Preface

This book is based on lectures regularly taught in the fourth and fifth year graduate courses in transport phenomena and chemical reactor modeling, and in a post-graduate course in modern reactor modeling at the Norwegian University of Science and Technology, Department of Chemical Engineering, Trondheim, Norway. The objective of the book is to present the fundamentals of the single-fluid and multi-fluid models for the analysis of single- and multiphase reactive flows in chemical reactors with a chemical reactor engineering rather than mathematical bias. Organized into 13 chapters, it combines theoretical aspects and practical applications and covers some of the recent research in several areas of chemical reactor engineering. This book contains a survey of the modern literature in the field of chemical reactor modeling.

This monograph consists of three parts printed in three volumes:

Part I: Single Phase Fundamentals.
Part II: Multiphase Fundamentals.
Part III: Applications.

In part I most of the fundamental theory of single phase reactive flows is presented. In part II most of the fundamental theory of multiphase reactive flows is presented. In both parts a few numerical model simulation application examples are given to elucidate the link between theory and applications. In part III the chemical reactor equipment to be modeled are described. Several engineering models are introduced and discussed. A survey of the frequently used numerical methods, algorithms, and schemes is provided. A few practical engineering applications of the modeling tools are presented and discussed. The working principles of several experimental techniques employed in order to get data for model validation are outlined.

I hope this book can serve as a guide for my future Ph.D. students, as well as other interested scientists, to get a thorough introduction to this field of research without spending too much of their invaluable time searching for and reading a large number of books and papers.

Comments on the contents of the book:
In Chap. 1, a survey of the elements of transport phenomena for single phase multi-component mixtures is given. This theory serves as basis for the

development of most chemical engineering models as well as the multiphase flow concepts to be presented in the following chapters. The first part of the chapter considers single phase Newtonian fluid flows for multi-component mixtures. In the second part of the chapter the governing equations are applied to turbulent flows.

Chapter 2 contains a summary of the basic concepts of kinetic theory of dilute and dense gases. This theory serves as basis for the development of the continuum scale conservation equations by averaging the governing equations determining the discrete molecular scale phenomena. This method is an alternative to, or rather both a verification and an extension of, the continuum approach described in Chap. 1. These kinetic theory concepts also determine the basis for a group of models used describing granular flows, further outlined in Chap. 4.

Chapter 3 contains a survey of a large number of books and journal papers dealing with the basic theory of multi-fluid flow modeling. Emphasis is placed on applying the multi-fluid model framework to describe reactive flows. In the more advanced textbooks the basic multi-component multiphase theory is introduced in a rather mathematical context, thus there is a need for a less demanding presentation easily accessible for chemical reaction engineering students.

Chapter 4 contains a summary of the basic theory of granular flow. These concepts have been adopted describing particulate flows in fluidized bed reactors. The theory was primarily used for dense bed reactors, but modified closures of this type have been employed for more dilute flows as well. Compared to the continuum theory presented in the previous chapter, the granular theory is considered more complex. The main purpose of introducing this theory, in the context of reactor modeling, is to improve the description of the particle (e.g., catalyst) transport and distribution in the reactor system.

In Chap. 5, an outline of the basic theory of the required closure laws and constitutive equations is provided. The first sections describe models for the interfacial transport phenomena occurring in multiphase reactive systems. An overview of the important models for the different forces acting on a single particle, bubble, or droplet is given. Model modifications due to swarm or cluster effects are discussed. In the following sections the standard theories for interfacial heat and mass transfer are examined. In the last section the literature controversy originating from the fact that with the present level of knowledge, there is no general mathematical theory available to determine whether the 3D multi-fluid model is *well posed* as an initial-boundary value problem, is examined.

In Chap. 6 the derivation of the classical reactor models is examined starting out from the microscopic heat and species mass balances. In chemical reactor engineering the idealized models like the plug flow reactor (PFR)—and continuous stirred tank reactor (CSTR) models are well known from basic courses in chemical reaction engineering. For non-ideal flows the dispersion models (DMs) are frequently used. These standard models are deduced from the local heat and species mass balances employing a cross-sectional area averaging procedure. Similar, but not identical, models can be obtained by simplifying the governing local transport equations. Two models for chemical reaction equilibrium calculations are examined.

In Chap. 7, a brief summary of the agitation and fluid mixing technology is given. The main emphasis is placed on examining the modern strategies used to model the momentum transfer from the impeller to the fluid. The methods are sketched and the basic equations are listed. A few model simulation examples are presented.

In Chap. 8, the basic bubble column constructions and the principles of operation of these reactors are described. The classical models for two- and three phase simple bubble column reactors are defined based on heat and species mass balances. The state of the art on fluid dynamic modeling of bubble column reactors is then summarized including a few simulations of reactive flows.

In Chap. 9, an outline of the basic theory of the population balance equation is provided. Three different modeling frameworks are defined, the macroscopic formulation, the local continuum, and the kinetic theory formulations. The macroscopic model is formulated directly on the macroscopic scales, enabling a suitable framework for practical engineering calculations. In this framework simple and inaccurate numerical approximations, quadrature rules and merged functions have become integrated parts of many such macroscopic closure laws. Since these numerical approximations are difficult to split from the physical parts of the closure laws and the fundamental functions can be hard to extract from the merged functions, the more popular macroscopic closures for bubble coalescence and breakage rates are also discussed in this chapter. The more rigorous local formulations are presented and future reactor analysis should preferably be based on these concepts, enabling more accurate closure laws to be formulated and more optimized solution methods to be used. The status on population balance modeling of bubble coalescence and breakage phenomena is summarized.

Chapter 10 contains a literature survey of the basic fluidized bed reactor designs, principles of operation, and modeling. The classical two- and three phase fluidized bed models for bubbling beds, risers, and circulating fluidized beds are defined based on heat and species mass balances.

In Chap. 11, an overview of the basic designs, principles of operation, and modeling of fixed packed bed reactors is presented. The basic theory is applied to describe the performance of particular chemical processes operated in fixed packed bed reactors.

In Chap. 12, a group of finite volume solution algorithms for solving the multi-fluid model equations is described. The basic single-phase finite volume method solution strategies, spatial discretization schemes, and ODE solution methods in time are examined. The selected multiphase algorithms are extended versions of the single-phase SIMPLE-like algorithms. However, alternative algorithms can be found in the literature. Some of these methods are briefly outlined in this chapter. Moreover, several numerical methods for solving the population balance equation for dispersed flows are outlined. Finally, several solution methods for the resulting algebraic discretization equations are mentioned.

In Chap. 13, a survey of several frequently used experimental techniques for characterization of dispersed multiphase flows is provided. The working principle

of these techniques are outlined. The application of these techniques to chemical reactor flows is critically examined.

The book may be used as a reference book of the multi-fluid theory, or for teaching purposes at different educational levels. For example, at the graduate level, an introductory graduate course in single phase transport phenomena can be based on Chap. 1 (and parts of Chap. 2). Suitable numerical solution methods for the governing single phase equations can be found in Chap. 12. An introduction to reactor modeling can be based on Chaps. 6–11. The material in Chaps. 2–5 the multiphase parts of Chap. 12 and Chap. 13 may be better suited at the postgraduate level. Taking these three courses in sequence, I hope the Ph.D. students get the necessary knowledge to give useful future contributions in this field of science.

I have received a great deal of help from numerous persons over the 30 years of association with this subject, in formulating and revising my views on both reactor modeling and chemical reactor engineering. I would like to acknowledge the inspiring discussions I have had with colleagues at NTNU during my work on this book. Moreover, I wish to thank the Ph.D. students who have taken my graduate subjects and thus read the lecture notes carefully and supplied me with constructive criticisms (among other comments) and suggestions for further improvements on the text. It is fair to mention that my students, especially Dr.-Ing. Lars Hagesæther, Prof. Dr.-Ing. Carlos A. Dorao, Dr.-Ing. Håvard Lindborg, Dr.-Ing. Hans Kristian Rusten, Dr.-Ing. Cecilie Gotaas Johnsen, Ph.D., Zhengjie Zhu, Ph.D. Luciano E. Patruno, Ph.D. Federico Sporleder, Ph.D. Kumar Ranjan Rout, Ph.D. Zhongxi Chao, and M.Sc. Jannike Solsvik, have contributed to this book in many ways. This includes technical contributions either in a direct or indirect way, and reading parts of the draft manuscript. Finally, I must thank B.Sc. Itishree Mohallick for drawing many of the figures in the book.

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