trapezoidal rule fits a straight line (first-order polynomial) between the two points. Simpson's rule, on the other hand, fits a second-order polynomial between the two points. In this case the general formula is

$$\begin{aligned}
 I &= \int_a^b f(x) dx \\
 &= \frac{\Delta x}{3} f(a) + 4 \sum_{i=1,3,5}^{n-1} f(a + i\Delta x) + 2 \sum_{i=2,4,6}^{n-2} f(a + i\Delta x) + f(b) \quad (\text{A.8-11})
 \end{aligned}$$

where

$$n = \frac{b - a}{\Delta x} \quad (\text{A.8-12})$$

Note that this formula requires the division of the interval of integration into an even number of subdivisions.

**Example A.6** Determine the heat required to increase the temperature of benzene vapor from 300 K to 1000 K at atmospheric pressure. The heat capacity of benzene vapor varies as a function of temperature as follows:

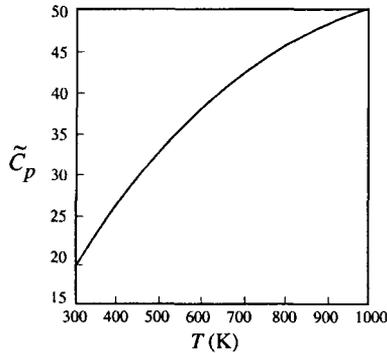
$T$ (K)	$\tilde{C}_P$ (cal/mol.K)
300	19.65
400	26.74
500	32.80
600	37.74
700	41.75
800	45.06
900	47.83
1000	50.16

**Solution**

The amount of heat necessary to increase the temperature of benzene vapor from 300 K to 1000 K under constant pressure is calculated from the formula

$$\tilde{Q} = \Delta\tilde{H} = \int_{300}^{1000} \tilde{C}_P dT$$

The variation of  $\tilde{C}_P$  as a function of temperature is shown in the figure below:



Since the function is monotonically increasing, the bounding values are

$$\tilde{Q}_{\min} = (19.65)(1000 - 300) = 13,755 \text{ cal/mol}$$

$$\tilde{Q}_{\max} = (50.16)(1000 - 300) = 35,112 \text{ cal/mol}$$

**Trapezoidal rule with  $n = 8$** 

From Eq. (A.8-10)

$$\Delta T = \frac{1000 - 300}{8 - 1} = 100$$

The value of the integral can be calculated from Eq. (A.8-9) as

$$\begin{aligned}\tilde{Q} &= \frac{100}{2} [19.65 + 2(26.74 + 32.80 + 37.74 + 41.75 + 45.06 + 47.83) + 50.16] \\ &= 26,683 \text{ cal/mol}\end{aligned}$$

**Simpson's rule with  $n = 4$**

From Eq. (A.8-12)

$$\Delta T = \frac{1000 - 300}{4} = 175$$

Therefore, the values of  $\tilde{C}_P$  at 5 equally spaced points are given in the following table:

$T$ (K)	$\tilde{C}_P$ (cal/mol.K)
300	19.65
475	31.50
650	39.50
825	45.75
1000	50.16

The value of the integral using Eq. (A.8-11) is

$$\begin{aligned}\tilde{Q} &= \frac{175}{3} [19.65 + 4(31.50 + 45.75) + 2(39.50) + 50.16] \\ &= 26,706 \text{ cal/mol}\end{aligned}$$

## A.8.4 Numerical Integration When the Integrand is a Continuous Function

### A.8.4.1 Gauss-Legendre quadrature

The evaluation of an integral given by Eq. (A.8-1), where  $a$  and  $b$  are arbitrary but finite, using the Gauss-Legendre quadrature requires the following transformation:

$$x = \left( \frac{b-a}{2} \right) u + \frac{a+b}{2} \quad (\text{A.8-13})$$

Then Eq. (A.8-1) becomes

$$\begin{aligned}I &= \int_a^b f(x) dx \\ &= \frac{b-a}{2} \int_{-1}^1 F(u) du = \frac{b-a}{2} \sum_{i=0}^n w_i F(u_i)\end{aligned} \quad (\text{A.8-14})$$

where the roots and weight factors for  $n = 1, 2, 3,$  and  $4$  are given in Table A.3.

**Table A.3** Roots and weight factors for Gauss-Legendre quadrature (Abramowitz and Stegun, 1970).

$n$	Roots ( $u_i$ )	Weight Factors ( $w_i$ )
1	$\pm 0.57735\ 02691\ 89626$	1.00000 00000 00000
2	0.00000 00000 00000	0.88888 88888 88889
	$\pm 0.77459\ 66692\ 41483$	0.55555 55555 55556
3	$\pm 0.33998\ 10435\ 84856$	0.65214 51548 62546
	$\pm 0.86113\ 63115\ 94053$	0.34785 48451 37454
4	0.00000 00000 00000	0.56888 88888 88889
	$\pm 0.53846\ 93101\ 05683$	0.47862 86704 99366
	$\pm 0.90617\ 98459\ 38664$	0.23692 68850 56189

**Example A.7** Evaluate

$$I = \int_1^2 \frac{1}{x+2} dx$$

using the five-point ( $n = 4$ ) Gauss-Legendre quadrature formula and compare with the analytical solution.

**Solution**

Since  $b = 2$  and  $a = 1$ , from Eq. (A.8-13)

$$x = \frac{u+3}{2}$$

Then

$$F(u) = \frac{1}{\left(\frac{u+3}{2}\right) + 2} = \frac{2}{u+7}$$

The five-point quadrature is given by

$$I = \int_1^2 \frac{1}{x+2} dx = \frac{1}{2} \sum_{i=0}^4 w_i F(u_i)$$

The values of  $w_i$  and  $F(u_i)$  are given in the table below:

$i$	$u_i$	$w_i$	$F(u_i) = \frac{2}{u_i + 7}$	$w_i F(u_i)$
0	0.00000000	0.56888889	0.28571429	0.16253969
1	+0.53846931	0.47862867	0.26530585	0.12698299
2	-0.53846931	0.47862867	0.30952418	0.14814715
3	+0.90617985	0.23692689	0.25296667	0.05993461
4	-0.90617985	0.23692689	0.32820135	0.07775973
$\sum_{i=0}^{i=4} w_i F(u_i) = 0.57536417$				

Therefore

$$I = (0.5)(0.57536417) = 0.28768209$$

Analytically,

$$I = \ln(x+2) \Big|_{x=1}^{x=2} = \ln\left(\frac{4}{3}\right) = 0.28768207$$

#### A.8.4.2 Gauss-Laguerre quadrature

The Gauss-Laguerre quadrature can be used to evaluate integrals of the form

$$I = \int_a^\infty e^{-x} f(x) dx \quad (\text{A.8-15})$$

where  $a$  is arbitrary and finite. The transformation

$$x = u + a \quad (\text{A.8-16})$$

reduces Eq. (A.8-15) to

$$I = \int_a^\infty e^{-x} f(x) dx = e^{-a} \int_0^\infty e^{-u} F(u) du = e^{-a} \sum_{i=0}^n w_i F(u_i) \quad (\text{A.8-17})$$

where the  $w_i$  and  $u_i$  are given in Table A.4.

**Example A.8** The gamma function,  $\Gamma(n)$ , is defined by

$$\Gamma(n) = \int_0^\infty \beta^{n-1} e^{-\beta} d\beta$$

where the variable  $\beta$  in the integrand is the dummy variable of integration. Estimate  $\Gamma(1.5)$  by using the Gauss-Laguerre quadrature with  $n = 3$ .

**Table A.4** Roots and weight factors for Gauss-Laguerre quadrature (Abramowitz and Stegun, 1970).

$n$	Roots ( $u_i$ )	Weight Factors ( $w_i$ )
1	0.58578 64376 27	0.85355 33905 93
	3.41421 35623 73	0.14644 66094 07
2	0.41577 45567 83	0.71109 30099 29
	2.29428 03602 79	0.27851 77335 69
	6.28994 50829 37	0.01038 92565 02
3	0.32254 76896 19	0.60315 41043 42
	1.74576 11011 58	0.35741 86924 38
	4.53662 02969 21	0.03888 79085 15
	9.39507 09123 01	0.00053 92947 06
4	0.26356 03197 18	0.52175 56105 83
	1.41340 30591 07	0.39866 68110 83
	3.59642 57710 41	0.07594 24496 82
	7.08581 00058 59	0.00361 17586 80
	12.64080 08442 76	0.00002 33699 72

**Solution**

Since  $a = 0$ , then

$$\beta = u$$

and

$$F(u) = \sqrt{u}$$

The four-point quadrature is given by

$$\Gamma(1.5) = \int_0^\infty \sqrt{\beta} e^{-\beta} d\beta = \sum_{i=0}^3 w_i F(u_i)$$

The values of  $w_i$  and  $F(u_i)$  are given in the table below:

$i$	$u_i$	$w_i$	$F(u_i) = \sqrt{u_i}$	$w_i F(u_i)$
0	0.32254769	0.60315410	0.56793282	0.34255101
1	1.74576110	0.35741869	1.32127253	0.47224750
2	4.53662030	0.03888791	2.12993434	0.08282869
3	9.39507091	0.00053929	3.06513799	0.00165300

$$\Gamma(1.5) = \sum_{i=0}^{i=3} w_i F(u_i) = 0.8992802$$

The exact value of  $\Gamma(1.5)$  is 0.8862269255.

### A.8.4.3 Gauss-Hermite quadrature

The Gauss-Hermite quadrature can be used to evaluate integrals of the form

$$I = \int_{-\infty}^{\infty} e^{-x^2} f(x) dx = \sum_{i=0}^n w_i f(x_i) \quad (\text{A.8-18})$$

The weight factors and appropriate roots for the first few quadrature formulas are given in Table A.5.

**Table A.5** Roots and weight factors for Gauss-Hermite quadrature (Abramowitz and Stegun, 1970).

$n$	Roots ( $x_i$ )	Weight Factors ( $w_i$ )
1	$\pm 0.70710\ 67811$	0.88622 69255
2	$\pm 1.22474\ 48714$	0.29540 89752
	0.00000 00000	1.18163 59006
3	$\pm 1.65068\ 01239$	0.08131 28354
	$\pm 0.52464\ 76233$	0.80491 40900
	$\pm 2.02018\ 28705$	0.01995 32421
4	$\pm 0.95857\ 24646$	0.39361 93232
	0.00000 00000	0.94530 87205

## A.9 MATRICES

A rectangular array of elements or functions is called a *matrix*. If the array has  $m$  rows and  $n$  columns, it is called an  $m \times n$  matrix and expressed in the form

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mn} \end{bmatrix} \quad (\text{A.9-1})$$

The numbers or functions  $a_{ij}$  are called the elements of a matrix. Equation (A.9-1) is also expressed as

$$\mathbf{A} = (a_{ij}) \quad (\text{A.9-2})$$

in which the subscripts  $i$  and  $j$  represent the row and the column of the matrix, respectively.

A matrix having only one row is called a *row matrix* (or, *row vector*) while a matrix having only one column is called a *column matrix* (or, *column vector*). When the number of rows and the number of columns are the same, i.e.,  $m = n$ , the matrix is called a *square matrix* or a matrix of order  $n$ .

### A.9.1 Fundamental Algebraic Operations

1. Two matrices  $\mathbf{A} = (a_{ij})$  and  $\mathbf{B} = (b_{ij})$  of the same order are equal if and only if  $a_{ij} = b_{ij}$ .
2. If  $\mathbf{A} = (a_{ij})$  and  $\mathbf{B} = (b_{ij})$  have the same order, the sum of  $\mathbf{A}$  and  $\mathbf{B}$  is defined as

$$\mathbf{A} + \mathbf{B} = (a_{ij} + b_{ij}) \quad (\text{A.9-3})$$

If  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  are the matrices of the same order, addition is commutative and associative, i.e.,

$$\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A} \quad (\text{A.9-4})$$

$$\mathbf{A} + (\mathbf{B} + \mathbf{C}) = (\mathbf{A} + \mathbf{B}) + \mathbf{C} \quad (\text{A.9-5})$$

3. If  $\mathbf{A} = (a_{ij})$  and  $\mathbf{B} = (b_{ij})$  have the same order, the difference of  $\mathbf{A}$  and  $\mathbf{B}$  is defined as

$$\mathbf{A} - \mathbf{B} = (a_{ij} - b_{ij}) \quad (\text{A.9-6})$$

**Example A.9** *If*

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ 1 & 0 \\ 3 & 5 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 2 & -4 \\ 3 & 0 \\ 0 & 1 \end{bmatrix}$$

*determine*  $\mathbf{A} + \mathbf{B}$  *and*  $\mathbf{A} - \mathbf{B}$ .

**Solution**

$$\begin{aligned} \mathbf{A} + \mathbf{B} &= \begin{bmatrix} 2+2 & -1-4 \\ 1+3 & 0+0 \\ 3+0 & 5+1 \end{bmatrix} = \begin{bmatrix} 4 & -5 \\ 4 & 0 \\ 3 & 6 \end{bmatrix} \\ \mathbf{A} - \mathbf{B} &= \begin{bmatrix} 2-2 & -1+4 \\ 1-3 & 0-0 \\ 3-0 & 5-1 \end{bmatrix} = \begin{bmatrix} 0 & 3 \\ -2 & 0 \\ 3 & 4 \end{bmatrix} \end{aligned}$$

4. If  $\mathbf{A} = (a_{ij})$  and  $\lambda$  is any number, the product of  $\mathbf{A}$  by  $\lambda$  is defined as

$$\lambda \mathbf{A} = \mathbf{A} \lambda = (\lambda a_{ij}) \quad (\text{A.9-7})$$

5. The product of two matrices  $\mathbf{A}$  and  $\mathbf{B}$ ,  $\mathbf{AB}$ , is defined only if the number of columns in  $\mathbf{A}$  is equal to the number of rows in  $\mathbf{B}$ . In this case, the two

matrices are said to be *conformable* in the order stated. For example, if  $\mathbf{A}$  is of order  $4 \times 2$  and  $\mathbf{B}$  is of order  $2 \times 3$ , then the product  $\mathbf{A}\mathbf{B}$  is

$$\begin{aligned} \mathbf{A}\mathbf{B} &= \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \\ a_{41} & a_{42} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix} & (\text{A.9-8}) \\ &= \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} & a_{11}b_{13} + a_{12}b_{23} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} & a_{21}b_{13} + a_{22}b_{23} \\ a_{31}b_{11} + a_{32}b_{21} & a_{31}b_{12} + a_{32}b_{22} & a_{31}b_{13} + a_{32}b_{23} \\ a_{41}b_{11} + a_{42}b_{21} & a_{41}b_{12} + a_{42}b_{22} & a_{41}b_{13} + a_{42}b_{23} \end{bmatrix} \end{aligned}$$

In general, if a matrix of order  $(m, r)$  is multiplied by a matrix of order  $(r, n)$ , the product is a matrix of order  $(m, n)$ . Symbolically, this may be expressed as

$$(m, r) \times (r, n) = (m, n) \quad (\text{A.9-9})$$

**Example A.10** *If*

$$\mathbf{A} = \begin{bmatrix} 1 & -1 \\ 2 & 0 \\ -1 & 5 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

*determine*  $\mathbf{A}\mathbf{B}$ .

**Solution**

$$\begin{aligned} \mathbf{A}\mathbf{B} &= \begin{bmatrix} 1 & -1 \\ 2 & 0 \\ -1 & 5 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} \\ &= \begin{bmatrix} (1)(1) + (-1)(2) \\ (2)(1) + (0)(2) \\ (-1)(1) + (5)(2) \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \\ 9 \end{bmatrix} \end{aligned}$$

6. A matrix  $\mathbf{A}$  can be multiplied by itself if and only if it is a square matrix. The product  $\mathbf{A}\mathbf{A}$  can be expressed as  $\mathbf{A}^2$ . If the relevant products are defined, multiplication of matrices is associative, i.e.,

$$\mathbf{A}(\mathbf{B}\mathbf{C}) = (\mathbf{A}\mathbf{B})\mathbf{C} \quad (\text{A.9-10})$$

and distributive, i.e.,

$$\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{A}\mathbf{B} + \mathbf{A}\mathbf{C} \quad (\text{A.9-11})$$

$$(\mathbf{B} + \mathbf{C})\mathbf{A} = \mathbf{B}\mathbf{A} + \mathbf{C}\mathbf{A} \quad (\text{A.9-12})$$

but, in general, not commutative.

### A.9.2 Determinants

For each square matrix  $\mathbf{A}$ , it is possible to associate a scalar quantity called the determinant of  $\mathbf{A}$ ,  $|\mathbf{A}|$ . If the matrix  $\mathbf{A}$  in Eq. (A.9-1) is a square matrix, then the determinant of  $\mathbf{A}$  is given by

$$|\mathbf{A}| = \begin{vmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{vmatrix} \quad (\text{A.9-13})$$

If the row and column containing an element  $a_{ij}$  in a square matrix  $\mathbf{A}$  are deleted, the determinant of the remaining square array is called the *minor* of  $a_{ij}$  and denoted by  $M_{ij}$ . The cofactor of  $a_{ij}$ , denoted by  $A_{ij}$ , is then defined by the relation

$$A_{ij} = (-1)^{i+j} M_{ij} \quad (\text{A.9-14})$$

Thus, if the sum of the row and column indices of an element is even, the cofactor and the minor of that element are identical; otherwise they differ in sign.

The determinant of a square matrix  $\mathbf{A}$  can be calculated by the following formula:

$$|\mathbf{A}| = \sum_{k=1}^n a_{ik} A_{ik} = \sum_{k=1}^n a_{kj} A_{kj} \quad (\text{A.9-15})$$

where  $i$  and  $j$  may stand for any row and column, respectively. Therefore, the determinant of  $2 \times 2$  and  $3 \times 3$  matrices are

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21} \quad (\text{A.9-16})$$

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} - a_{13}a_{22}a_{31} \quad (\text{A.9-17})$$

**Example A.11** Determine  $|\mathbf{A}|$  if

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 \\ 3 & 2 & 1 \\ -1 & 1 & 0 \end{bmatrix}$$

**Solution**

Expanding on the first row, i.e.,  $i = 1$ , gives

$$|\mathbf{A}| = 1 \begin{vmatrix} 2 & 1 \\ 1 & 0 \end{vmatrix} - 0 \begin{vmatrix} 3 & 1 \\ -1 & 0 \end{vmatrix} + 1 \begin{vmatrix} 3 & 2 \\ -1 & 1 \end{vmatrix} = -1 + 5 = 4$$

### A.9.2.1 Some properties of determinants

1. If all elements in a row or column are zero, the determinant is zero, i.e.,

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ 0 & 0 & 0 \end{vmatrix} = 0 \qquad \begin{vmatrix} 0 & b_1 & c_1 \\ 0 & b_2 & c_2 \\ 0 & b_3 & c_3 \end{vmatrix} = 0 \qquad (\text{A.9-18})$$

2. The value of a determinant is not altered when the rows are changed to columns and the columns to rows, i.e., when the rows and columns are interchanged.
3. The interchange of any two columns or any two rows of a determinant changes the sign of the determinant.
4. If two columns or two rows of a determinant are identical, the determinant is equal to zero.
5. If each element in any column or row of a determinant is expressed as the sum of two quantities, the determinant can be expressed as the sum of two determinants of the same order, i.e.,

$$\begin{vmatrix} a_1 + d_1 & b_1 & c_1 \\ a_2 + d_2 & b_2 & c_2 \\ a_3 + d_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} + \begin{vmatrix} d_1 & b_1 & c_1 \\ d_2 & b_2 & c_2 \\ d_3 & b_3 & c_3 \end{vmatrix} \qquad (\text{A.9-19})$$

6. Adding the same multiple of each element of one row to the corresponding element of another row does not change the value of the determinant. The same holds true for the columns.

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} (a_1 + nb_1) & b_1 & c_1 \\ (a_2 + nb_2) & b_2 & c_2 \\ (a_3 + nb_3) & b_3 & c_3 \end{vmatrix} \qquad (\text{A.9-20})$$

This result follows immediately from Properties 4 and 5.

7. If all the elements in any column or row are multiplied by any factor, the determinant is multiplied by that factor, i.e.,

$$\begin{vmatrix} \lambda a_1 & b_1 & c_1 \\ \lambda a_2 & b_2 & c_2 \\ \lambda a_3 & b_3 & c_3 \end{vmatrix} = \lambda \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} \qquad (\text{A.9-21})$$

$$\begin{vmatrix} (1/\lambda)a_1 & b_1 & c_1 \\ (1/\lambda)a_2 & b_2 & c_2 \\ (1/\lambda)a_3 & b_3 & c_3 \end{vmatrix} = \frac{1}{\lambda} \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} \qquad (\text{A.9-22})$$

### A.9.3 Types of Matrices

#### A.9.3.1 The transpose of a matrix

The matrix which is obtained from  $\mathbf{A}$  by interchanging rows and columns is called the *transpose* of  $\mathbf{A}$  and denoted by  $\mathbf{A}^T$ .

The transpose of the product  $\mathbf{A}\mathbf{B}$  is the product of the transposes in the form

$$(\mathbf{A}\mathbf{B})^T = \mathbf{B}^T \mathbf{A}^T \quad (\text{A.9-23})$$

#### A.9.3.2 Unit matrix

The *unit matrix*  $\mathbf{I}$  of order  $n$  is the square  $n \times n$  matrix having ones in its principal diagonal and zeros elsewhere, i.e.,

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \end{pmatrix} \quad (\text{A.9-24})$$

For any matrix

$$\mathbf{A}\mathbf{I} = \mathbf{I}\mathbf{A} = \mathbf{A} \quad (\text{A.9-25})$$

#### A.9.3.3 Symmetric and skew-symmetric matrices

A square matrix  $\mathbf{A}$  is said to be *symmetric* if

$$\mathbf{A} = \mathbf{A}^T \quad \text{or} \quad a_{ij} = a_{ji} \quad (\text{A.9-26})$$

A square matrix  $\mathbf{A}$  is said to be *skew-symmetric* (or, *antisymmetric*) if

$$\mathbf{A} = -\mathbf{A}^T \quad \text{or} \quad a_{ij} = -a_{ji} \quad (\text{A.9-27})$$

Equation (A.9-27) implies that the diagonal elements of a skew-symmetric matrix are all zero.

#### A.9.3.4 Singular matrix

A square matrix  $\mathbf{A}$  for which the determinant  $|\mathbf{A}|$  of its elements is zero, is termed a *singular* matrix. If  $|\mathbf{A}| \neq 0$ , then  $\mathbf{A}$  is *nonsingular*.

#### A.9.3.5 The inverse matrix

If the determinant  $|\mathbf{A}|$  of a square matrix  $\mathbf{A}$  does not vanish, i.e., nonsingular matrix, it then possesses an *inverse* (or, *reciprocal*) matrix  $\mathbf{A}^{-1}$  such that

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I} \quad (\text{A.9-28})$$

The inverse of a matrix  $\mathbf{A}$  is defined by

$$\mathbf{A}^{-1} = \frac{\text{Adj } \mathbf{A}}{|\mathbf{A}|} \tag{A.9-29}$$

where  $\text{Adj } \mathbf{A}$  is called the *adjoint* of  $\mathbf{A}$ . It is obtained from a square matrix  $\mathbf{A}$  by replacing each element by its cofactor and then interchanging rows and columns.

**Example A.12** Find the inverse of the matrix  $\mathbf{A}$  given in Example A.11.

**Solution**

The minor of  $\mathbf{A}$  is given by

$$M_{ij} = \begin{bmatrix} \begin{vmatrix} 2 & 1 \\ 1 & 0 \end{vmatrix} & \begin{vmatrix} 3 & 1 \\ -1 & 0 \end{vmatrix} & \begin{vmatrix} 3 & 2 \\ -1 & 1 \end{vmatrix} \\ \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} & \begin{vmatrix} 1 & 1 \\ -1 & 0 \end{vmatrix} & \begin{vmatrix} 1 & 0 \\ -1 & 1 \end{vmatrix} \\ \begin{vmatrix} 0 & 1 \\ 2 & 1 \end{vmatrix} & \begin{vmatrix} 1 & 1 \\ 3 & 1 \end{vmatrix} & \begin{vmatrix} 1 & 0 \\ 3 & 2 \end{vmatrix} \end{bmatrix} = \begin{bmatrix} -1 & 1 & 5 \\ -1 & 1 & 1 \\ -2 & -2 & 2 \end{bmatrix}$$

The cofactor matrix is

$$A_{ij} = \begin{bmatrix} -1 & -1 & 5 \\ 1 & 1 & -1 \\ -2 & 2 & 2 \end{bmatrix}$$

The transpose of the cofactor matrix gives the adjoint of  $\mathbf{A}$  as

$$\text{Adj } \mathbf{A} = \begin{bmatrix} -1 & 1 & -2 \\ -1 & 1 & 2 \\ 5 & -1 & 2 \end{bmatrix}$$

Since  $|\mathbf{A}| = 4$ , the use of Eq. (A.9-29) gives the inverse of  $\mathbf{A}$  in the form

$$\mathbf{A}^{-1} = \frac{\text{Adj } \mathbf{A}}{|\mathbf{A}|} = \begin{bmatrix} -0.25 & 0.25 & -0.5 \\ -0.25 & 0.25 & 0.5 \\ 1.25 & -0.25 & 0.5 \end{bmatrix}$$

### A.9.4 Solution of Simultaneous Algebraic Equations

Consider the system of  $n$  nonhomogeneous algebraic equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n &= c_1 \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n &= c_2 \\ \dots &= \dots \\ a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n &= c_n \end{aligned} \tag{A.9-30}$$

in which the coefficients  $a_{ij}$  and the constants  $c_i$  are independent of  $x_1, x_2, \dots, x_n$  but are otherwise arbitrary. In matrix notation, Eq. (A.9-30) is expressed as

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \dots \\ c_n \end{bmatrix} \quad (\text{A.9-31})$$

or,

$$\mathbf{A} \mathbf{X} = \mathbf{C} \quad (\text{A.9-32})$$

Multiplication of Eq. (A.9-32) by the inverse of the coefficient matrix  $\mathbf{A}$  gives

$$\mathbf{X} = \mathbf{A}^{-1} \mathbf{C} \quad (\text{A.9-33})$$

#### A.9.4.1 Cramer's rule

Cramer's rule states that, if the determinant of  $\mathbf{A}$  is not equal to zero, the system of linear algebraic equations has a solution given by

$$x_j = \frac{|\mathbf{A}_j|}{|\mathbf{A}|} \quad (\text{A.9-34})$$

where  $|\mathbf{A}|$  and  $|\mathbf{A}_j|$  are the determinants of the coefficient and substituted matrices, respectively. The *substituted matrix*,  $\mathbf{A}_j$ , is obtained by replacing the  $j^{\text{th}}$  column of  $\mathbf{A}$  by the column of  $c$ 's, i.e.,

$$\mathbf{A}_j = \begin{bmatrix} a_{11} & a_{12} & \dots & c_1 & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & c_2 & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & c_n & \dots & a_{nn} \end{bmatrix} \quad (\text{A.9-35})$$

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# Appendix B

## Solutions of Differential Equations

A *differential equation* is an equation involving derivatives or differentials of one or more dependent variables with respect to one or more independent variables.

The *order* of a differential equation is the order of the highest derivative in the equation.

The *degree* of a differential equation is the power of the highest derivative after the equation has been rationalized and cleared of fractions.

A differential equation is *linear* when: (i) every dependent variable and every derivative involved occurs to the first-degree only, (ii) neither products nor powers of dependent variables nor products of dependent variables with differentials exist.

### B.1 TYPES OF FIRST-ORDER EQUATIONS WITH EXACT SOLUTIONS

There are 5 types of differential equations for which solutions may be obtained by exact methods. These are:

- Separable equations,
- Exact equations,
- Homogeneous equations,
- Linear equations,
- Bernoulli equations.

### B.1.1 Separable Equations

An equation of the form

$$f_1(x)g_1(y) dx + f_2(x)g_2(y) dy = 0 \quad (\text{B.1-1})$$

is called a *separable equation*. Division of Eq. (B.1-1) by  $g_1(y)f_2(x)$  results in

$$\frac{f_1(x)}{f_2(x)} dx + \frac{g_2(y)}{g_1(y)} dy = 0 \quad (\text{B.1-2})$$

Integration of Eq. (B.1-2) gives

$$\int \frac{f_1(x)}{f_2(x)} dx + \int \frac{g_2(y)}{g_1(y)} dy = C \quad (\text{B.1-3})$$

where  $C$  is the integration constant.

**Example B.1** Solve the following equation

$$(2x + xy^2) dx + (3y + x^2y) dy = 0$$

**Solution**

The differential equation can be rewritten in the form

$$x(2 + y^2) dx + y(3 + x^2) dy = 0 \quad (1)$$

Note that Eq. (1) is a separable equation and can be expressed as

$$\frac{x}{3 + x^2} dx + \frac{y}{2 + y^2} dy = 0 \quad (2)$$

Integration of Eq. (2) gives

$$(3 + x^2)(2 + y^2) = C \quad (3)$$

### B.1.2 Exact Equations

The expression  $M dx + N dy$  is called an *exact differential*<sup>1</sup> if there exists some  $\phi = \phi(x, y)$  for which this expression is the total differential  $d\phi$ , i.e.,

$$M dx + N dy = d\phi \quad (\text{B.1-4})$$

A necessary and sufficient condition for the expression  $M dx + N dy$  to be expressed as a total differential is that

$$\frac{\partial M}{\partial y} = \frac{\partial N}{\partial x} \quad (\text{B.1-5})$$

---

<sup>1</sup>In thermodynamics, an exact differential is called a state function.

If  $M dx + N dy$  is an exact differential, then the differential equation

$$M dx + N dy = 0 \quad (\text{B.1-6})$$

is called an *exact differential equation*. Since an exact differential can be expressed in the form of a total differential  $d\phi$ , then

$$M dx + N dy = d\phi = 0 \quad (\text{B.1-7})$$

and the solution can easily be obtained as

$$\phi = C \quad (\text{B.1-8})$$

where  $C$  is a constant.

**Example B.2** Solve the following differential equation

$$(4x - 3y)dx + (1 - 3x)dy = 0$$

**Solution**

Note that  $M = 4x - 3y$  and  $N = 1 - 3x$ . Since

$$\frac{\partial M}{\partial y} = \frac{\partial N}{\partial x} = -3 \quad (1)$$

the differential equation is exact and can be expressed in the form of a total differential  $d\phi$ ,

$$(4x - 3y) dx + (1 - 3x) dy = d\phi = \frac{\partial\phi}{\partial x} dx + \frac{\partial\phi}{\partial y} dy = 0 \quad (2)$$

From Eq. (2) we see that

$$\frac{\partial\phi}{\partial x} = 4x - 3y \quad (3)$$

$$\frac{\partial\phi}{\partial y} = 1 - 3x \quad (4)$$

Partial integration of Eq. (3) with respect to  $x$  gives

$$\phi = 2x^2 - 3xy + h(y) \quad (5)$$

Substitution of Eq. (5) into Eq. (4) yields

$$\frac{dh}{dy} = 1 \quad (6)$$

Integration of Eq. (6) gives the function  $h$  as

$$h = y + C \quad (7)$$

where  $C$  is a constant. Substitution of Eq. (7) into Eq. (5) gives the function  $\phi$  as

$$\phi = 2x^2 - 3xy + y + C \quad (8)$$

Hence, the solution is

$$2x^2 - 3xy + y = C^* \quad (9)$$

where  $C^*$  is a constant.

If the equation  $M dx + N dy$  is not exact, multiplication of it by some function  $\mu$ , called an *integrating factor*, may make it an exact equation, i.e.,

$$\mu M dx + \mu N dy = 0 \quad \Rightarrow \quad \frac{\partial(\mu M)}{\partial y} = \frac{\partial(\mu N)}{\partial x} \quad (\text{B.1-9})$$

For example, all thermodynamic functions except heat and work are state functions. Although  $dQ$  is a path function,  $dQ/T$  is a state function. Therefore,  $1/T$  is an integrating factor in this case.

### B.1.3 Homogeneous Equations

A function  $f(x, y)$  is said to be *homogeneous of degree  $n$*  if

$$f(\lambda x, \lambda y) = \lambda^n f(x, y) \quad (\text{B.1-10})$$

for all  $\lambda$ . For an equation

$$M dx + N dy = 0 \quad (\text{B.1-11})$$

if  $M$  and  $N$  are homogeneous of the same degree, the transformation

$$y = u x \quad (\text{B.1-12})$$

will make the equation separable.

For a homogeneous function of degree  $n$ , *Euler's theorem* states that

$$n f(x_1, x_2, \dots, x_\alpha) = \sum_{i=1}^{\alpha} \left( \frac{\partial f}{\partial x_i} \right) x_i \quad (\text{B.1-13})$$

Note that the *extensive properties* in thermodynamics can be regarded as homogeneous functions of order unity. Therefore, for every extensive property we can write

$$f(x_1, x_2, \dots, x_\alpha) = \sum_{i=1}^{\alpha} \left( \frac{\partial f}{\partial x_i} \right) x_i \quad (\text{B.1-14})$$

On the other hand, the *intensive properties* are homogeneous functions of order zero and can be expressed as

$$0 = \sum_{i=1}^{\alpha} \left( \frac{\partial f}{\partial x_i} \right) x_i \quad (\text{B.1-15})$$

**Example B.3** Solve the following differential equation

$$xy \, dx - (x^2 + y^2) \, dy = 0$$

**Solution**

Since both of the functions

$$M = xy \quad (1)$$

$$N = -(x^2 + y^2) \quad (2)$$

are homogeneous of degree 2, the transformation

$$y = ux \quad \text{and} \quad dy = u \, dx + x \, du \quad (3)$$

reduces the equation to the form

$$\frac{dx}{x} + \frac{1+u^2}{u^3} \, du = 0 \quad (4)$$

Integration of Eq. (4) gives

$$xu = C \exp\left(\frac{1}{2u^2}\right) \quad (5)$$

where  $C$  is an integration constant. Substitution of  $u = y/x$  into Eq. (5) gives the solution as

$$y = C \exp\left[\frac{1}{2}\left(\frac{x}{y}\right)^2\right] \quad (6)$$

### B.1.4 Linear Equations

In order to solve an equation of the form

$$\frac{dy}{dx} + P(x)y = Q(x) \quad (\text{B.1-16})$$

the first step is to find out an *integrating factor*,  $\mu$ , which is defined by

$$\mu = \exp\left[\int P(x) \, dx\right] \quad (\text{B.1-17})$$

Multiplication of Eq. (B.1-16) by the integrating factor gives

$$\frac{d(\mu y)}{dx} = Q \mu \quad (\text{B.1-18})$$

Integration of Eq. (B.1-18) gives the solution as

$$y = \frac{1}{\mu} \int Q \mu dx + \frac{C}{\mu} \quad (\text{B.1-19})$$

where  $C$  is an integration constant.

**Example B.4** Solve the following differential equation

$$x \frac{dy}{dx} - 2y = x^3 \sin x$$

**Solution**

The differential equation can be rewritten as

$$\frac{dy}{dx} - \frac{2}{x} y = x^2 \sin x \quad (1)$$

The integrating factor,  $\mu$ , is

$$\mu = \exp\left(-\int \frac{2}{x} dx\right) = x^{-2} \quad (2)$$

Multiplication of Eq. (1) by the integrating factor gives

$$\frac{1}{x^2} \frac{dy}{dx} - \frac{2}{x^3} y = \sin x \quad (3)$$

Note that Eq. (3) can also be expressed in the form

$$\frac{d}{dx} \left( \frac{y}{x^2} \right) = \sin x \quad (4)$$

Integration of Eq. (4) gives

$$y = -x^2 \cos x + C x^2 \quad (5)$$

### B.1.5 Bernoulli Equations

Bernoulli equation has the form

$$\frac{dy}{dx} + P(x)y = Q(x)y^n \quad n \neq 0, 1 \quad (\text{B.1-20})$$

The transformation

$$z = y^{1-n} \quad (\text{B.1-21})$$

reduces Bernoulli equation to a linear equation, Eq. (B.1-16).

## B.2 SECOND-ORDER LINEAR DIFFERENTIAL EQUATIONS

A general second-order linear differential equation with constant coefficients is written as

$$a_0 \frac{d^2 y}{dx^2} + a_1 \frac{dy}{dx} + a_2 y = R(x) \quad (\text{B.2-1})$$

If  $R(x) = 0$ , the equation

$$a_0 \frac{d^2 y}{dx^2} + a_1 \frac{dy}{dx} + a_2 y = 0 \quad (\text{B.2-2})$$

is called a *homogeneous equation*.

The second-order homogeneous equation can be solved by proposing a solution of the form

$$y = e^{mx} \quad (\text{B.2-3})$$

where  $m$  is a constant. Substitution of Eq. (B.2-3) into Eq. (B.2-2) gives

$$a_0 m^2 + a_1 m + a_2 = 0 \quad (\text{B.2-4})$$

which is known as the *characteristic* or *auxiliary equation*. Solution of the given differential equation depends on the roots of the characteristic equation.

### Distinct real roots

When the roots of Eq. (B.2-4),  $m_1$  and  $m_2$ , are real and distinct, then the solution is

$$y = C_1 e^{m_1 x} + C_2 e^{m_2 x} \quad (\text{B.2-5})$$

### Repeated real roots

When the roots of Eq. (B.2-4),  $m_1$  and  $m_2$ , are real and equal to each other, i.e.,  $m_1 = m_2 = m$ , then the solution is

$$y = (C_1 + C_2 x) e^{mx} \quad (\text{B.2-6})$$

### Conjugate complex roots

When the roots of Eq. (B.2-4),  $m_1$  and  $m_2$ , are complex and conjugate, i.e.,  $m_{1,2} = a \pm ib$ , then the solution is

$$y = e^{ax} (C_1 \cos bx + C_2 \sin bx) \quad (\text{B.2-7})$$

### B.2.1 Special Case of a Second-Order Equation

A second-order ordinary differential equation of the form

$$\frac{d^2y}{dx^2} - \lambda^2 y = 0 \quad (\text{B.2-8})$$

where  $\lambda$  is a constant, is frequently encountered in heat and mass transfer problems. Since the roots of the characteristic equation are

$$m_{1,2} = \pm \lambda \quad (\text{B.2-9})$$

the solution becomes

$$y = C_1 e^{\lambda x} + C_2 e^{-\lambda x} \quad (\text{B.2-10})$$

Using the identities

$$\cosh \lambda x = \frac{e^{\lambda x} + e^{-\lambda x}}{2} \quad \text{and} \quad \sinh \lambda x = \frac{e^{\lambda x} - e^{-\lambda x}}{2} \quad (\text{B.2-11})$$

Equation (B.2-10) can be rewritten as

$$y = C_1^* \sinh \lambda x + C_2^* \cosh \lambda x \quad (\text{B.2-12})$$

### B.2.2 Solution of a Non-Homogenous Differential Equation

Consider the second-order differential equation

$$\frac{d^2y}{dx^2} + P(x) \frac{dy}{dx} + Q(x)y = R(x) \quad (\text{B.2-13})$$

If one solution of the homogeneous solution is known, i.e., say  $y = y_1(x)$ , then the complete solution is (Murray, 1924)

$$y = C_1 y_1(x) + C_2 y_1(x) \int \frac{\exp(-\int P(x)dx)}{y_1^2} dx + y_1 \int \frac{\exp(-\int P(x)dx)}{y_1^2} \times \left[ \int^x y_1(u)R(u) \exp\left(\int P(u)du\right) \right] dx \quad (\text{B.2-14})$$

**Example B.5** Obtain the complete solution of the following non-homogeneous differential equation if one of the solutions of the homogeneous part is  $y_1 = e^{2x}$ .

$$\frac{d^2y}{dx^2} - \frac{dy}{dx} - 2y = 3e^{-x} + 10 \sin x - 4x$$

**Solution**

Comparison of the equation with Eq. (B.2-13) indicates that

$$\begin{aligned} P(x) &= -1 \\ Q(x) &= -2 \\ R(x) &= 3e^{-x} + 10\sin x - 4x \end{aligned}$$

Therefore, Eq. (B.2-14) takes the form

$$y = C_1 e^{2x} + C_2 e^{2x} \int e^{-3x} dx + e^{2x} \int e^{-3x} \left[ \int^x e^u (3e^{-u} + 10\sin u - 4u) du \right] dx$$

The use of the integral formulas

$$\begin{aligned} \int x e^{ax} dx &= \frac{e^{ax}}{a} \left( x - \frac{1}{a} \right) \\ \int e^{ax} \sin bx dx &= e^{ax} \left( \frac{a \sin bx - b \cos bx}{a^2 + b^2} \right) \\ \int e^{ax} \cos bx dx &= e^{ax} \left( \frac{a \cos bx + b \sin bx}{a^2 + b^2} \right) \end{aligned}$$

gives the complete solution as

$$y = C_1 e^{2x} + C_2^* e^{-x} - x e^{-x} - \frac{1}{3} e^{-x} - 3\sin x + \cos x + 2x - 1$$

**B.2.3 Bessel's Equation**

There is large class of ordinary differential equations that cannot be solved in closed form in terms of elementary functions. Over certain intervals, the differential equation may possess solutions in power series or *Frobenius series*.

An expression of the form

$$a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \dots + a_n(x - x_0)^n = \sum_{n=0}^{\infty} a_n(x - x_0)^n \quad (\text{B.2-15})$$

is called a power series in powers of  $(x - x_0)$  with  $x_0$  being the center of expansion. Such a series is said to *converge* if it approaches a finite value as  $n$  approaches infinity.

An ordinary differential equation given in the general form

$$\frac{d}{dx} \left( x^p \frac{dy}{dx} \right) + (ax^j + bx^k)y = 0 \quad j > k \quad (\text{B.2-16})$$

with either  $k = p - 2$  or  $b = 0$ , is known as the *Bessel's equation*. Solutions to Bessel's equations are expressed in the form of power series.

**Example B.6** Show that the equation

$$x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} - \left(x^2 + \frac{1}{4}\right) y = 0$$

is reducible to Bessel's equation.

**Solution**

A second-order differential equation

$$a_o(x) \frac{d^2 y}{dx^2} + a_1(x) \frac{dy}{dx} + a_2(x) y = 0 \quad (1)$$

can be expressed in the form of Eq. (B.2-16) as follows. Dividing each term in Eq. (1) by  $a_o(x)$  gives

$$\frac{d^2 y}{dx^2} + \frac{a_1(x)}{a_o(x)} \frac{dy}{dx} + \frac{a_2(x)}{a_o(x)} y = 0 \quad (2)$$

The integrating factor,  $\mu$ , is

$$\mu = \exp \left( \int \frac{a_1(x)}{a_o(x)} dx \right) \quad (3)$$

Multiplication of Eq. (2) with the integrating factor results in

$$\frac{d}{dx} \left( \mu \frac{dy}{dx} \right) + q y = 0 \quad (4)$$

where

$$q = \frac{a_2(x)}{a_o(x)} \mu \quad (5)$$

To express the given equation in the form of Eq. (B.2-16), the first step is to divide each term by  $x^2$  to get

$$\frac{d^2 y}{dx^2} + \frac{1}{x} \frac{dy}{dx} - \left(1 + \frac{1}{4} x^{-2}\right) y = 0 \quad (6)$$

Note that the integrating factor is

$$\mu = \exp \left( \int \frac{1}{x} dx \right) = x \quad (7)$$

Multiplication of Eq. (6) by the integrating factor and rearrangement gives

$$\frac{d}{dx} \left( x \frac{dy}{dx} \right) - \left( x + \frac{1}{4} x^{-1} \right) y = 0 \quad (8)$$

Comparison of Eq. (8) with Eq. (B.2-16) gives  $p = 1$ ;  $a = -1$ ;  $b = -\frac{1}{4}$ ;  $j = 1$ ; and  $k = -1$ . Since  $k = p - 2$ , then Eq. (8) is Bessel's equation.

**B.2.3.1 Solution of Bessel's equation**

If an ordinary differential equation is reducible to the Bessel's equation, then the constants  $\alpha$ ,  $\beta$ , and  $n$  are defined by

$$\alpha = \frac{2 - p + j}{2} \tag{B.2-17}$$

$$\beta = \frac{1 - p}{2 - p + j} \tag{B.2-18}$$

$$n = \frac{\sqrt{(1 - p)^2 - 4b}}{2 - p + j} \tag{B.2-19}$$

The solution depends on whether the term  $a$  is positive or negative.

**Case (i)  $a > 0$**

In this case the solution is given by

$$y = x^{\alpha\beta} [C_1 J_n(\Omega x^\alpha) + C_2 J_{-n}(\Omega x^\alpha)] \quad n \neq \text{integer} \tag{B.2-20}$$

$$y = x^{\alpha\beta} [C_1 J_n(\Omega x^\alpha) + C_2 Y_n(\Omega x^\alpha)] \quad n = \text{integer} \tag{B.2-21}$$

where  $C_1$  and  $C_2$  are constants, and  $\Omega$  is defined by

$$\Omega = \frac{\sqrt{a}}{\alpha} \tag{B.2-22}$$

The term  $J_n(x)$  is known as the *Bessel function of the first kind of order  $n$*  and is given by

$$J_n(x) = \sum_{i=0}^{\infty} \frac{(-1)^i (x/2)^{2i+n}}{i! \Gamma(i + n + 1)} \tag{B.2-23}$$

$J_{-n}(x)$  is obtained by simply replacing  $n$  in Eq. (B.2-23) with  $-n$ . When  $n$  is not an integer, the functions  $J_n(x)$  and  $J_{-n}(x)$  are linearly independent solutions of Bessel's equation as given by Eq. (B.2-20). When  $n$  is an integer, however, these two functions are no longer linearly independent. In this case, the solution is given by Eq. (B.2-21) in which  $Y_n(x)$  is known as *Weber's Bessel function of the second kind of order  $n$*  and is given by

$$Y_n(x) = \frac{(\cos n\pi)J_n(x) - J_{-n}(x)}{\sin n\pi} \tag{B.2-24}$$

Case (ii)  $a < 0$

In this case the solution is given by

$$y = x^{\alpha\beta} [C_1 I_n(\Omega x^\alpha) + C_2 I_{-n}(\Omega x^\alpha)] \quad n \neq \text{integer} \quad (\text{B.2-25})$$

$$y = x^{\alpha\beta} [C_1 I_n(\Omega x^\alpha) + C_2 K_n(\Omega x^\alpha)] \quad n = \text{integer} \quad (\text{B.2-26})$$

where  $C_1$  and  $C_2$  are constants, and  $\Omega$  is defined by

$$\Omega = -i \frac{\sqrt{a}}{\alpha} \quad (\text{B.2-27})$$

The term  $I_n(x)$  is known as the *modified Bessel function of the first kind of order  $n$*  and is given by

$$I_n(x) = \sum_{i=0}^{\infty} \frac{(x/2)^{2i+n}}{i! \Gamma(i+n+1)} \quad (\text{B.2-28})$$

$I_{-n}(x)$  is obtained by simply replacing  $n$  in Eq. (B.2-28) with  $-n$ . When  $n$  is not an integer, the functions  $I_n(x)$  and  $I_{-n}(x)$  are linearly independent solutions of Bessel's equation as given by Eq. (B.2-25). However, when  $n$  is an integer, the functions  $I_n(x)$  and  $I_{-n}(x)$  are linearly dependent. In this case, the solution is given by Eq. (B.2-26) in which  $K_n(x)$  is known as the *modified Bessel function of the second kind of order  $n$*  and is given by

$$K_n(x) = \frac{\pi}{2} \frac{I_{-n}(x) - I_n(x)}{\sin n\pi} \quad (\text{B.2-29})$$

**Example B.7** Obtain the general solution of the following equations in terms of Bessel functions:

a)  $x \frac{d^2 y}{dx^2} - 3 \frac{dy}{dx} + xy = 0$

b)  $\frac{d^2 y}{dx^2} - x^2 y = 0$

**Solution**

a) Note that the integrating factor is  $x^{-3}$  and the equation can be rewritten as

$$\frac{d}{dx} \left( x^{-3} \frac{dy}{dx} \right) + x^{-3} y = 0 \quad (1)$$

Therefore,  $p = -3$ ;  $a = 1$ ;  $j = -3$ ;  $b = 0$ . Since  $b = 0$ , the equation is reducible to Bessel's equation. The terms  $\alpha$ ,  $\beta$ , and  $n$  are calculated from Eqs. (B.2-17)-(B.2-19) as

$$\begin{aligned} \alpha &= \frac{2-p+j}{2} \\ &= \frac{2+3-3}{2} = 1 \end{aligned} \quad (2)$$

$$\begin{aligned} \beta &= \frac{1-p}{2-p+j} \\ &= \frac{1+3}{2+3-3} = 2 \end{aligned} \tag{3}$$

$$\begin{aligned} n &= \frac{\sqrt{(1-p)^2 - 4b}}{2-p+j} \\ &= \frac{\sqrt{(1+3)^2 - (4)(0)}}{2+3-3} = 2 \end{aligned} \tag{4}$$

Note that  $a > 0$  and  $\Omega$  is calculated from Eq. (B.2-22) as

$$\begin{aligned} \Omega &= \frac{\sqrt{a}}{\alpha} \\ &= \frac{\sqrt{1}}{1} = 1 \end{aligned} \tag{5}$$

Since  $n$  is an integer, the solution is given in the form of Eq. (B.2-21)

$$y = x^2 [C_1 J_2(x) + C_2 Y_2(x)] \tag{6}$$

b) The equation can be rearranged in the form

$$\frac{d}{dx} \left( \frac{dy}{dx} \right) - x^2 y = 0 \tag{7}$$

Therefore,  $p = 0$ ;  $a = -1$ ;  $j = 2$ ;  $b = 0$ . Since  $b = 0$ , the equation is reducible to Bessel's equation. The terms  $\alpha$ ,  $\beta$ , and  $n$  are calculated from Eqs. (B.2-17)-(B.2-19) as

$$\begin{aligned} \alpha &= \frac{2-p+j}{2} \\ &= \frac{2-0+2}{2} = 2 \end{aligned} \tag{8}$$

$$\begin{aligned} \beta &= \frac{1-p}{2-p+j} \\ &= \frac{1-0}{2-0+2} = \frac{1}{4} \end{aligned} \tag{9}$$

$$\begin{aligned} n &= \frac{\sqrt{(1-p)^2 - 4b}}{2-p+j} \\ &= \frac{\sqrt{(1-0)^2 - (4)(0)}}{2-0+2} = \frac{1}{4} \end{aligned} \tag{10}$$

Note that  $a < 0$  and  $\Omega$  is calculated from Eq. (B.2-27) as

$$\begin{aligned}\Omega &= -i \frac{\sqrt{a}}{\alpha} \\ &= -i \frac{\sqrt{-1}}{2} = \frac{1}{2}\end{aligned}\quad (11)$$

Since  $n$  is not an integer, the solution is given in the form of Eq. (B.2-25)

$$y = \sqrt{x} [C_1 I_{1/4}(x^2/2) + C_2 I_{-1/4}(x^2/2)]$$

The properties of the Bessel functions are summarized in Table B.1.

### B.2.4 Numerical Solution of Initial Value Problems

Consider an initial value problem of the type

$$\frac{dy}{dt} = f(t, y) \quad (B.2-30)$$

$$y(0) = a = \text{given} \quad (B.2-31)$$

Among the various numerical methods available for the integration of Eq. (B.2-30), *fourth-order Runge-Kutta method* is the most frequently used one. It is expressed by the following algorithm:

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + k_4) + \frac{1}{3}(k_2 + k_3) \quad (B.2-32)$$

The terms  $k_1$ ,  $k_2$ ,  $k_3$ , and  $k_4$  in Eq. (B.2-32) are defined by

$$k_1 = h f(t_n, y_n) \quad (B.2-33)$$

$$k_2 = h f\left(t_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) \quad (B.2-34)$$

$$k_3 = h f\left(t_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2\right) \quad (B.2-35)$$

$$k_4 = h f(t_n + h, y_n + k_3) \quad (B.2-36)$$

in which  $h$  is the time step used in the numerical solution of the differential equation.

#### Example B.8 An irreversible chemical reaction



takes place in an isothermal batch reactor. The rate of reaction is given by

$$r = k c_A$$

**Table B.1** Properties of the Bessel functions.

**BEHAVIOR NEAR THE ORIGIN**

$$\begin{aligned}
 J_0(0) &= I_0(0) = 1 \\
 -Y_n(0) &= K_n(0) = \infty \quad \text{for all } n \\
 J_n(0) &= I_n(0) = 0 \quad \text{for } n > 0
 \end{aligned}$$

Note that if the origin is a point in the calculation field, then  $J_n(x)$  and  $I_n(x)$  are the only physically permissible solutions.

**BESSEL FUNCTIONS OF NEGATIVE ORDER**

$$\begin{aligned}
 J_{-n}(\lambda x) &= (-1)^n J_n(\lambda x) & Y_{-n}(\lambda x) &= (-1)^n Y_n(\lambda x) \\
 I_{-n}(\lambda x) &= I_n(\lambda x) & K_{-n}(\lambda x) &= K_n(\lambda x)
 \end{aligned}$$

**RECURRENCE FORMULAS**

$$\begin{aligned}
 J_n(\lambda x) &= \frac{\lambda x}{2n} [J_{n+1}(\lambda x) + J_{n-1}(\lambda x)] \\
 Y_n(\lambda x) &= \frac{\lambda x}{2n} [Y_{n+1}(\lambda x) + Y_{n-1}(\lambda x)] \\
 I_n(\lambda x) &= -\frac{\lambda x}{2n} [I_{n+1}(\lambda x) - I_{n-1}(\lambda x)] \\
 K_n(\lambda x) &= -\frac{\lambda x}{2n} [K_{n+1}(\lambda x) - K_{n-1}(\lambda x)]
 \end{aligned}$$

**INTEGRAL PROPERTIES**

$$\begin{aligned}
 \int \lambda x^n J_{n-1}(\lambda x) dx &= x^n J_n(\lambda x) & \int \lambda x^n Y_{n-1}(\lambda x) dx &= x^n Y_n(\lambda x) \\
 \int \lambda x^n I_{n-1}(\lambda x) dx &= x^n I_n(\lambda x) & \int \lambda x^n K_{n-1}(\lambda x) dx &= -x^n K_n(\lambda x)
 \end{aligned}$$

**DIFFERENTIAL RELATIONS**

$$\begin{aligned}
 \frac{d}{dx} J_n(\lambda x) &= \lambda J_{n-1}(\lambda x) - \frac{n}{x} J_n(\lambda x) = -\lambda J_{n+1}(\lambda x) + \frac{n}{x} J_n(\lambda x) \\
 \frac{d}{dx} Y_n(\lambda x) &= \lambda Y_{n-1}(\lambda x) - \frac{n}{x} Y_n(\lambda x) = -\lambda Y_{n+1}(\lambda x) + \frac{n}{x} Y_n(\lambda x) \\
 \frac{d}{dx} I_n(\lambda x) &= \lambda I_{n-1}(\lambda x) - \frac{n}{x} I_n(\lambda x) = \lambda I_{n+1}(\lambda x) + \frac{n}{x} I_n(\lambda x) \\
 \frac{d}{dx} K_n(\lambda x) &= -\lambda K_{n-1}(\lambda x) - \frac{n}{x} K_n(\lambda x) = -\lambda K_{n+1}(\lambda x) + \frac{n}{x} K_n(\lambda x)
 \end{aligned}$$

with a rate constant of  $k = 2 \text{ h}^{-1}$ . If the initial number of moles of species  $A$  is 1.5 mol, determine the variation in the number of moles of  $A$  during the first one hour of the reaction. Compare your results with the analytical solution.

### Solution

The inventory rate equation based on the moles of species  $A$  is

$$-(k c_A)V = \frac{dn_A}{dt} \quad (1)$$

or,

$$\frac{dn_A}{dt} = -k n_A \quad (2)$$

### Analytical solution

Equation (2) is a separable equation with the solution

$$n_A = n_{A_0} \exp(-kt) \quad (3)$$

in which  $n_{A_0}$  is the initial number of moles of species  $A$ .

### Numerical solution

In terms of the notation of the Runge-Kutta method, Eq. (2) is expressed as

$$\frac{dy}{dt} = -2y \quad (4)$$

with an initial condition of

$$y(0) = 1.5 \quad (5)$$

Therefore,

$$f(t, y) = -2y \quad (6)$$

$$y_0 = 1.5 \quad (7)$$

Integration of Eq. (4) from  $t = 0$  to  $t = 1$  by using fourth-order Runge-Kutta method with a time step of  $h = 0.1$  is given as follows:

#### Calculation of $y$ at $t = 0.1$ hour

First, it is necessary to determine  $k_1$ ,  $k_2$ ,  $k_3$ , and  $k_4$ :

$$\begin{aligned} k_1 &= h f(y_0) \\ &= (0.1)(-2)(1.5) = -0.3000 \end{aligned} \quad (8)$$

$$\begin{aligned} k_2 &= h f\left(y_0 + \frac{1}{2}k_1\right) \\ &= (0.1)(-2)\left(1.5 - \frac{0.3}{2}\right) = -0.2700 \end{aligned} \quad (9)$$

$$\begin{aligned}
 k_3 &= h f \left( y_0 + \frac{1}{2} k_2 \right) \\
 &= (0.1)(-2) \left( 1.5 - \frac{0.2700}{2} \right) = -0.2730
 \end{aligned} \tag{10}$$

$$\begin{aligned}
 k_4 &= h f(y_0 + k_3) \\
 &= (0.1)(-2)(1.5 - 0.2730) = -0.2454
 \end{aligned} \tag{11}$$

Substitution of these values into Eq. (B.2-32) gives the value of  $y$  at  $t = 0.1$  hour as

$$y_1 = 1.5 - \frac{1}{6}(0.3 + 0.2454) - \frac{1}{3}(0.2700 + 0.2730) = 1.2281 \tag{12}$$

### Calculation of $y$ at $t = 0.2$ hour

The constants  $k_1$ ,  $k_2$ ,  $k_3$ , and  $k_4$  are calculated as

$$\begin{aligned}
 k_1 &= h f(y_1) \\
 &= (0.1)(-2)(1.2281) = -0.2456
 \end{aligned} \tag{13}$$

$$\begin{aligned}
 k_2 &= h f \left( y_1 + \frac{1}{2} k_1 \right) \\
 &= (0.1)(-2) \left( 1.2281 - \frac{0.2456}{2} \right) = -0.2211
 \end{aligned} \tag{14}$$

$$\begin{aligned}
 k_3 &= h f \left( y_1 + \frac{1}{2} k_2 \right) \\
 &= (0.1)(-2) \left( 1.2281 - \frac{0.2211}{2} \right) = -0.2235
 \end{aligned} \tag{15}$$

$$\begin{aligned}
 k_4 &= h f(y_1 + k_3) \\
 &= (0.1)(-2)(1.2281 - 0.2235) = -0.2009
 \end{aligned} \tag{16}$$

Substitution of these values into Eq. (B.2-32) gives the value of  $y$  at  $t = 0.2$  hour as

$$y_2 = 1.2281 - \frac{1}{6}(0.2456 + 0.2009) - \frac{1}{3}(0.2211 + 0.2235) = 1.0055 \tag{17}$$

Repeated application of this procedure gives the value of  $y$  at every 0.1 hour. The results of such calculations are given in Table 1. The last column of Table 1 gives the analytical results obtained from Eq. (3). In this case, the numerical and analytical results are equal to each other. However, this is not always the case. The accuracy of the numerical results depends on the time step chosen for the calculations. For example, for a time step of  $h = 0.5$ , the numerical results are slightly different from the exact ones as shown in Table 2.

**Table 1** Comparison of numerical and exact values for  $h = 0.1$ .

$t$ (h)	$k_1$	$k_2$	$k_3$	$k_4$	$y$ (num.)	$y$ (exact)
0.1	-0.3000	-0.2700	-0.2730	-0.2454	1.2281	1.2281
0.2	-0.2456	-0.2211	-0.2235	-0.2009	1.0055	1.0055
0.3	-0.2011	-0.1810	-0.1830	-0.1645	0.8232	0.8232
0.4	-0.1646	-0.1482	-0.1498	-0.1347	0.6740	0.6740
0.5	-0.1348	-0.1213	-0.1227	-0.1103	0.5518	0.5518
0.6	-0.1104	-0.0993	-0.1004	-0.0903	0.4518	0.4518
0.7	-0.0904	-0.0813	-0.0822	-0.0739	0.3699	0.3699
0.8	-0.0740	-0.0666	-0.0673	-0.0605	0.3028	0.3028
0.9	-0.0606	-0.0545	-0.0551	-0.0495	0.2479	0.2479
1.0	-0.0496	-0.0446	-0.0451	-0.0406	0.2030	0.2030

**Table 2** Comparison of numerical and exact values for  $h = 0.5$ .

$t$ (h)	$k_1$	$k_2$	$k_3$	$k_4$	$y$ (num.)	$y$ (exact)
0.5	-1.5000	-0.7500	-1.1250	-0.3750	0.5625	0.5518
1.0	-0.5625	-0.2813	-0.4219	-0.1406	0.2109	0.2030

## B.2.5 Solution of Simultaneous Differential Equations

The solution procedure presented for a single ordinary differential equation can be easily extended to solve sets of simultaneous differential equations. For example, for the case of two simultaneous ordinary differential equations

$$\frac{dy}{dx} = f(t, y, z) \quad (\text{B.2-37})$$

$$\frac{dz}{dt} = g(t, y, z) \quad (\text{B.2-38})$$

the fourth-order Runge-Kutta solution algorithm is given by

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + k_4) + \frac{1}{3}(k_2 + k_3) \quad (\text{B.2-39})$$

and

$$z_{n+1} = z_n + \frac{1}{6}(\ell_1 + \ell_4) + \frac{1}{3}(\ell_2 + \ell_3) \quad (\text{B.2-40})$$

The terms  $k_1 \rightarrow k_4$  and  $\ell_1 \rightarrow \ell_4$  are defined by

$$k_1 = h f(t_n, y_n, z_n) \quad (\text{B.2-41})$$

$$\ell_1 = h g(t_n, y_n, z_n) \quad (\text{B.2-42})$$

$$k_2 = h f \left( t_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1, z_n + \frac{1}{2}\ell_1 \right) \quad (\text{B.2-43})$$

$$\ell_2 = h g \left( t_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1, z_n + \frac{1}{2}\ell_1 \right) \quad (\text{B.2-44})$$

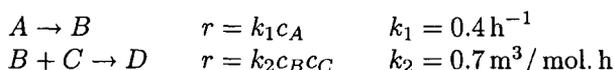
$$k_3 = h f \left( t_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2, z_n + \frac{1}{2}\ell_2 \right) \quad (\text{B.2-45})$$

$$\ell_3 = h g \left( t_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2, z_n + \frac{1}{2}\ell_2 \right) \quad (\text{B.2-46})$$

$$k_4 = h f(t_n + h, y_n + k_3, z_n + \ell_3) \quad (\text{B.2-47})$$

$$\ell_4 = h g(t_n + h, y_n + k_3, z_n + \ell_3) \quad (\text{B.2-48})$$

**Example B.9** The following liquid phase reactions are carried out in a batch reactor under isothermal conditions:



If the initial concentration of species A and C are  $1 \text{ mol/m}^3$ , determine the concentration of species D after 18 min. Compare your results with the analytical solution.

### Solution

The inventory rate expression for species A and D are given by

$$\frac{dc_A}{dt} = -k_1 c_A \quad (1)$$

$$\frac{dc_D}{dt} = k_2 c_B c_C \quad (2)$$

From the stoichiometry of the reactions, the concentrations of B and C are expressed in terms of A and D as

$$c_B = c_{A_0} - c_A - c_D \quad (3)$$

$$c_C = c_{C_0} - c_D \quad (4)$$

Substitution of Eqs. (3) and (4) into Eq. (2) yields

$$\frac{dc_D}{dt} = k_2 (c_{A_0} - c_A - c_D)(c_{C_0} - c_D) \quad (5)$$

### Analytical solution

Equation (1) is a separable equation with the solution

$$c_A = c_{A_0} \exp(-k_1 t) \quad (6)$$

in which  $c_{A_0}$  is the initial concentration of species A. Substitution of Eq. (6) into Eq. (5) gives

$$\frac{dc_D}{dt} = k_2 c_D^2 + k_2 (c_{A_0} e^{-k_1 t} - c_{A_0} - c_{C_0}) c_D + k_2 c_{A_0} c_{C_0} (1 - e^{-k_1 t}) \quad (7)$$

In terms of numerical values, Eq. (7) becomes

$$\frac{dc_D}{dt} = 0.7 c_D^2 + 0.7 (e^{-0.4t} - 2) c_D + 0.7 (1 - e^{-0.4t}) \quad (8)$$

The non-linear first-order differential equation

$$\frac{dy}{dx} = a(x) y^2 + b(x) y + c(x)$$

is called a Riccati equation. If  $y_1(x)$  is any known solution of the given equation, then the transformation

$$y = y_1(x) + \frac{1}{u}$$

leads to a linear equation in  $u$ . Equation (8) is in the form of a Riccati equation and note that  $c_D = 1$  is a solution. Therefore, the solution is

$$c_D = 1 - e^{-1.75\tau} \left( 1.75 \int_{\tau}^1 \frac{e^{-1.75\eta}}{\eta} d\eta + e^{-1.75} \right)^{-1} \quad (9)$$

where

$$\tau = e^{-0.4t} \quad (10)$$

When  $t = 0.3$  h, Eq. (9) gives  $c_D = 0.0112$  mol/m<sup>3</sup>.

### Numerical solution

In terms of the notation of the Runge-Kutta method, Eqs. (1) and (5) are expressed in the form

$$\frac{dy}{dt} = -0.4y \quad (11)$$

$$\frac{dz}{dt} = 0.7(1 - y - z)(1 - z) \quad (12)$$

with initial conditions of

$$y(0) = 1 \quad \text{and} \quad z(0) = 0 \quad (13)$$

Therefore,

$$f(t, y, z) = -0.4y \quad (14)$$

$$g(t, y, z) = 0.7(1 - y - z)(1 - z) \quad (15)$$

with the initial conditions

$$y_o = 1 \quad (16)$$

$$z_o = 0 \quad (17)$$

Choosing  $h = 0.05$ , the values of  $y_1$  and  $z_1$  are calculated as follows:

$$\begin{aligned} k_1 &= h f(y_o, z_o) \\ &= (0.05)(-0.4)(1) = -0.0200 \end{aligned} \quad (18)$$

$$\begin{aligned} \ell_1 &= h g(y_o, z_o) \\ &= (0.05)(0.7)(1 - 1 - 0)(1 - 0) = 0 \end{aligned} \quad (19)$$

$$\begin{aligned} k_2 &= h f\left(y_o + \frac{1}{2}k_1, z_o + \frac{1}{2}\ell_1\right) \\ &= (0.05)(-0.4)\left(1 - \frac{0.0200}{2}\right) = -0.0198 \end{aligned} \quad (20)$$

$$\begin{aligned} \ell_2 &= h g\left(y_o + \frac{1}{2}k_1, z_o + \frac{1}{2}\ell_1\right) \\ &= (0.05)(0.7)\left[1 - \left(1 - \frac{0.0200}{2}\right) - 0\right](1 - 0) = 3.5 \times 10^{-4} \end{aligned} \quad (21)$$

$$\begin{aligned} k_3 &= h f\left(y_o + \frac{1}{2}k_2, z_o + \frac{1}{2}\ell_2\right) \\ &= (0.05)(-0.4)\left(1 - \frac{0.0198}{2}\right) = -0.0198 \end{aligned} \quad (22)$$

$$\begin{aligned} \ell_3 &= h g\left(y_o + \frac{1}{2}k_2, z_o + \frac{1}{2}\ell_2\right) \\ &= (0.05)(0.7)\left[1 - \left(1 - \frac{0.0198}{2}\right) - \frac{3.5 \times 10^{-4}}{2}\right]\left(1 - \frac{3.5 \times 10^{-4}}{2}\right) \\ &= 3.4032 \times 10^{-4} \end{aligned} \quad (23)$$

$$\begin{aligned} k_4 &= h f(y_o + k_3, z_o + \ell_3) \\ &= (0.05)(-0.4)(1 - 0.0198) = -0.0196 \end{aligned} \quad (24)$$

$$\begin{aligned} \ell_4 &= h g(y_o + k_3, z_o + \ell_3) \\ &= (0.05)(0.7)\left[1 - (1 - 0.0198) - 3.4032 \times 10^{-4}\right](1 - 3.4032 \times 10^{-4}) \\ &= 6.8086 \times 10^{-4} \end{aligned} \quad (25)$$

Substitution of  $k_1 \rightarrow k_4$  and  $\ell_1 \rightarrow \ell_4$  into Eqs. (B.2-39) and (B.2-40), respectively, gives the values of  $y_1$  and  $z_1$  as

$$y_1 = 1 - \frac{1}{6}(0.0200 + 0.0196) - \frac{1}{3}(0.0198 + 0.0198) = 0.9802 \quad (26)$$

$$\begin{aligned} z_1 &= 0 + \frac{1}{6}(0 + 6.8086 \times 10^{-4}) + \frac{1}{3}(3.5 \times 10^{-4} + 3.4032 \times 10^{-4}) \\ &= 3.4358 \times 10^{-4} \end{aligned} \quad (27)$$

Repeated application of this procedure gives the values of  $y$  and  $z$  at every 0.05 h. The results are given in Tables 1 and 2.

**Table 1** Values of  $y$  as a function of time.

$t$ (h)	$k_1$	$k_2$	$k_3$	$k_4$	$y$
0.05	-0.0200	-0.0198	-0.0198	-0.0196	0.9802
0.10	-0.0196	-0.0194	-0.0194	-0.0192	0.9608
0.15	-0.0192	-0.0190	-0.0190	-0.0188	0.9418
0.20	-0.0188	-0.0186	-0.0186	-0.0185	0.9232
0.25	-0.0185	-0.0183	-0.0183	-0.0181	0.9049
0.30	-0.0181	-0.0179	-0.0179	-0.0177	0.8870

**Table 2** Values of  $z$  as a function of time.

$t$ (h)	$\ell_1$	$\ell_2$	$\ell_3$	$\ell_4$	$z$
0.05	0.0000	0.0004	0.0003	0.0007	0.0003
0.10	0.0007	0.0010	0.0010	0.0013	0.0013
0.15	0.0013	0.0016	0.0016	0.0019	0.0029
0.20	0.0019	0.0022	0.0022	0.0025	0.0051
0.25	0.0025	0.0028	0.0028	0.0030	0.0079
0.30	0.0030	0.0033	0.0033	0.0035	0.0112

## B.3 SECOND-ORDER PARTIAL DIFFERENTIAL EQUATIONS

### B.3.1 Classification of Partial Differential Equations

As a function of two independent variables,  $x$  and  $y$ , the most general form of a second-order linear partial differential equation has the form

$$\begin{aligned} A(x, y) \frac{\partial^2 u}{\partial x^2} + 2B(x, y) \frac{\partial^2 u}{\partial x \partial y} + C(x, y) \frac{\partial^2 u}{\partial y^2} + D(x, y) \frac{\partial u}{\partial x} \\ + E(x, y) \frac{\partial u}{\partial y} + F(x, y) u = G(x, y) \end{aligned} \quad (\text{B.3-1})$$

It is assumed that the coefficient functions and the given function  $G$  are real-valued and twice continuously differentiable on a region  $\mathbb{R}$  of the  $x, y$  plane.

When  $G = 0$ , the equation is *homogeneous*, otherwise the equation is *non-homogeneous*.

The criteria,  $B^2 - AC$ , that will indicate whether the second-order equation is a graph of a parabola, ellipse or hyperbola is called the discriminant,  $\Delta$ , i.e.,

$$\Delta = B^2 - AC \begin{cases} > 0 & \text{Hyperbolic} \\ = 0 & \text{Parabolic} \\ < 0 & \text{Elliptic} \end{cases}$$

### B.3.2 Orthogonal Functions

Let  $f(x)$  and  $g(x)$  be real-valued functions defined on the interval  $a \leq x \leq b$ . The *inner product* of  $f(x)$  and  $g(x)$  with respect to  $w(x)$  is defined by

$$\langle f, g \rangle = \int_a^b w(x) f(x) g(x) dx \quad (\text{B.3-2})$$

in which the *weight function*  $w(x)$  is considered positive on the interval  $(a, b)$ .

**Example B.10** Find the inner product of  $f(x) = x$  and  $g(x) = 1$  with respect to the weight function  $w(x) = x^{1/2}$  on the interval  $0 \leq x \leq 1$ .

#### Solution

Application of Eq. (B.3-2) gives the inner product as

$$\langle f, g \rangle = \int_0^1 \sqrt{x} x dx = \frac{2}{5} x^{5/2} \Big|_0^1 = \frac{2}{5}$$

The inner product has the following properties:

$$\langle f, g \rangle = \langle g, f \rangle \quad (\text{B.3-3})$$

$$\langle f, g + h \rangle = \langle f, g \rangle + \langle f, h \rangle \quad (\text{B.3-4})$$

$$\langle \alpha f, g \rangle = \alpha \langle f, g \rangle \quad \alpha \text{ is a scalar} \quad (\text{B.3-5})$$

The inner product of  $f$  with respect to itself is

$$\langle f, f \rangle = \int_a^b w(x) f^2(x) dx = \|f(x)\|^2 > 0 \quad (\text{B.3-6})$$

in which *norm* of  $f(x)$  is defined as

$$\|f(x)\| = \sqrt{\langle f, f \rangle} \quad (\text{B.3-7})$$

When  $\langle f, g \rangle = 0$  on  $(a, b)$ , then  $f(x)$  is *orthogonal* to  $g(x)$  with respect to the weight function  $w(x)$  on  $(a, b)$ , and when  $\langle f, f \rangle = 1$ , then  $f(x)$  is an *orthonormal* function. In the special case where  $w(x) = 1$  for  $a \leq x \leq b$ ,  $f(x)$  and  $g(x)$  are said to be *simply orthogonal*.

A sequence of functions  $\{f_n\}_{n=0}^{\infty}$  is an *orthogonal set* of functions if

$$\langle f_n, f_m \rangle = 0 \quad n \neq m \quad (\text{B.3-8})$$

The orthogonal set is a linearly independent set. If

$$\langle f_n, f_m \rangle = \begin{cases} 0 & \text{if } n \neq m \\ 1 & \text{if } n = m \end{cases} \quad (\text{B.3-9})$$

such a set is called an *orthonormal set*. Note that an orthonormal set can be obtained from an orthogonal set by dividing each function by its norm on the interval under consideration.

**Example B.11** Let  $\phi_n(x) = \sin(n\pi x)$  for  $n = 1, 2, 3, \dots$  and for  $0 < x < 1$ . Show that the sequence  $\{\phi_n\}_{n=1}^{\infty}$  is simply orthogonal on  $(0, 1)$ . Find the norms of the functions  $\phi_n$ .

### Solution

The inner product is

$$\langle \phi_n, \phi_m \rangle = \int_0^1 \sin(n\pi x) \sin(m\pi x) dx \quad (1)$$

The use of the identity

$$\sin A \sin B = \frac{1}{2} [\cos(A - B) - \cos(A + B)] \quad (2)$$

reduces Eq. (1) to the form

$$\begin{aligned} \langle \phi_n, \phi_m \rangle &= \frac{1}{2} \int_0^1 \{\cos[(n - m)\pi x] - \cos[(n + m)\pi x]\} dx \\ &= \frac{1}{2} \left\{ \frac{\sin[(n - m)\pi x]}{(n - m)\pi} - \frac{\sin[(n + m)\pi x]}{(n + m)\pi} \right\}_0^1 = 0 \end{aligned} \quad (3)$$

On the other hand,

$$\begin{aligned} \langle \phi_n, \phi_n \rangle &= \int_0^1 \sin^2(n\pi x) dx \\ &= \frac{1}{2} \int_0^1 [(1 - \cos(2n\pi x))] dx = \frac{1}{2} \left[ x - \frac{\sin(2n\pi x)}{2n\pi} \right]_0^1 = \frac{1}{2} \end{aligned} \quad (4)$$

Therefore, the norm is

$$\|\phi_n\| = \sqrt{\langle \phi_n, \phi_n \rangle} = \frac{1}{\sqrt{2}} \quad (5)$$

Hence, the corresponding orthonormal set is  $\{\sqrt{2}\sin(n\pi x)\}_{n=1}^{\infty}$ .

### B.3.3 Self-Adjoint Problems

Consider a second-order ordinary differential equation of the form

$$a_o(x) \frac{d^2y}{dx^2} + a_1(x) \frac{dy}{dx} + a_2(x) y = 0 \quad (\text{B.3-10})$$

Multiplication of Eq. (B.3-10) by  $p(x)/a_o(x)$  in which  $p(x)$  is the integrating factor defined by

$$p(x) = \exp \left( \int_0^x \frac{a_1(u)}{a_o(u)} du \right) \quad (\text{B.3-11})$$

gives

$$\frac{d^2y}{dx^2} + \frac{a_1(x)}{a_o(x)} p(x) \frac{dy}{dx} + \frac{a_2(x)}{a_o(x)} p(x) y = 0 \quad (\text{B.3-12})$$

Equation (B.3-12) can be rewritten as

$$p(x) \frac{d^2y}{dx^2} + \frac{dp(x)}{dx} \frac{dy}{dx} + q(x) y = 0 \quad (\text{B.3-13})$$

where

$$q(x) = \frac{a_2(x)}{a_o(x)} p(x) \quad (\text{B.3-14})$$

Rearrangement of Eq. (B.3-13) yields

$$\frac{d}{dx} \left[ p(x) \frac{dy}{dx} \right] + q(x) y = 0 \quad (\text{B.3-15})$$

A second-order differential equation in this form is said to be in *self-adjoint form*.

**Example B.12** Write the following differential equation in self-adjoint form:

$$x^2 \frac{d^2y}{dx^2} - x \frac{dy}{dx} + (x - 3)y = 0$$

**Solution**

Dividing the given equation by  $x^2$  gives

$$\frac{d^2y}{dx^2} - \frac{1}{x} \frac{dy}{dx} + \left( \frac{1}{x} - \frac{3}{x^2} \right) y = 0 \quad (1)$$

Note that

$$p(x) = \exp \left( - \int_0^x \frac{du}{u} \right) = \frac{1}{x} \quad (2)$$

Multiplication of Eq. (1) by  $p(x)$  gives

$$\frac{1}{x} \frac{d^2y}{dx^2} - \frac{1}{x^2} \frac{dy}{dx} + \left( \frac{1}{x^2} - \frac{3}{x^3} \right) y = 0 \quad (3)$$

Note that Eq. (3) can be rearranged as

$$\frac{d}{dx} \left( \frac{1}{x} \frac{dy}{dx} \right) + \left( \frac{1}{x^2} - \frac{3}{x^3} \right) y = 0 \quad (4)$$

### B.3.4 The Sturm-Liouville Problem

The linear, homogeneous, second-order equation

$$\frac{1}{w(x)} \frac{d}{dx} \left[ p(x) \frac{dy}{dx} \right] + q(x)y = -\lambda y \quad (\text{B.3-16})$$

on some interval  $a \leq x \leq b$  satisfying boundary conditions of the form

$$\alpha_1 y(a) + \alpha_2 \left. \frac{dy}{dx} \right|_{x=a} = 0 \quad (\text{B.3-17})$$

$$\beta_1 y(b) + \beta_2 \left. \frac{dy}{dx} \right|_{x=b} = 0 \quad (\text{B.3-18})$$

where  $\alpha_1, \alpha_2, \beta_1, \beta_2$  are given constants;  $p(x), q(x), w(x)$  are given functions which are differentiable and  $\lambda$  is an unspecified parameter independent of  $x$ , is called the *Sturm-Liouville equation*.

The values of  $\lambda$  for which the problem given by Eqs. (B.3-16)-(B.3-18) has a nontrivial solution, i.e., a solution other than  $y = 0$ , are called the *eigenvalues*. The corresponding solutions are the *eigenfunctions*.

Eigenfunctions corresponding to different eigenvalues are orthogonal with respect to the weight function  $w(x)$ . All the eigenvalues are positive. In particular,  $\lambda = 0$  is not an eigenvalue.

**Example B.13** Solve

$$\frac{d^2 y}{dx^2} + \lambda y = 0$$

subject to the boundary conditions

$$\text{at } x = 0 \quad y = 0$$

$$\text{at } x = \pi \quad y = 0$$

**Solution**

The equation can be rewritten in the form

$$\frac{d}{dx} \left( \frac{dy}{dx} \right) = -\lambda y \quad (1)$$

Comparison of Eq. (1) with Eq. (B.3-16) indicates that this is a Sturm-Liouville problem with  $p(x) = 1$ ,  $q(x) = 0$  and  $w(x) = 1$ .

The solution of Eq. (1) is

$$y = A \sin(\sqrt{\lambda} x) + B \cos(\sqrt{\lambda} x) \quad (2)$$

Application of the boundary condition at  $x = 0$  implies that  $B = 0$ . On the other hand, the use of the boundary condition at  $x = \pi$  gives

$$A \sin(\sqrt{\lambda} \pi) = 0 \tag{3}$$

In order to have a nontrivial solution

$$\sin(\sqrt{\lambda} \pi) = 0 \quad \Rightarrow \quad \sqrt{\lambda} \pi = n\pi \quad n = 1, 2, 3, \dots \tag{4}$$

or,

$$\sqrt{\lambda} = n \quad \Rightarrow \quad \lambda_n = n^2 \quad n = 1, 2, 3, \dots \tag{5}$$

Equation (5) represents the eigenvalues of the problem. The corresponding eigenfunctions are

$$y_n = A_n \sin(nx) \quad n = 1, 2, 3, \dots \tag{6}$$

where  $A_n$  is an arbitrary non-zero constant.

Since the eigenfunctions are orthogonal to each other with respect to the weight function  $w(x)$ , it is possible to write

$$\int_0^\pi \overline{\sin(nx)} \sin(mx) dx = 0 \quad n \neq m \tag{7}$$

### B.3.4.1 The method of Stodola and Vianello

The method of Stodola and Vianello (Bird *et al.*, 1987; Hildebrand, 1976) is an iterative procedure which makes use of successive approximation to estimate  $\lambda$  value in the following differential equation

$$\frac{d}{dx} \left[ p(x) \frac{dy}{dx} \right] = -\lambda w(x) y \tag{B.3-19}$$

with appropriate homogeneous boundary conditions at  $x = a$  and  $x = b$ .

The procedure is as follows:

1. Assume a trial function for  $y_1(x)$  which satisfies the boundary conditions  $x = a$  and  $x = b$ .
2. On the right side of Eq. (B.3-19), replace  $y(x)$  by  $y_1(x)$ .
3. Solve the resulting differential equation and express the solution in the form

$$y(x) = \lambda f_1(x) \tag{B.3-20}$$

4. Repeat step (2) with a second trial function  $y_2(x)$  defined by

$$y_2(x) = f_1(x) \tag{B.3-21}$$

5. Solve the resulting differential equation and express the solution in the form

$$y(x) = \lambda f_2(x) \quad (\text{B.3-22})$$

6. Continue the process as long as desired. The  $n^{\text{th}}$  approximation to the smallest permissible value of  $\lambda$  is given by

$$\lambda_1^n = \frac{\int_a^b w(x) f_n(x) y_n(x) dx}{\int_a^b w(x) [f_n(x)]^2 dx} \quad (\text{B.3-23})$$

### B.3.5 Fourier Series

Let  $f(x)$  be an arbitrary function defined on  $a \leq x \leq b$  and let  $\{\phi_n\}_{n=1}^{\infty}$  be an orthogonal set of functions over the same interval with weight function  $w(x)$ . Let us assume that  $f(x)$  can be represented by an infinite series of the form

$$f(x) = \sum_{n=1}^{\infty} C_n \phi_n(x) \quad (\text{B.3-24})$$

The series  $\sum C_n \phi_n(x)$  is called the *Fourier series* of  $f(x)$ , and the coefficients  $C_n$  are called the *Fourier coefficients* of  $f(x)$  with respect to the orthogonal functions  $\phi_n(x)$ .

To determine the Fourier coefficients, multiply both sides of Eq. (B.3-24) by  $w(x)\phi_m(x)$  and integrate from  $x = a$  to  $x = b$ ,

$$\int_a^b f(x) w(x) \phi_m(x) dx = \sum_{n=1}^{\infty} C_n \int_a^b \phi_n(x) \phi_m(x) w(x) dx \quad (\text{B.3-25})$$

Because of the orthogonality, all the integrals on the right-side of Eq. (B.3-25) are zero except when  $n = m$ . Therefore, the summation drops and Eq. (B.3-25) takes the form

$$\int_a^b f(x) w(x) \phi_n(x) dx = C_n \int_a^b \phi_n^2(x) w(x) dx \quad (\text{B.3-26})$$

or,

$$C_n = \frac{\langle f, \phi_n \rangle}{\|\phi_n\|^2} \quad (\text{B.3-27})$$

**Example B.14** Let  $f(x) = x$  for  $0 \leq x \leq \pi$ . Find the Fourier series of  $f(x)$  with respect to the simply orthogonal set  $\{\sin(nx)\}_{n=1}^{\infty}$ .

**Solution**

The function  $f(x) = x$  is represented in the form of a Fourier series

$$x = \sum_{n=1}^{\infty} C_n \sin(nx) \quad (1)$$

The Fourier coefficients can be calculated from Eq. (B.3-27) as

$$C_n = \frac{\int_0^{\pi} x \sin(nx) dx}{\int_0^{\pi} \sin^2(nx) dx} = -2 \frac{\cos(n\pi)}{n} \quad (2)$$

Since

$$\cos(n\pi) = (-1)^n \quad (3)$$

the coefficients  $C_n$  become

$$C_n = -2 \frac{(-1)^n}{n} = 2 \frac{(-1)^{n+1}}{n} \quad (4)$$

Substitution of Eq. (4) into Eq. (1) yields

$$x = 2 \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin(nx) \quad (5)$$

**B.3.6 Solution of Partial Differential Equations**

Various analytical methods are available to solve partial differential equations. In the determination of the method to be used, the structure of the equation is not the only factor that should be taken into consideration as in the case for ordinary differential equations. The boundary conditions are almost as important as the equation itself.

**B.3.6.1 The method of separation of variables**

The method of separation of variables requires the partial differential equation to be homogeneous and the boundary conditions be defined over a limited interval, i.e., semi-infinite and infinite domains do not permit the use of the separation of variables method. Besides, boundary conditions must be homogeneous in at least one dimension.

Let us apply the method of separation of variables to an unsteady-state heat transfer problem. Consider a slab which is initially at temperature  $T_0$ . At time  $t = 0$ , both surfaces are suddenly subjected to a constant temperature  $T_1$  with

$T_1 > T_o$ . The governing differential equation together with the initial and boundary conditions are

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (\text{B.3-28})$$

$$\text{at } t = 0 \quad T = T_o \quad \text{for all } x \quad (\text{B.3-29})$$

$$\text{at } x = 0 \quad T = T_1 \quad t > 0 \quad (\text{B.3-30})$$

$$\text{at } x = L \quad T = T_1 \quad t > 0 \quad (\text{B.3-31})$$

Note that the differential equation is linear and homogeneous. On the other hand, the boundary conditions, although linear, are not homogeneous. The boundary conditions in the  $x$ -direction become homogeneous by introducing the dimensionless quantities

$$\theta = \frac{T_1 - T}{T_1 - T_o} \quad (\text{B.3-32})$$

$$\xi = \frac{z}{L} \quad (\text{B.3-33})$$

$$\tau = \frac{\alpha t}{L^2} \quad (\text{B.3-34})$$

In dimensionless form, Eqs. (B.3-28)-(B.3-31) become

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} \quad (\text{B.3-35})$$

$$\text{at } \tau = 0 \quad \theta = 1 \quad (\text{B.3-36})$$

$$\text{at } \xi = 0 \quad \theta = 0 \quad (\text{B.3-37})$$

$$\text{at } \xi = 1 \quad \theta = 0 \quad (\text{B.3-38})$$

The separation of variables method assumes that the solution can be represented as a product of two functions of the form

$$\theta(\tau, \xi) = F(\tau) G(\xi) \quad (\text{B.3-39})$$

Substitution of Eq. (B.3-39) into Eq. (B.3-35) and rearrangement gives

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2 G}{d\xi^2} \quad (\text{B.3-40})$$

While the left side of Eq. (B.3-40) is a function of  $\tau$  only, the right side is dependent only on  $\xi$ . This is possible only if both sides of Eq. (B.3-40) are equal to a constant, say  $-\lambda^2$ , i.e.,

$$\frac{1}{F} \frac{dF}{d\tau} = \frac{1}{G} \frac{d^2 G}{d\xi^2} = -\lambda^2 \quad (\text{B.3-41})$$

The choice of a negative constant is due to the fact that the solution will decay to zero as time increases. The choice of a positive constant would give a solution that becomes infinite as time increases.

Note that Eq. (B.3-41) results in two ordinary differential equations. The equation for  $F$  is given by

$$\frac{dF}{d\tau} + \lambda^2 F = 0 \tag{B.3-42}$$

The solution of Eq. (B.3-42) is

$$F(\tau) = e^{-\lambda^2 \tau} \tag{B.3-43}$$

On the other hand, the equation for  $G$  is

$$\frac{d^2 G}{d\xi^2} + \lambda^2 G = 0 \tag{B.3-44}$$

subject to the boundary conditions

$$\text{at } \xi = 0 \quad G = 0 \tag{B.3-45}$$

$$\text{at } \xi = 1 \quad G = 0 \tag{B.3-46}$$

Note that Eq. (B.3-44) is a Sturm-Liouville equation with a weight function of unity. The solution of Eq. (B.3-44) is

$$G(\xi) = A \sin(\lambda \xi) + B \cos(\lambda \xi) \tag{B.3-47}$$

where  $A$  and  $B$  are constants. The use of the boundary condition defined by Eq. (B.3-45) implies  $B = 0$ . Application of the boundary condition defined by Eq. (B.3-46) gives

$$A \sin \lambda = 0 \tag{B.3-48}$$

For a nontrivial solution, the eigenvalues are given by

$$\sin \lambda = 0 \quad \Rightarrow \quad \lambda_n = n\pi \quad n = 1, 2, 3, \dots \tag{B.3-49}$$

The corresponding eigenfunctions are

$$G_n(\xi) = \sin(n\pi \xi) \tag{B.3-50}$$

Note that each of the product functions

$$\theta_n(\tau, \xi) = e^{-n^2 \pi^2 \tau} \sin(n\pi \xi) \quad n = 1, 2, 3, \dots \tag{B.3-51}$$

is a solution of Eq. (B.3-35) and satisfies the initial and boundary conditions, Eqs. (B.3-36)-(B.3-38).

If  $\theta_1$  and  $\theta_2$  are the solutions satisfying the linear and homogeneous partial differential equation and the boundary conditions, then the linear combination of

the solutions, i.e.,  $C_1\theta_1 + C_2\theta_2$ , also satisfies the partial differential equation and the boundary conditions. Therefore, the complete solution is

$$\theta = \sum_{n=1}^{\infty} C_n e^{-n^2\pi^2\tau} \sin(n\pi\xi) \quad (\text{B.3-52})$$

The unknown coefficients  $C_n$  can be determined by using the initial condition. The use of Eq. (B.3-36) results in

$$1 = \sum_{n=1}^{\infty} C_n \sin(n\pi\xi) \quad (\text{B.3-53})$$

Since the eigenfunctions are simply orthogonal, multiplication of Eq. (B.3-53) by  $\sin(m\pi\xi)$  and integration from  $\xi = 0$  to  $\xi = 1$  gives

$$\int_0^1 \sin(m\pi\xi) d\xi = \sum_{n=1}^{\infty} C_n \int_0^1 \sin(n\pi\xi) \sin(m\pi\xi) d\xi \quad (\text{B.3-54})$$

Note that the integral on the right side of Eq. (B.3-54) is zero when  $m \neq n$  and nonzero when  $m = n$ . Therefore, when  $m = n$  the summation drops out and Eq. (B.3-54) reduces to the form

$$\int_0^1 \sin(n\pi\xi) d\xi = C_n \int_0^1 \sin^2(n\pi\xi) d\xi \quad (\text{B.3-55})$$

Evaluation of the integrals show that

$$C_n = \frac{2}{\pi n} [1 - (-1)^n] \quad (\text{B.3-56})$$

The coefficients  $C_n$  take the following values depending on the value of  $n$ :

$$C_n = \begin{cases} 0 & n = 2, 4, 6, \dots \\ \frac{4}{\pi n} & n = 1, 3, 5, \dots \end{cases} \quad (\text{B.3-57})$$

Therefore, the solution becomes

$$\theta = \frac{4}{\pi} \sum_{n=1,3,5}^{\infty} e^{-n^2\pi^2\tau} \frac{\sin(n\pi\xi)}{n} \quad (\text{B.3-58})$$

Replacing  $n$  by  $2k + 1$  gives

$$\theta = \frac{4}{\pi} \sum_{k=0}^{\infty} e^{-(2k+1)^2\pi^2\tau} \frac{\sin[(2k+1)\pi\xi]}{2k+1} \quad (\text{B.3-59})$$

**B.3.6.2 Similarity solution**

This is also known as the *method of combination of variables*. Similarity solutions are a special class of solutions used to solve parabolic second-order partial differential equations when there is no geometric length scale in the problem, i.e., the domain must be either semi-infinite or infinite. Besides, the initial condition should match the boundary condition at infinity.

The basis of this method is to combine the two independent variables in a single variable so as to transform the second-order partial differential equation into an ordinary differential equation.

Let us consider the following parabolic second-order partial differential equation together with the initial and boundary conditions:

$$\frac{\partial v_z}{\partial t} = \nu \frac{\partial^2 v_z}{\partial x^2} \tag{B.3-60}$$

$$\text{at } t \leq 0 \quad v_z = 0 \quad \text{for all } x \tag{B.3-61}$$

$$\text{at } x = 0 \quad v_z = V \quad \text{for } t > 0 \tag{B.3-62}$$

$$\text{at } x = \infty \quad v_z = 0 \quad \text{for } t > 0 \tag{B.3-63}$$

Such a problem represents the velocity profile in a fluid adjacent to a wall suddenly set in motion and is also known as *Stokes' first problem*.

The solution is sought in the form

$$\frac{v_z}{V} = f(\eta) \tag{B.3-64}$$

where

$$\eta = \beta t^m x^n \tag{B.3-65}$$

The term  $\eta$  is called the *similarity variable*. The proportionality constant  $\beta$  is included in Eq. (B.3-65) so as to make  $\eta$  dimensionless.

The chain rule of differentiation gives

$$\begin{aligned} \frac{\partial(v_z/V)}{\partial t} &= \frac{df}{d\eta} \frac{\partial\eta}{\partial t} \\ &= \beta m t^{m-1} x^n \frac{df}{d\eta} \end{aligned} \tag{B.3-66}$$

$$\begin{aligned} \frac{\partial^2(v_z/V)}{\partial x^2} &= \frac{d^2 f}{d\eta^2} \left( \frac{\partial\eta}{\partial x} \right)^2 + \frac{df}{d\eta} \frac{\partial^2\eta}{\partial x^2} \\ &= \beta^2 n^2 t^{2m} x^{2(n-1)} \frac{d^2 f}{d\eta^2} + \beta n(n-1)t^m x^{n-2} \frac{df}{d\eta} \end{aligned} \tag{B.3-67}$$

Substitution of Eqs. (B.3-66) and (B.3-67) into Eq. (B.3-60) gives

$$\left( \frac{\nu\beta n^2 t^{m+1}}{m x^{2-n}} \right) \frac{d^2 f}{d\eta^2} + \left[ \frac{\nu n(n-1)t}{m x^2} - 1 \right] \frac{df}{d\eta} = 0 \tag{B.3-68}$$

or,

$$\left[ \left( \frac{\nu n^2 \eta}{m} \right) t x^{-2} \right] \frac{d^2 f}{d\eta^2} + \left\{ \left[ \frac{\nu n(n-1)}{m} \right] t x^{-2} - 1 \right\} \frac{df}{d\eta} = 0 \quad (\text{B.3-69})$$

It should be kept in mind that the purpose of introducing the similarity variable is to reduce the order of the partial differential equation by one. Therefore, the coefficients of  $d^2 f/d\eta^2$  and  $df/d\eta$  in Eq. (B.3-69) must depend only on  $\eta$ . This can be achieved if

$$t x^{-2} \propto t^m x^n \quad (\text{B.3-70})$$

which implies that

$$n = -2m \quad (\text{B.3-71})$$

If  $n = 1$ , then  $m = -1/2$  and the similarity variable defined by Eq. (B.3-65) becomes

$$\eta = \beta \frac{x}{\sqrt{t}} \quad (\text{B.3-72})$$

Note that  $x/\sqrt{t}$  has the units of  $\text{m/s}^{1/2}$ . Since the kinematic viscosity,  $\nu$ , has the units of  $\text{m}^2/\text{s}$ ,  $\eta$  becomes dimensionless if  $\beta = 1/\sqrt{\nu}$ . It is also convenient to introduce a factor 2 in the denominator so that the similarity variable takes the form

$$\beta = \frac{x}{2\sqrt{\nu t}} \quad (\text{B.3-73})$$

Hence, Eq. (B.3-69) becomes

$$\frac{d^2 f}{d\eta^2} + 2\eta \frac{df}{d\eta} = 0 \quad (\text{B.3-74})$$

The boundary conditions associated with Eq. (B.3-74) are

$$\text{at } \eta = 0 \quad f = 1 \quad (\text{B.3-75})$$

$$\text{at } \eta = \infty \quad f = 0 \quad (\text{B.3-76})$$

The integrating factor for Eq. (B.3-74) is  $\exp(\eta^2)$ . Multiplication of Eq. (B.3-74) by the integrating factor yields<sup>2</sup>

$$\frac{d}{d\eta} \left( e^{\eta^2} \frac{df}{d\eta} \right) = 0 \quad (\text{B.3-77})$$

which implies that

$$\frac{df}{d\eta} = C_1 e^{-\eta^2} \quad (\text{B.3-78})$$

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<sup>2</sup>The advantage of including the term 2 in the denominator of the similarity variable can be seen here. Without it, the result would have been

$$\frac{d}{d\eta} \left( e^{\eta^2/2} \frac{df}{d\eta} \right) = 0$$

Integration of Eq. (B.3-78) gives

$$f = C_1 \int_0^\eta e^{-u^2} du + C_2 \quad (\text{B.3-79})$$

where  $u$  is a dummy variable of integration. Application of the boundary condition defined by Eq. (B.3-75) gives  $C_2 = 1$ . On the other hand, the use of the boundary condition defined by Eq. (B.3-76) gives

$$C_1 = - \frac{1}{\int_0^\infty e^{-u^2} du} = - \frac{2}{\sqrt{\pi}} \quad (\text{B.3-80})$$

Therefore, the solution becomes

$$f = 1 - \frac{2}{\sqrt{\pi}} \int_0^\eta e^{-u^2} du = 1 - \text{erf}(\eta) \quad (\text{B.3-81})$$

where  $\text{erf}(x)$  is the *error function* defined by

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du \quad (\text{B.3-82})$$

Finally, the velocity distribution as a function of  $t$  and  $x$  is given by

$$\frac{v_z}{V} = 1 - \text{erf} \left( \frac{x}{2\sqrt{\nu t}} \right) \quad (\text{B.3-83})$$

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## Appendix C

# Flux Expressions for Mass, Momentum, and Energy

**Table C.1** Components of the stress tensor for Newtonian fluids in rectangular coordinates.

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$$\tau_{xx} = -\mu \left[ 2 \frac{\partial v_x}{\partial x} - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{A})$$

$$\tau_{yy} = -\mu \left[ 2 \frac{\partial v_y}{\partial y} - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{B})$$

$$\tau_{zz} = -\mu \left[ 2 \frac{\partial v_z}{\partial z} - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{C})$$

$$\tau_{xy} = \tau_{yx} = -\mu \left( \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) \quad (\text{D})$$

$$\tau_{yz} = \tau_{zy} = -\mu \left( \frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right) \quad (\text{E})$$

$$\tau_{zx} = \tau_{xz} = -\mu \left( \frac{\partial v_z}{\partial x} + \frac{\partial v_x}{\partial z} \right) \quad (\text{F})$$

$$(\nabla \cdot \mathbf{v}) = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \quad (\text{G})$$

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**Table C.2** Components of the stress tensor for Newtonian fluids in cylindrical coordinates.

---


$$\tau_{rr} = -\mu \left[ 2 \frac{\partial v_r}{\partial r} - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{A})$$

$$\tau_{\theta\theta} = -\mu \left[ 2 \left( \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right) - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{B})$$

$$\tau_{zz} = -\mu \left[ 2 \frac{\partial v_z}{\partial z} - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{C})$$

$$\tau_{r\theta} = \tau_{\theta r} = -\mu \left[ r \frac{\partial}{\partial r} \left( \frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} \right] \quad (\text{D})$$

$$\tau_{\theta z} = \tau_{z\theta} = -\mu \left( \frac{\partial v_\theta}{\partial z} + \frac{1}{r} \frac{\partial v_z}{\partial \theta} \right) \quad (\text{E})$$

$$\tau_{zr} = \tau_{rz} = -\mu \left( \frac{\partial v_z}{\partial r} + \frac{\partial v_r}{\partial z} \right) \quad (\text{F})$$

$$(\nabla \cdot \mathbf{v}) = \frac{1}{r} \frac{\partial}{\partial r} (r v_r) + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z} \quad (\text{G})$$


---

**Table C.3** Components of the stress tensor for Newtonian fluids in spherical coordinates.

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$$\tau_{rr} = -\mu \left[ 2 \frac{\partial v_r}{\partial r} - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{A})$$

$$\tau_{\theta\theta} = -\mu \left[ 2 \left( \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right) - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{B})$$

$$\tau_{\phi\phi} = -\mu \left[ 2 \left( \frac{1}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} + \frac{v_r}{r} + \frac{v_\theta \cot \theta}{r} \right) - \frac{2}{3} (\nabla \cdot \mathbf{v}) \right] \quad (\text{C})$$

$$\tau_{r\theta} = \tau_{\theta r} = -\mu \left[ r \frac{\partial}{\partial r} \left( \frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} \right] \quad (\text{D})$$

$$\tau_{\theta\phi} = \tau_{\phi\theta} = -\mu \left[ \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left( \frac{v_\phi}{\sin \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} \right] \quad (\text{E})$$

$$\tau_{\phi r} = \tau_{r\phi} = -\mu \left[ \frac{1}{r \sin \theta} \frac{\partial v_r}{\partial \phi} + r \frac{\partial}{\partial r} \left( \frac{v_\phi}{r} \right) \right] \quad (\text{F})$$

$$(\nabla \cdot \mathbf{v}) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (v_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} \quad (\text{G})$$


---

**Table C.4** Flux expressions for energy transport in rectangular coordinates.

Total Flux	Molecular Flux	Convective Flux	Constraint
$e_x$	$q_x = -k \frac{\partial T}{\partial x}$	$(\rho \hat{C}_P T) v_x$	None
	$q_x = -\alpha \frac{\partial(\rho \hat{C}_P T)}{\partial x}$		$\rho \hat{C}_P = \text{constant}$
$e_y$	$q_y = -k \frac{\partial T}{\partial y}$	$(\rho \hat{C}_P T) v_y$	None
	$q_y = -\alpha \frac{\partial(\rho \hat{C}_P T)}{\partial y}$		$\rho \hat{C}_P = \text{constant}$
$e_z$	$q_z = -k \frac{\partial T}{\partial z}$	$(\rho \hat{C}_P T) v_z$	None
	$q_z = -\alpha \frac{\partial(\rho \hat{C}_P T)}{\partial z}$		$\rho \hat{C}_P = \text{constant}$

**Table C.5** Flux expressions for energy transport in cylindrical coordinates.

Total Flux	Molecular Flux	Convective Flux	Constraint
$e_r$	$q_r = -k \frac{\partial T}{\partial r}$	$(\rho \hat{C}_P T) v_r$	None
	$q_r = -\alpha \frac{\partial(\rho \hat{C}_P T)}{\partial r}$		$\rho \hat{C}_P = \text{constant}$
$e_\theta$	$q_\theta = -\frac{k}{r} \frac{\partial T}{\partial \theta}$	$(\rho \hat{C}_P T) v_\theta$	None
	$q_\theta = -\frac{\alpha}{r} \frac{\partial(\rho \hat{C}_P T)}{\partial \theta}$		$\rho \hat{C}_P = \text{constant}$
$e_z$	$q_z = -k \frac{\partial T}{\partial z}$	$(\rho \hat{C}_P T) v_z$	None
	$q_z = -\alpha \frac{\partial(\rho \hat{C}_P T)}{\partial z}$		$\rho \hat{C}_P = \text{constant}$

**Table C.6** Flux expressions for energy transport in spherical coordinates.

Total Flux	Molecular Flux	Convective Flux	Constraint
$e_r$	$q_r = -k \frac{\partial T}{\partial r}$	$(\rho \hat{C}_P T) v_r$	None
	$q_r = -\alpha \frac{\partial(\rho \hat{C}_P T)}{\partial r}$		$\rho \hat{C}_P = \text{constant}$
$e_\theta$	$q_\theta = -\frac{k}{r} \frac{\partial T}{\partial \theta}$	$(\rho \hat{C}_P T) v_\theta$	None
	$q_\theta = -\frac{\alpha}{r} \frac{\partial(\rho \hat{C}_P T)}{\partial \theta}$		$\rho \hat{C}_P = \text{constant}$
$e_\phi$	$q_\phi = -\frac{k}{r \sin \theta} \frac{\partial T}{\partial \phi}$	$(\rho \hat{C}_P T) v_\phi$	None
	$q_\phi = -\frac{\alpha}{r \sin \theta} \frac{\partial(\rho \hat{C}_P T)}{\partial \phi}$		$\rho \hat{C}_P = \text{constant}$

Table C.7 Flux expressions for mass transport in rectangular coordinates.

Total Flux	Molecular Flux	Convective Flux	Constraint
$W_{A_x}$	$j_{A_x} = -\rho D_{AB} \frac{\partial \omega_A}{\partial x}$	$\rho_A v_x$	None
	$j_{A_x} = -D_{AB} \frac{\partial \rho_A}{\partial x}$		$\rho = \text{constant}$
$W_{A_y}$	$j_{A_y} = -\rho D_{AB} \frac{\partial \omega_A}{\partial y}$	$\rho_A v_y$	None
	$j_{A_y} = -D_{AB} \frac{\partial \rho_A}{\partial y}$		$\rho = \text{constant}$
$W_{A_z}$	$j_{A_z} = -\rho D_{AB} \frac{\partial \omega_A}{\partial z}$	$\rho_A v_z$	None
	$j_{A_z} = -D_{AB} \frac{\partial \rho_A}{\partial z}$		$\rho = \text{constant}$
$N_{A_x}$	$J_{A_x}^* = -c D_{AB} \frac{\partial x_A}{\partial x}$	$c_A v_x^*$	None
	$J_{A_x}^* = -D_{AB} \frac{\partial c_A}{\partial x}$		$c = \text{constant}$
$N_{A_y}$	$J_{A_y}^* = -c D_{AB} \frac{\partial x_A}{\partial y}$	$c_A v_y^*$	None
	$J_{A_y}^* = -D_{AB} \frac{\partial c_A}{\partial y}$		$c = \text{constant}$
$N_{A_z}$	$J_{A_z}^* = -c D_{AB} \frac{\partial x_A}{\partial z}$	$c_A v_z^*$	None
	$J_{A_z}^* = -D_{AB} \frac{\partial c_A}{\partial z}$		$c = \text{constant}$

**Table C.8** Flux expressions for mass transport in cylindrical coordinates.

Total Flux	Molecular Flux	Convective Flux	Constraint
$W_{A_r}$	$j_{A_r} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial r}$	$\rho_A v_r$	None
	$j_{A_r} = -\mathcal{D}_{AB} \frac{\partial \rho_A}{\partial r}$		$\rho = \text{constant}$
$W_{A_\theta}$	$j_{A_\theta} = -\frac{\rho \mathcal{D}_{AB}}{r} \frac{\partial \omega_A}{\partial \theta}$	$\rho_A v_\theta$	None
	$j_{A_\theta} = -\frac{\mathcal{D}_{AB}}{r} \frac{\partial \rho_A}{\partial \theta}$		$\rho = \text{constant}$
$W_{A_z}$	$j_{A_z} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial z}$	$\rho_A v_z$	None
	$j_{A_z} = -\mathcal{D}_{AB} \frac{\partial \rho_A}{\partial z}$		$\rho = \text{constant}$
$N_{A_r}$	$J_{A_r}^* = -c \mathcal{D}_{AB} \frac{\partial x_A}{\partial r}$	$c_A v_r^*$	None
	$J_{A_r}^* = -\mathcal{D}_{AB} \frac{\partial c_A}{\partial r}$		$c = \text{constant}$
$N_{A_\theta}$	$J_{A_\theta}^* = -\frac{c \mathcal{D}_{AB}}{r} \frac{\partial x_A}{\partial \theta}$	$c_A v_\theta^*$	None
	$J_{A_\theta}^* = -\frac{\mathcal{D}_{AB}}{r} \frac{\partial c_A}{\partial \theta}$		$c = \text{constant}$
$N_{A_z}$	$J_{A_z}^* = -c \mathcal{D}_{AB} \frac{\partial x_A}{\partial z}$	$c_A v_z^*$	None
	$J_{A_z}^* = -\mathcal{D}_{AB} \frac{\partial c_A}{\partial z}$		$c = \text{constant}$

Table C.9 Flux expressions for mass transport in spherical coordinates.

Total Flux	Molecular Flux	Convective Flux	Constraint
$W_{A_r}$	$j_{A_r} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial r}$	$\rho_A v_r$	None
	$j_{A_r} = -\mathcal{D}_{AB} \frac{\partial \rho_A}{\partial r}$		$\rho = \text{constant}$
$W_{A_\theta}$	$j_{A_\theta} = -\frac{\rho \mathcal{D}_{AB}}{r} \frac{\partial \omega_A}{\partial \theta}$	$\rho_A v_\theta$	None
	$j_{A_\theta} = -\frac{\mathcal{D}_{AB}}{r} \frac{\partial \rho_A}{\partial \theta}$		$\rho = \text{constant}$
$W_{A_\phi}$	$j_{A_\phi} = -\frac{\rho \mathcal{D}_{AB}}{r \sin \theta} \frac{\partial \omega_A}{\partial \phi}$	$\rho_A v_\phi$	None
	$j_{A_\phi} = -\frac{\mathcal{D}_{AB}}{r \sin \theta} \frac{\partial \rho_A}{\partial \phi}$		$\rho = \text{constant}$
$N_{A_r}$	$J_{A_r}^* = -c \mathcal{D}_{AB} \frac{\partial x_A}{\partial r}$	$c_A v_r^*$	None
	$J_{A_r}^* = -\mathcal{D}_{AB} \frac{\partial c_A}{\partial r}$		$c = \text{constant}$
$N_{A_\theta}$	$J_{A_\theta}^* = -\frac{c \mathcal{D}_{AB}}{r} \frac{\partial x_A}{\partial \theta}$	$c_A v_\theta^*$	None
	$J_{A_\theta}^* = -\frac{\mathcal{D}_{AB}}{r} \frac{\partial c_A}{\partial \theta}$		$c = \text{constant}$
$N_{A_\phi}$	$J_{A_\phi}^* = -\frac{c \mathcal{D}_{AB}}{r \sin \theta} \frac{\partial x_A}{\partial \phi}$	$c_A v_\phi^*$	None
	$J_{A_\phi}^* = -\frac{\mathcal{D}_{AB}}{r \sin \theta} \frac{\partial c_A}{\partial \phi}$		$c = \text{constant}$

# Appendix D

## Physical Properties

This appendix contains physical properties of some frequently encountered materials in the transport of momentum, energy and mass. The reader should refer to either Perry's Chemical Engineers' Handbook (1997) or CRC Handbook of Chemistry and Physics (2001) for a more extensive list of physical properties.

Table D.1 contains viscosities of gases and liquids, as taken from Reid *et al.* (1977). Table D.2 contains thermal conductivities of gases, liquids and solids. While gas and liquid thermal conductivities are compiled from Reid *et al.* (1977), solid thermal conductivity values are taken from Perry's Chemical Engineers' Handbook (1997). The values of the diffusion coefficients given in Table D.3 are compiled from Reid *et al.* (1977), Perry's Chemical Engineers' Handbook (1997) and Geankoplis (1972).

Table D.4 contains the physical properties of dry air at standard atmospheric pressure. The values are taken from Kays and Crawford (1980) who obtained the data from the three volumes of Touloukian *et al.* (1970). The physical properties of saturated liquid water, given in Table D.5, are taken from Incropera and DeWitt (1996) who adapted the data from Liley (1984).

A widely used vapor pressure correlation over limited temperature ranges is the *Antoine equation* expressed in the form

$$\ln P^{sat} = A - \frac{B}{T + C}$$

where  $P^{sat}$  is in mmHg and  $T$  is in degrees Kelvin. The Antoine constants  $A$ ,  $B$  and  $C$ , given in Table D.6 for various substances, are taken from Reid *et al.* (1977).

**Table D.1** Viscosities of various substances.

Substance	$T$ K	$\mu \times 10^4$ kg/ m. s
<b>Gases</b>		
Ammonia	273	0.9
	373	1.31
Carbon dioxide	303	1.51
	373.5	1.81
Ethanol	383	1.11
	423	1.23
Sulfur dioxide	313	1.35
	373	1.63
<b>Liquids</b>		
Benzene	313	4.92
	353	3.18
Carbon tetrachloride	303	8.56
	343	5.34
Ethanol	313	8.26
	348	4.65

**Table D.2** Thermal conductivities of various substances.

Substance	$T$ K	$k$ W/m. K
<b>Gases</b>		
Ammonia	273	0.0221
	373	0.0320
Carbon dioxide	300	0.0167
	473	0.0283
Ethanol	293	0.0150
	375	0.0222
Sulfur dioxide	273	0.0083
<b>Liquids</b>		
Benzene	293	0.148
	323	0.137
Carbon tetrachloride	293	0.103
Ethanol	293	0.165
	313	0.152
<b>Solids</b>		
Aluminum	300	273
Brick	300	0.72
Copper	300	398
Glass Fiber	300	0.036
Steel	300	45

**Table D.3** Experimental values of binary diffusion coefficients at 101.325 kPa.

Substance	$T$ K	$D_{AB}$ $\text{m}^2/\text{s}$
<b>Gases</b>		
Air - CO <sub>2</sub>	317.2	$1.77 \times 10^{-5}$
Air - Ethanol	313	$1.45 \times 10^{-5}$
Air - Naphthalene	300	$0.62 \times 10^{-5}$
Air - H <sub>2</sub> O	313	$2.88 \times 10^{-5}$
H <sub>2</sub> - Acetone	296	$4.24 \times 10^{-5}$
N <sub>2</sub> - SO <sub>2</sub>	263	$1.04 \times 10^{-5}$
<b>Liquids</b>		
NH <sub>3</sub> - H <sub>2</sub> O	288	$1.77 \times 10^{-9}$
Benzoic acid - H <sub>2</sub> O	298	$1.21 \times 10^{-9}$
CO <sub>2</sub> - H <sub>2</sub> O	298	$1.92 \times 10^{-9}$
Ethanol - H <sub>2</sub> O	283	$0.84 \times 10^{-9}$
<b>Solids</b>		
Bi - Pb	293	$1.1 \times 10^{-20}$
H <sub>2</sub> - Nickel	358	$1.16 \times 10^{-12}$
O <sub>2</sub> - Vulc. Rubber	298	$0.21 \times 10^{-9}$

Table D.4 Properties of air at  $P = 101.325$  kPa.

$T$ K	$\rho$ kg/m <sup>3</sup>	$\mu \times 10^6$ kg/m.s	$\nu \times 10^6$ m <sup>2</sup> /s	$\hat{C}_P$ kJ/kg.K	$k \times 10^3$ W/m.K	Pr
100	3.5985	7.060	1.962	1.028	9.220	0.787
150	2.3673	10.38	4.385	1.011	13.75	0.763
200	1.7690	13.36	7.552	1.006	18.10	0.743
250	1.4119	16.06	11.37	1.003	22.26	0.724
263	1.3421	16.70	12.44	1.003	23.28	0.720
273	1.2930	17.20	13.30	1.004	24.07	0.717
275	1.2836	17.30	13.48	1.004	24.26	0.716
280	1.2607	17.54	13.92	1.004	24.63	0.715
283	1.2473	17.69	14.18	1.004	24.86	0.714
285	1.2385	17.79	14.36	1.004	25.00	0.714
288	1.2256	17.93	14.63	1.004	25.22	0.714
290	1.2172	18.03	14.81	1.004	25.37	0.714
293	1.2047	18.17	15.08	1.004	25.63	0.712
295	1.1966	18.27	15.27	1.005	25.74	0.713
298	1.1845	18.41	15.54	1.005	25.96	0.712
300	1.1766	18.53	15.75	1.005	26.14	0.711
303	1.1650	18.64	16.00	1.005	26.37	0.710
305	1.1573	18.74	16.19	1.005	26.48	0.711
308	1.1460	18.88	16.47	1.005	26.70	0.711
310	1.1386	18.97	16.66	1.005	26.85	0.710
313	1.1277	19.11	16.95	1.005	27.09	0.709
315	1.1206	19.20	17.14	1.006	27.22	0.709
320	1.1031	19.43	17.62	1.006	27.58	0.709
323	1.0928	19.57	17.91	1.006	27.80	0.708
325	1.0861	19.66	18.10	1.006	27.95	0.708
330	1.0696	19.89	18.59	1.006	28.32	0.707
333	1.0600	20.02	18.89	1.007	28.51	0.707
343	1.0291	20.47	19.89	1.008	29.21	0.706
350	1.0085	20.81	20.63	1.008	29.70	0.706
353	1.0000	20.91	20.91	1.008	29.89	0.705
363	0.9724	21.34	21.95	1.009	30.58	0.704
373	0.9463	21.77	23.01	1.010	31.26	0.703
400	0.8825	22.94	26.00	1.013	33.05	0.703
450	0.7844	24.93	31.78	1.020	36.33	0.700
500	0.7060	26.82	37.99	1.029	39.51	0.699
550	0.6418	28.60	44.56	1.039	42.60	0.698
600	0.5883	30.30	51.50	1.051	45.60	0.699
650	0.5431	31.93	58.80	1.063	48.40	0.701
700	0.5043	33.49	66.41	1.075	51.30	0.702

Table D.5 Properties of saturated liquid water.

$T$	$P^{sat}$	$\hat{V} \times 10^3$	$\hat{\lambda}$	$\hat{C}_P$	$\mu \times 10^6$	$k \times 10^3$	Pr
273	0.00611	1.000	2502	4.217	1750	569	12.99
275	0.00697	1.000	2497	4.211	1652	574	12.22
280	0.00990	1.000	2485	4.198	1422	582	10.26
285	0.01387	1.000	2473	4.189	1225	590	8.70
288	0.01703	1.001	2466	4.186	1131	595	7.95
290	0.01917	1.001	2461	4.184	1080	598	7.56
293	0.02336	1.001	2454	4.182	1001	603	6.94
295	0.02617	1.002	2449	4.181	959	606	6.62
298	0.03165	1.003	2442	4.180	892	610	6.11
300	0.03531	1.003	2438	4.179	855	613	5.83
303	0.04240	1.004	2430	4.178	800	618	5.41
305	0.04712	1.005	2426	4.178	769	620	5.20
308	0.05620	1.006	2418	4.178	721	625	4.82
310	0.06221	1.007	2414	4.178	695	628	4.62
313	0.07373	1.008	2407	4.179	654	632	4.32
315	0.08132	1.009	2402	4.179	631	634	4.16
320	0.1053	1.011	2390	4.180	577	640	3.77
325	0.1351	1.013	2378	4.182	528	645	3.42
330	0.1719	1.016	2366	4.184	489	650	3.15
335	0.2167	1.018	2354	4.186	453	656	2.88
340	0.2713	1.021	2342	4.188	420	660	2.66
345	0.3372	1.024	2329	4.191	389	664	2.45
350	0.4163	1.027	2317	4.195	365	668	2.29
355	0.5100	1.030	2304	4.199	343	671	2.14
360	0.6209	1.034	2291	4.203	324	674	2.02
365	0.7514	1.038	2278	4.209	306	677	1.91
370	0.9040	1.041	2265	4.214	289	679	1.80
373	1.0133	1.044	2257	4.217	279	680	1.76
375	1.0815	1.045	2252	4.220	274	681	1.70
380	1.2869	1.049	2239	4.226	260	683	1.61
385	1.5233	1.053	2225	4.232	248	685	1.53
390	1.794	1.058	2212	4.239	237	686	1.47
400	2.455	1.067	2183	4.256	217	688	1.34

$T = \text{K}$ ;  $P^{sat} = \text{bar}$ ;  $\hat{V} = \text{m}^3/\text{kg}$ ;  $\hat{\lambda} = \text{kJ}/\text{kg}$ ;  $\hat{C}_P = \text{kJ}/\text{kg}\cdot\text{K}$ ;  
 $\mu = \text{kg}/\text{m}\cdot\text{s}$ ;  $k = \text{W}/\text{m}\cdot\text{K}$

**Table D.6** Antoine equation constants.

Substance	Range (K)	<i>A</i>	<i>B</i>	<i>C</i>
Acetone	241 – 350	16.6513	2940.46	– 35.93
Benzene	280 – 377	15.9008	2788.51	– 52.36
Benzoic acid	405 – 560	17.1634	4190.70	– 125.2
Chloroform	260 – 370	15.9732	2696.79	– 46.16
Ethanol	270 – 369	18.9119	3803.98	– 41.68
Methanol	257 – 364	18.5875	3626.55	– 34.29
Naphthalene	360 – 525	16.1426	3992.01	– 71.29

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# Appendix E

## Constants and Conversion Factors

### PHYSICAL CONSTANTS

Gas constant ( $\mathcal{R}$ )	$= 82.05 \text{ cm}^3 \cdot \text{atm}/\text{mol} \cdot \text{K}$ $= 0.08205 \text{ m}^3 \cdot \text{atm}/\text{kmol} \cdot \text{K}$ $= 1.987 \text{ cal}/\text{mol} \cdot \text{K}$ $= 8.314 \text{ J}/\text{mol} \cdot \text{K}$ $= 8.314 \times 10^{-3} \text{ kPa} \cdot \text{m}^3/\text{mol} \cdot \text{K}$ $= 8.314 \times 10^{-5} \text{ bar} \cdot \text{m}^3/\text{mol} \cdot \text{K}$ $= 8.314 \times 10^{-2} \text{ bar} \cdot \text{m}^3/\text{kmol} \cdot \text{K}$ $= 8.314 \times 10^{-6} \text{ MPa} \cdot \text{m}^3/\text{mol} \cdot \text{K}$
Acceleration of gravity ( $g$ )	$= 9.8067 \text{ m}/\text{s}^2$ $= 32.1740 \text{ ft}/\text{s}^2$
Stefan-Boltzmann constant ( $\sigma$ )	$= 5.67051 \times 10^{-8} \text{ W}/\text{m}^2 \cdot \text{K}^4$ $= 0.1713 \times 10^{-8} \text{ Btu}/\text{h} \cdot \text{ft}^2 \cdot \text{R}^4$

## CONVERSION FACTORS

Density	$1 \text{ kg/m}^3 = 10^{-3} \text{ g/cm}^3 = 10^{-3} \text{ kg/L}$ $1 \text{ kg/m}^3 = 0.06243 \text{ lb/ft}^3$
Diffusivity (Kinematic, Mass, Thermal)	$1 \text{ m}^2/\text{s} = 10^4 \text{ cm}^2/\text{s}$ $1 \text{ m}^2/\text{s} = 10.7639 \text{ ft}^2/\text{s} = 3.875 \times 10^4 \text{ ft}^2/\text{h}$
Energy, Heat, Work	$1 \text{ J} = 1 \text{ W} \cdot \text{s} = 1 \text{ N} \cdot \text{m} = 10^{-3} \text{ kJ}$ $1 \text{ cal} = 4.184 \text{ J}$ $1 \text{ kJ} = 2.7778 \times 10^{-4} \text{ kW} \cdot \text{h} = 0.94783 \text{ Btu}$
Heat capacity	$1 \text{ kJ/kg} \cdot \text{K} = 0.239 \text{ cal/g} \cdot \text{K}$ $1 \text{ kJ/kg} \cdot \text{K} = 0.239 \text{ Btu/lb} \cdot ^\circ\text{R}$
Force	$1 \text{ N} = 1 \text{ kg} \cdot \text{m}/\text{s}^2 = 10^5 \text{ g} \cdot \text{cm}/\text{s}^2 \text{ (dyne)}$ $1 \text{ N} = 0.2248 \text{ lbf} = 7.23275 \text{ lb} \cdot \text{ft}/\text{s}^2 \text{ (poundals)}$
Heat flux	$1 \text{ W}/\text{m}^2 = 1 \text{ J}/\text{s} \cdot \text{m}^2$ $1 \text{ W}/\text{m}^2 = 0.31709 \text{ Btu}/\text{h} \cdot \text{ft}^2$
Heat transfer coefficient	$1 \text{ W}/\text{m}^2 \cdot \text{K} = 1 \text{ J}/\text{s} \cdot \text{m}^2 \cdot \text{K}$ $1 \text{ W}/\text{m}^2 \cdot \text{K} = 2.39 \times 10^{-5} \text{ cal}/\text{s} \cdot \text{cm}^2 \cdot \text{K}$ $1 \text{ W}/\text{m}^2 \cdot \text{K} = 0.1761 \text{ Btu}/\text{h} \cdot \text{ft}^2 \cdot ^\circ\text{R}$
Length	$1 \text{ m} = 100 \text{ cm} = 10^6 \mu\text{m}$ $1 \text{ m} = 39.370 \text{ in} = 3.2808 \text{ ft}$
Mass	$1 \text{ kg} = 1000 \text{ g}$ $1 \text{ kg} = 2.2046 \text{ lb}$
Mass flow rate	$1 \text{ kg}/\text{s} = 2.2046 \text{ lb}/\text{s} = 7936.6 \text{ lb}/\text{h}$
Mass flux	$1 \text{ kg}/\text{s} \cdot \text{m}^2 = 0.2048 \text{ lb}/\text{s} \cdot \text{ft}^2 = 737.3 \text{ lb}/\text{h} \cdot \text{ft}^2$
Mass transfer coefficient	$1 \text{ m}/\text{s} = 3.2808 \text{ ft}/\text{s}$
Power	$1 \text{ W} = 1 \text{ J}/\text{s} = 10^{-3} \text{ kW}$ $1 \text{ kW} = 3412.2 \text{ Btu}/\text{h} = 1.341 \text{ hp}$
Pressure	$1 \text{ Pa} = 1 \text{ N}/\text{m}^2$ $1 \text{ kPa} = 10^3 \text{ Pa} = 10^{-3} \text{ MPa}$ $1 \text{ atm} = 101.325 \text{ kPa} = 1.01325 \text{ bar} = 760 \text{ mmHg}$ $1 \text{ atm} = 14.696 \text{ lbf}/\text{in}^2$
Temperature	$1 \text{ K} = 1.8 ^\circ\text{R}$ $T(^{\circ}\text{F}) = 1.8 T(^{\circ}\text{C}) + 32$

Thermal Conductivity	$1 \text{ W/m.K} = 1 \text{ J/s.m.K} = 2.39 \times 10^{-3} \text{ cal/s.cm.K}$ $1 \text{ W/m.K} = 0.5778 \text{ Btu/h.ft.}^\circ\text{F}$
Velocity	$1 \text{ m/s} = 3.60 \text{ km/h}$ $1 \text{ m/s} = 3.2808 \text{ ft/s} = 2.237 \text{ mi/h}$
Viscosity	$1 \text{ kg/m.s} = 1 \text{ Pa.s}$ $1 \text{ P (poise)} = 1 \text{ g/cm.s}$ $1 \text{ kg/m.s} = 10 \text{ P} = 10^3 \text{ cP}$ $1 \text{ P (poise)} = 241.9 \text{ lb/ft.h}$
Volume	$1 \text{ m}^3 = 1000 \text{ L}$ $1 \text{ m}^3 = 6.1022 \times 10^4 \text{ in}^3 = 35.313 \text{ ft}^3 = 264.17 \text{ gal}$
Volumetric flow rate	$1 \text{ m}^3/\text{s} = 1000 \text{ L/s}$ $1 \text{ m}^3/\text{s} = 35.313 \text{ ft}^3/\text{s} = 1.27127 \times 10^5 \text{ ft}^3/\text{h}$

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