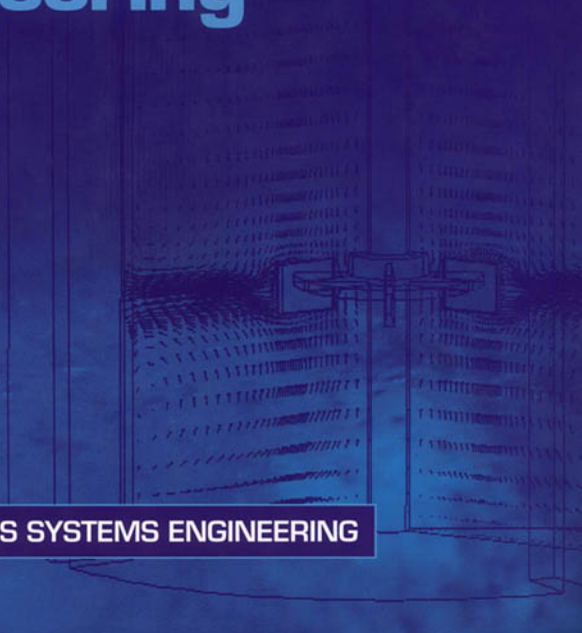
Vivek V. Ranade

Computational Flow Modeling for Chemical Reactor Engineering



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Computational Flow Modeling for Chemical Reactor Engineering
Vivek V Ranade

COMPUTATIONAL FLOW MODELING FOR CHEMICAL REACTOR ENGINEERING

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To Nanda & Vishakha

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PREFACE

Industrial Flow Modeling Group, *iFMg* at National Chemical Laboratory undertakes contract research and consultancy projects in the general area of reactor engineering. We use computational flow modeling to carry out these industrial projects. Computational flow modeling is a powerful tool for the design and analysis of industrial flow processes. Though it is routinely used as a design tool in aerospace engineering, chemical engineers have started exploiting the power of computational flow modeling only recently. Considering the central role played by reactors in chemical process industries, there is tremendous potential for applying computational flow-modeling tools to improve reactor engineering.

Through interactions with practicing engineers from industry, it has been realized that there is insufficient help available to harness state of the art computational flow modeling tools for complex, industrial reactor engineering applications. Many reactor engineers either consider that the flow complexities of industrial reactors are impossible to simulate, or expect miracles from off-the-shelf, commercial flow modeling tools. These two diverse views arise because of inadequate interactions between the flow modeling and industrial reactor engineering communities. It is essential to clearly understand the role of flow modeling in reactor engineering. It is necessary to relate the individual aspects of reactor engineering and computational flow modeling in a coherent and consistent way to realize the potential of computational flow modeling for reactor engineering research and practice. To assist practicing engineers in these aspects, workshops on 'computational flow modeling for chemical process industries' were started at the National Chemical Laboratory. The enthusiastic response to these workshops has encouraged me to write this book, which is an expanded and formalized presentation of workshop notes. I have tried to provide sufficient information to understand and to define the specific role of computational flow modeling for reactor engineering applications, to select appropriate tools and to apply these tools to link reactor hardware to reactor performance. The intended audience of the book is practicing chemical engineers working in industry as well as chemical engineering scientists and research students working in the area of reactor engineering. Some prior background in reactor engineering and numerical techniques is assumed.

The information in the book is organized to facilitate the central task of reactor engineer, that is, relating reactor hardware to reactor performance. Several steps to achieve such a task are discussed to clearly define the role of flow modeling in the overall reactor engineering activity. The necessity of using a hierarchy of modeling tools and establishing a clear relationship between the objectives of reactor engineering and the computational flow model is emphasized with the help of examples. The overall methodology of achieving the objectives of reactor engineering via computational flow modeling is discussed. Desirable characteristics and key issues in selecting appropriate computational fluid dynamics (CFD) codes are briefly discussed. A number of examples and case studies covering the four major reactor types used in chemical industries, namely, stirred reactors, bubble column reactors, fluidized bed reactors and fixed bed reactors are included. In view of the wide range of reactor types, however, it is impossible to cover all the reactor types and flows relevant to these reactor types. Emphasis on certain topics and the selection of examples is biased and is directly related to my own research and consulting experience. Some topics, like radiative heat transfer, laminar reactive flows are completely omitted. I have, however, made an attempt to evolve general guidelines, which will be useful for solving practical reactor engineering problems. Some comments on future trends in computational flow modeling and its use by the chemical engineering community are also included.

The material included in this book may be used in several ways and at various stages of flow modeling projects. It may be used as a basic resource for making appropriate decisions about investment in the application of CFD to reactor engineering. It may be used as a study material for an in-house course to facilitate the appreciation and application of computational flow modeling for reactor engineering. It may be used as a companion book while solving practical reactor engineering problems. I hope that this book will encourage chemical engineers to exploit the potential of computational flow modeling and will eventually lead to better reactor engineering.

This book is essentially the outcome of my last fifteen years of association with this subject. I have received a great deal of help from numerous persons over these years in formulating and revising my views on both computational flow modeling and chemical reactor engineering. I am particularly indebted to my teacher and mentor, Professor J.B. Joshi, who has been one of the leading practitioners of process fluid dynamics for three decades. There are not adequate words to express his contributions to this book. I was fortunate to have an opportunity to work with Dr R.V. Chaudhari and Dr R.A. Mashelkar at the National Chemical Laboratory. Both of them always extended their full support and encouragement in my every endeavor. Without their support, it would not have been possible to develop our industrial flow modeling activity, on which this book is based. I would like to acknowledge the support provided by Professor H.E.A. van den Akker of Delft University of Technology and by

Professors G.F. Versteeg and J.A.M. Kuipers of University of Twente, The Netherlands. My brief stay at Professor van den Akker's laboratory at Delft introduced me to different commercial CFD solvers and expanded my horizons. The idea of this book was formalized during my second visit to The Netherlands at University of Twente. I would also like to thank Dr Bharatan Patel of Fluent Inc. and Mr Paresh Patel of Fluent India for their support.

I am grateful to my associates and collaborators with whom I worked on different industrial projects. In particular, I owe much to Professor J.R. Bourne, Mr Vaibhav Deshpande, Ms S.M.S. Dommeti and Mr Yatin Tayalia. My students, especially Kapil Girotra, Ashwin Sunthankar, Ranjit Utikar, Aravind Rammohan, Sachin Muthian, Avinash Khopkar, Prashant Gunjal, Vivek Buwa and Shishir Sable have contributed to this book in different ways. This includes technical contributions either in a direct or indirect way, helping me to collect the required information and reading the draft manuscript. My father, Mr V.B. Ranade also has painstakingly read the entire manuscript and suggested several ways to enhance the clarity of presentation. The manuscript was improved wherever their suggestions were incorporated. Any remaining errors or shortcomings are, needless to say, the responsibility of the author. Finally, I wish to thank my wife, Nanda, for her patience, understanding and enthusiastic support, which carried me through this long and arduous writing process.

Vivek V. Ranade
December 2000
Pune

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PART I
INTRODUCTION

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1 REACTOR ENGINEERING AND FLOW MODELING

All industrial chemical processes are designed to transform cheap raw materials to high value products (usually via chemical reactions). A 'reactor', in which such chemical transformations take place, has to carry out several functions such as bringing reactants into intimate contact (to allow chemical reactions to occur), providing an appropriate environment (temperature and concentration fields, catalysts) for an adequate time and allowing for the removal of products. Chemical reactor engineering includes all the activities necessary to evolve the best possible hardware and operating protocol of the reactor to carry out the desired transformation of raw materials (or reactants) to value added products. A reactor engineer has to ensure that the reactor hardware and operating protocol satisfy various process demands without compromising safety, the environment and economics. To realize this, the reactor engineer has to establish a relationship between reactor hardware and operating protocols and various performance issues (Fig. 1.1).

Successful reactor engineering requires expertise from various fields including thermodynamics, chemistry, catalysis, reaction engineering, fluid dynamics, mixing and heat and mass transfer. The reactor engineer has to interact with chemists to understand the basic chemistry and peculiarities of the catalyst. Based on such an understanding and proposed performance targets, the reactor engineer has to abstract the information relevant to identifying the characteristics of the desired fluid dynamics of the reactor. The reactor engineer then has to conceive suitable reactor hardware and operating protocols to realize this desired fluid dynamics in practice. Thus, fluid

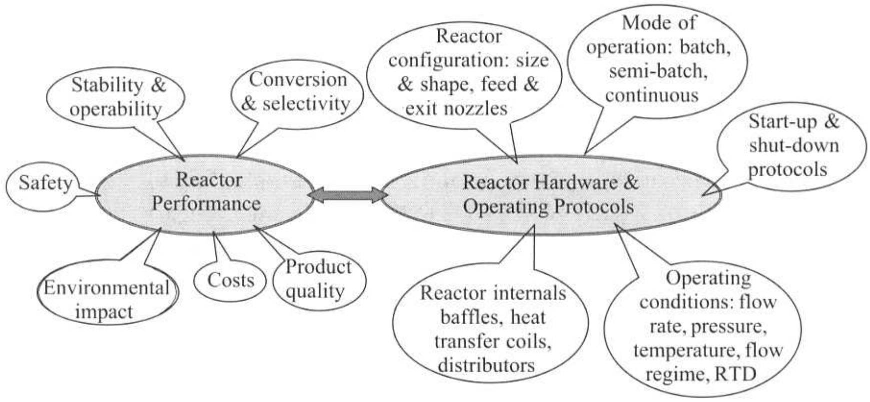

FIGURE 1.1 Chemical reactor engineering.

dynamics plays a pivotal role in establishing the relationship between reactor hardware and reactor performance.

To establish the relationship between reactor hardware and reactor performance, it is necessary to use a variety of different tools/models. Creative application of the best possible tools is required to evolve the best possible hardware configuration and operating protocol for the reactor under consideration. Various tools for modeling chemical kinetics and reactions are already well developed and routinely used in practice. This activity constitutes the major part of conventional chemical reaction engineering. Several excellent textbooks discussing these tools are available (for example, Aris, 1965; Levenspiel, 1972; Westerterp *et al.*, 1984; Naumann, 1987). Most models falling in this category make use of drastic simplifications when treating the reactor fluid dynamics. Indeed, sophisticated models and theories are available to predict the interaction between chemistry and transport processes such as mixing, heat and mass transfer. However, these models rarely attempt to rigorously relate transport properties with the reactor hardware and operating protocol. For a specific chemistry/catalyst, the reactor performance is a complex function of the underlying transport processes. These transport processes are, in turn, governed by the underlying fluid dynamics, and therefore by a variety of design and operating parameters of the process equipment. In conventional reaction engineering, experimental and semi-theoretical methods (like cold flow simulations or tracer studies) are used to relate fluid dynamics and mixing with reactor hardware and operating parameters. The information obtainable from these methods is usually described in an overall/global parametric form. This practice conceals detailed local information about turbulence and mixing, which may ultimately determine reactor performance. This approach essentially relies on prior experience and trial and error methods to evolve suitable reactor hardware. These tools, therefore, are increasingly perceived as being expensive and time consuming ways of developing better reactor technologies. It is necessary to adapt and develop better techniques and tools to relate reactor hardware with fluid dynamics and resultant transport processes.

Over the years, aerospace engineers, who are most concerned with the task of establishing the relationship between the hardware and resulting fluid dynamics, have developed and routinely use computational fluid dynamics. Computational fluid dynamics (CFD) is a body of knowledge and techniques used to solve mathematical models of fluid dynamics on digital computers. In recent years, chemical engineers have realized that, although establishing a relationship between reactor hardware and fluid dynamics is less central (compared to aerospace engineers) to their role, it is no less important. With the development of high performance computers and advances in numerical techniques and algorithms, chemical engineers have started exploiting the power of computational fluid dynamics tools. Considering the central role of reactors in chemical process industries, there is tremendous potential for applying these tools for better reactor engineering. If applied properly, computational flow modeling (CFM) may reduce development time, leading to reduced time to market, shorter payback time and better cash flow. It is, however, necessary to adapt CFD techniques and to develop a computational flow modeling approach to apply them to chemical reactor engineering. This book is written with the intention of assisting practicing engineers and researchers to develop such an approach. Individual aspects of chemical reactor engineering and computational flow modeling (CFM) are discussed and related in a coherent way to convey and clarify the potential of computational flow modeling for reactor engineering research and practice. The emphasis is not on providing a complete review but is on equipping the reader with adequate information and tips to undertake a complex flow-modeling project. The focus is on modeling fluid flows and developing tractable reactor engineering models. Numerical issues are dealt with in adequate detail to provide appreciation of the important aspects and to guide the development and incorporation of new models into available solvers. Readers interested in developing their own complete solvers may refer to specialized books on CFD (for example, Ferziger and Peric, 1995; Patankar, 1980).

The information in this book is organized to facilitate the central task of a reactor engineer, that is, relating reactor hardware to reactor performance. This chapter provides a brief introduction to the contents to be covered in detail in subsequent chapters. Here, the roles of flow modeling and computational flow modeling are discussed in the context of reactor engineering. Various aspects of chemical reaction and reactor engineering are discussed in Section 1.1 to clearly define the role of flow modeling in overall activity. Computational flow modeling, its advantages and limitations are discussed in Section 1.2. Introduction to the use of CFM for reactor engineering is given in Section 1.3. This chapter, as a whole, will be used to appreciate and identify the potential of CFM for reactor engineering.

The theoretical and numerical basis of computational flow modeling (CFM) is described in detail in Part II. The three major tasks involved in CFD, namely, mathematical modeling of fluid flows, numerical solution of model equations and computer implementation of numerical techniques are discussed. The discussion on mathematical modeling of fluid flows has been divided into four chapters (2 to 5). Basic governing equations (of mass, momentum and energy), ways of analysis and possible simplifications of these equations are discussed in Chapter 2. Formulation of different boundary conditions (inlet, outlet, walls, periodic/cyclic and so on) is also discussed. Most of the discussion is restricted to the modeling of Newtonian fluids (fluids exhibiting the linear dependence between strain rate and stress). In most cases, industrial