(Rate of Input of φ) − (Rate of Output of φ) + (Rate of Generation of φ) = (Rate of Accumulation of φ)

MODELLING IN TRANSPORT PHENOMENA

A Conceptual Approach

İSMAİL TOSUN

ELSEVIER

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A Conceptual Approach

ISMAIL TOSUN
Professor of Chemical Engineering
Middle East Technical University
Ankara, Turkey

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To Ayşe

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 φ :

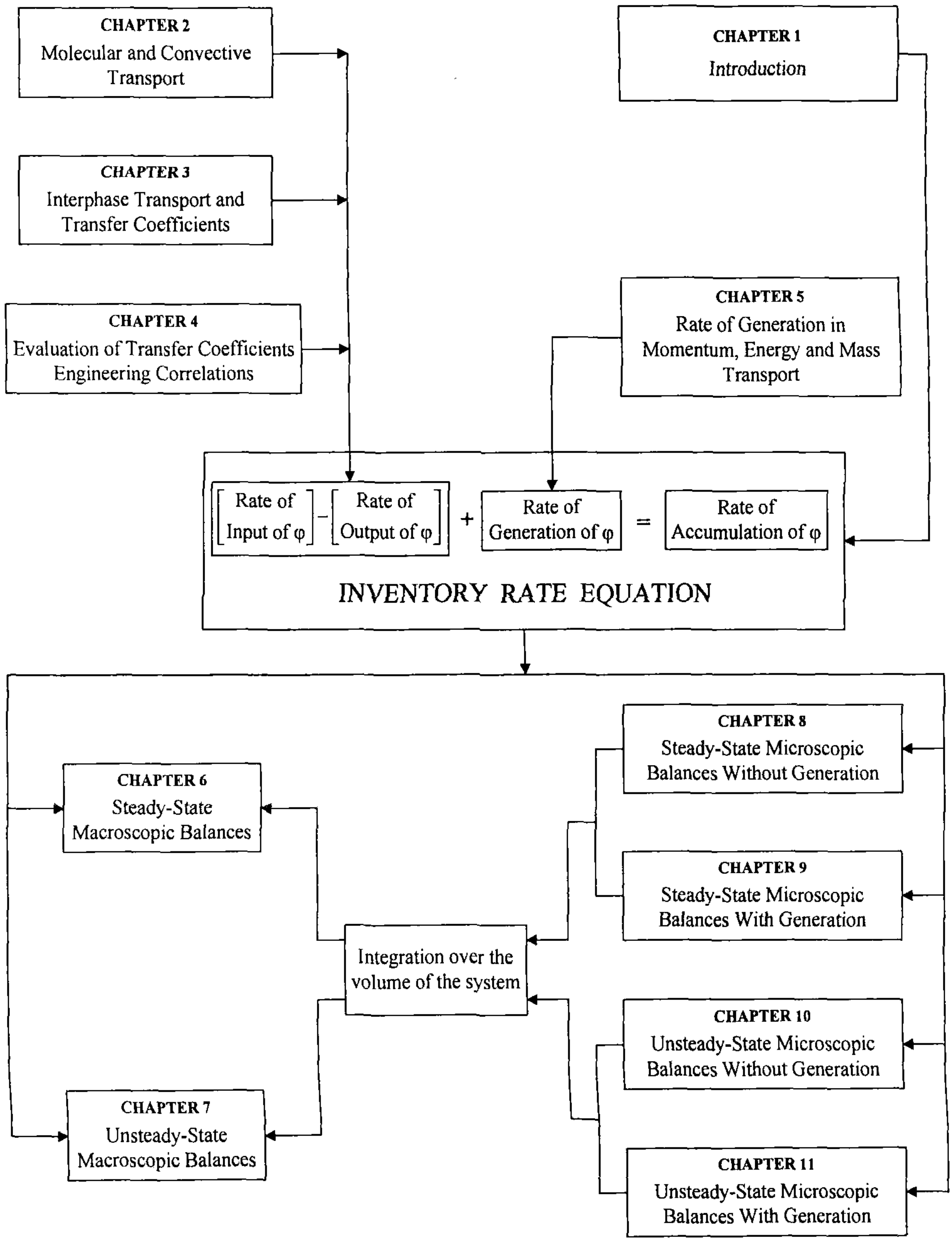
$$\begin{pmatrix} \text{Rate of} \\ \varphi \text{ in} \end{pmatrix} - \begin{pmatrix} \text{Rate of} \\ \varphi \text{ out} \end{pmatrix} + \begin{pmatrix} \text{Rate of } \varphi \\ \text{generation} \end{pmatrix} = \begin{pmatrix} \text{Rate of } \varphi \\ \text{accumulation} \end{pmatrix}$$

in which the term φ 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.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Evaluation of Transfer Coefficients Engineering Correlations
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Rate of Generation in Momentum, Energy and Mass Transport
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Rate of Accumulation of φ
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CHAPTER 8
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Integration over the volume of the system
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CHAPTER 7
Unsteady-State Macroscopic Balances
CHAPTER 11
Unsteady-State Microscopic Balances With Generation

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 Hiçşaşmaz 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

Contents

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 φ takes the form

$$\begin{pmatrix} \text{Rate of} \\ \text{input of } \varphi \end{pmatrix} - \begin{pmatrix} \text{Rate of} \\ \text{output of } \varphi \end{pmatrix} + \begin{pmatrix} \text{Rate of} \\ \text{generation of } \varphi \end{pmatrix} = \begin{pmatrix} \text{Rate of} \\ \text{accumulation of } \varphi \end{pmatrix} \qquad (1.1\text{-}1)$$

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[1]. 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

[1]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

$$\varphi = \varphi\,(t, x, y, z) \tag{1.2-1}$$

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

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 φ, then

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

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 φ is not a function of time, t. When an ordinary derivative is used, i.e., $d\varphi/dt = 0$, then this implies that φ is a constant. It is important to distinguish between partial and ordinary derivatives because the conclusions are very different.