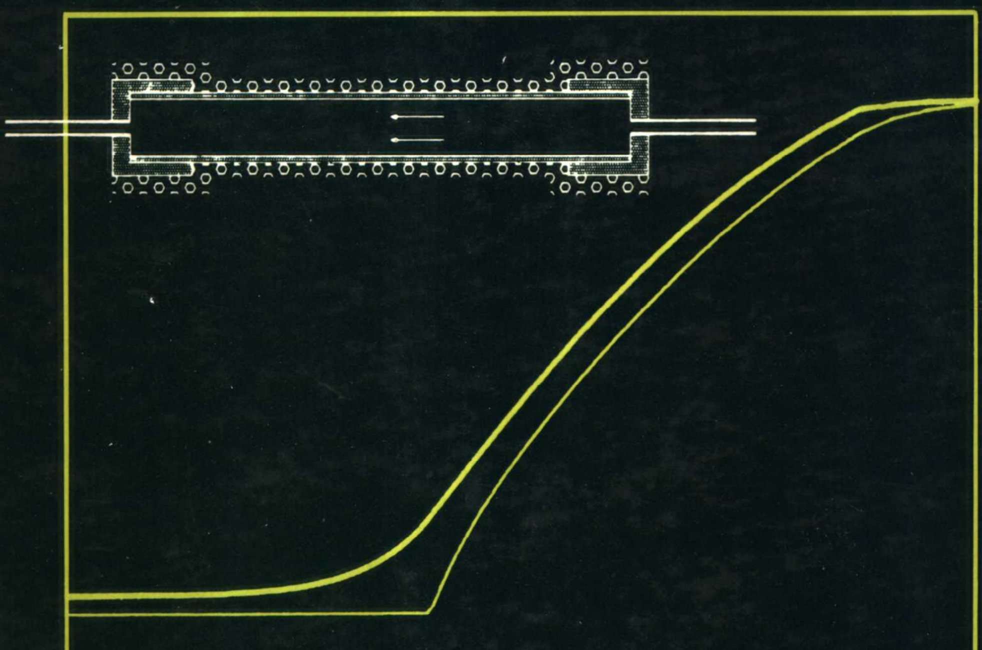
Computational Methods for Process Simulation

W. Fred Ramirez



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PREFACE

The purpose of this book is to help the reader develop the skills necessary for engineers and scientists to efficiently perform process modeling and computer simulations of chemical, physical, and biological processes. The book emphasizes techniques used to mathematically describe process systems and to arrange the mathematical relations of a process model into the solution strategy. Numerical methods necessary for machine computation are developed. Since most realistic process simulation problems require some form of high-speed machine computation, problems and examples in this text are formulated to develop necessary computer solution skills. The availability of personal computers has placed efficient computational machines at the disposal of professionals and students alike. The modern engineer and college student, with the aid of these machines and standard subroutines, can quickly obtain numerical solutions to rather large and complex problems.

Chapter 1 develops the macroscopic balances used in the simulation of lumped parameter systems. It is assumed that this is essentially a review and that the student or engineer is familiar with basic unit operations and transport phenomena. In this chapter the reader is first introduced via some simple examples to the information-flow diagram equation organization concept. Computationally, analytic solution techniques are stressed. Appendix A gives a review of analytical methods for the solution of differential equations.

Chapter 2 discusses the steady-state simulation of lumped systems. Computational techniques for the simultaneous solution of sets of linear and nonlinear algebraic equations are presented. The use of a scientific software library such as IMSL is discussed. Appendix B presents appropriate IMSL routines. Structural analysis techniques are also presented that use the interrelationships and interactions among variables and equations of an algebraic equation set to determine simple, efficient calculational strategies.

Chapter 3 introduces the dynamic simulation of lumped systems by studying various aspects of the modeling of stirred tanks. The information-flow concept is expanded and ordinary differential equation IMSL routines are used for the solution of several examples. Order-of-magnitude analysis is introduced as an efficient method for model reduction and simplification.

Chapter 4 gives several examples of the dynamic simulation of reaction kinetic systems. The IMSL ordinary differential equation routines are again used extensively.

Chapter 5 discusses vapor-liquid equilibrium operations, including examples ranging from the simple boiling of pure fluids to multicomponent distillation towers. These examples require both sophisticated algebraic and differential equation solution.

Chapter 6 develops the microscopic balances that are used in the simulation of distributed parameter systems. Initial-value examples are given that can be solved using computational techniques already introduced in the book. The value of order-of-magnitude scaling is stressed as a means of equation simplification.

Chapter 7 discusses techniques for the solution of split boundary-value problems. Shooting techniques, the principle of superposition, and the method of adjoints are discussed. Quasilinearization concepts for nonlinear problems are also presented.

Chapter 8 introduces finite difference techniques for the solution of partial differential equations. Centered-difference, Crank-Nicolson, and state-variable analogs are discussed. Quasilinearization is presented for solution of nonlinear problems. Special techniques for one-dimensional and two-dimensional multiphase flow through porous media are presented. The method of weighted residuals is also introduced.

ACKNOWLEDGMENTS

This book is a result of the author's efforts to teach process simulation and numerical methods to chemical engineering students for the past twenty years. During this period I have thoroughly enjoyed the educational process of discovering, debating, learning, and presenting both the theoretical, mathematical basis of process simulation and the many and varied applications of the material to the problems that we as engineers tackle. I feel that process modeling and computer simulation is a great blend of the theoretical and the practical that forms one of the cornerstones of engineering education and practice. Besides enjoying the interactions with my students, I am grateful for the guidance of those who have taught me both in the university and industry as well as for the many stimulating hours that were spent with my colleagues. I would like to acknowledge the superb word processing job done by Ellen Romig. A special word of thanks must go my family and especially my wife Marion, who has provided the environment which has made this project feasible. The book is dedicated to the memory of my father, who taught me fundamental lessons about hard work, the value of laughter, and genuine emotion.

W. Fred Ramirez

INTRODUCTION

Process modeling and computer simulation have proved to be extremely successful engineering tools for the design and optimization of physical, chemical, and biological processes. The use of simulation has expanded rapidly during the past two decades because of the availability of large high-speed computers. In the chemical process industry, large, realistic nonlinear problems are now routinely being solved via computer simulation. Also, the recent trend toward personal computing allows for the expanded availability of individual computer workstations. This means that virtually all engineering computations will shortly be computerized.

The increasing use of computer simulation techniques has broadened the usefulness of the scientific approach to engineering. Developing competency in process simulation requires that the engineer develop the following skills:

1. A sound understanding of engineering fundamentals: The engineer must be familiar with the physical system and its mechanisms in order to be able to intelligently simulate a real process and evaluate that simulation. The process cannot be viewed as a black box.

2. Modeling skills: The engineer has to be able to develop a set of mathematical relations which *adequately* describes the significant process behavior.

3. Computational skills: Rapid and inexpensive solutions to simulation problems must be obtained. The engineer must be capable of choosing and using the proper computational tool. For realistic problems, the tool of interest is usually a digital computer.

Since simulation relies upon a scientific rather than empirical approach to engineering, it has served to stimulate developments in interdisciplinary areas such as bioengineering and environmental engineering. Engineers have found that they have been able to make significant contributions to society through the successful simulations of biological and environmental systems. Future fruitful efforts should lie in the modeling of political and social systems. Chemical process simulations have investigated both the steady-state and dynamic behavior of processes.

The tremendous impact that simulation has had on the chemical process industry is due to the following benefits derived:

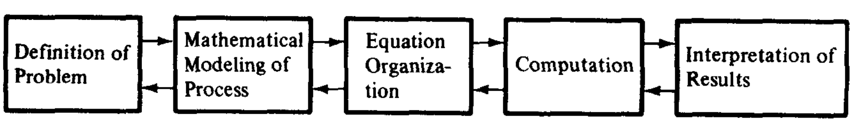
1. Economic desirability: For design purposes, it is usually cheaper to use simulation techniques incorporating fundamental laboratory data in the mathematical model than it is to build numerous different-sized pilot plants.

2. It is a convenient way to investigate the effects of system parameters and process disturbances upon operation. It is usually a lot easier to develop alternative operating approaches and evaluate these alternatives via a mathematical model than by experimental methods. In order to verify the simulation results some experiments are usually performed, but only the really critical ones are necessary.

3. Simulations are a reasonable way of extrapolating performance and scaling up processes. By incorporating fundamental mechanisms into process simulations, system performance can be predicted in new and different operating regions.

4. Understanding of the significant process behavior and mechanisms: By undertaking the rigors of mathematical modeling the engineer learns much about the process that is being simulated. In order to obtain a successful simulation, the significant process mechanisms must be quantitatively described. By solving the model, useful relations between the process and equipment variables are revealed and can be easily observed.

The general strategy for the simulation of complex processes follows a fairly well-defined path consisting of the commonsense steps given in the accompanying block diagram. Note that information travels in both directions, indicating the adaptive nature of the development of any successful simulation.



General Strategy of Process Simulation.

DEFINITION OF THE PROBLEM

This is a very important phase of a successful simulation but unfortunately there are very few precise general rules that apply. The real key to problem definition is an imaginative engineer. What is required is creative thought based upon sound engineering training. The engineer must spend sufficient time on this aspect of the problem before proceeding. A good problem definition comes from answering questions such as the following: What do I really want to find out? What are the important consequences of the study? Why should this job be done? What engineering effort should be required? How long should the job take?

MATHEMATICAL MODELING OF THE PROCESS

The engineer is now ready to write the appropriate balance equations and mechanistic relations for the process. Critical laboratory experiments must be designed and performed in order to determine unknown mechanisms and model parameters. Decisions must be made on which effects are important and which ones can be neglected. Order–of–magnitude analysis aids in making these critical simplifying decisions. It is imperative that the engineer be aware of and not overlook nor forget the assumptions made in the development of the mathematical model.

EQUATION ORGANIZATION

Once the mathematical relations have been assembled, they have to be arranged into a solution strategy, that is, decisions have to be made on which variable is to be solved for in each relation. For small problems, we usually perform this function routinely without much thought. However, for large problems care must be taken. Arranging the equations in an *information–flow diagram* is recommended. This block–diagram approach is useful for organizational purposes and illustrates the interrelationships among the equation variables. Also, equations should be arranged so that the solution strategy parallels the logical cause–and–effect relationships of the physical system. This "natural ordering" (see Franks, 1967) of equations usually leads to stable, efficient solution strategies.

COMPUTATION

For obtaining solutions to process simulation problems, the engineer has available several levels of computation—ranging from solution by inspection to analytical and high-speed computer solution. Because of the complexity and nonlinearity of process simulation problems, most solutions require high-speed digital computer solution. Digital computers are particularly useful for solving problems involving numerical manipulations. The FORTRAN language is designed for scientific usage and also has excellent logic capabilities; it is, therefore, used heavily by experienced process engineers. Numerical methods for the solution of sets of algebraic, ordinary differential, and partial differential equations are needed. To ease the programming effort in using numerical methods, generalized scientific subroutines have been written. A particularly useful and well-documented set is that of the IMSL library, which is available on both personal computers and mainframes (see Appendix B, IMSL Routines).

INTERPRETATION OF RESULTS

The real payoff of the simulation of chemical processes is in the intelligent interpretation of results by the engineer. At this point, the engineer must ascertain whether the model is a valid representation of the actual process or whether it needs revision and updating. The engineer must make sure that the results seem reasonable. Decisions have to be made on whether or not the simulated process achieves the objectives stated in the definition of the problem. Also, reasonable alternatives should be investigated in an effort to improve performance.

LIMITATIONS OF PROCESS SIMULATION

There are some definite limitations of process simulation of which the engineer must be aware. These include the following:

1. Lack of good data and knowledge of process mechanisms: The success of process simulation depends heavily on the basic information available to the engineer.

2. The character of the computational tools: There are certain types of equation sets that still pose a problem for numerical methods. These include some nonlinear algebraic and certain nonlinear partial differential equation sets.

3. The danger of forgetting the assumptions made in modeling the process: This can lead to placing too much significance on the model results.

USEFULNESS OF PROCESS SIMULATION

Computer simulation is playing an increasingly important role in the solution of chemical, biological, energy, and environmental problems. To develop some awareness of this emerging discipline, examine the literature of the past two years, and find a journal article with the application of computer computation and process modeling to the analysis and solution of a chemical engineering problem. Prepare a short, well-written summary of the article, in which you provide the following information:

1. The correctly written journal reference for each article.
2. The name of the author(s), where they are located, and their professional position.
3. The nature of the problem studied.
4. The method of computation and the size of the problem.
5. The value of the result.

Simulation, *I&EC Research*, *AIChE Journal*, *Chemical Engineering Communications*, and *Chemical Engineering Science* are good sources.

REFERENCE

Franks, R. G., *Mathematical Modeling in Chemical Engineering*, Wiley, New York (1967).