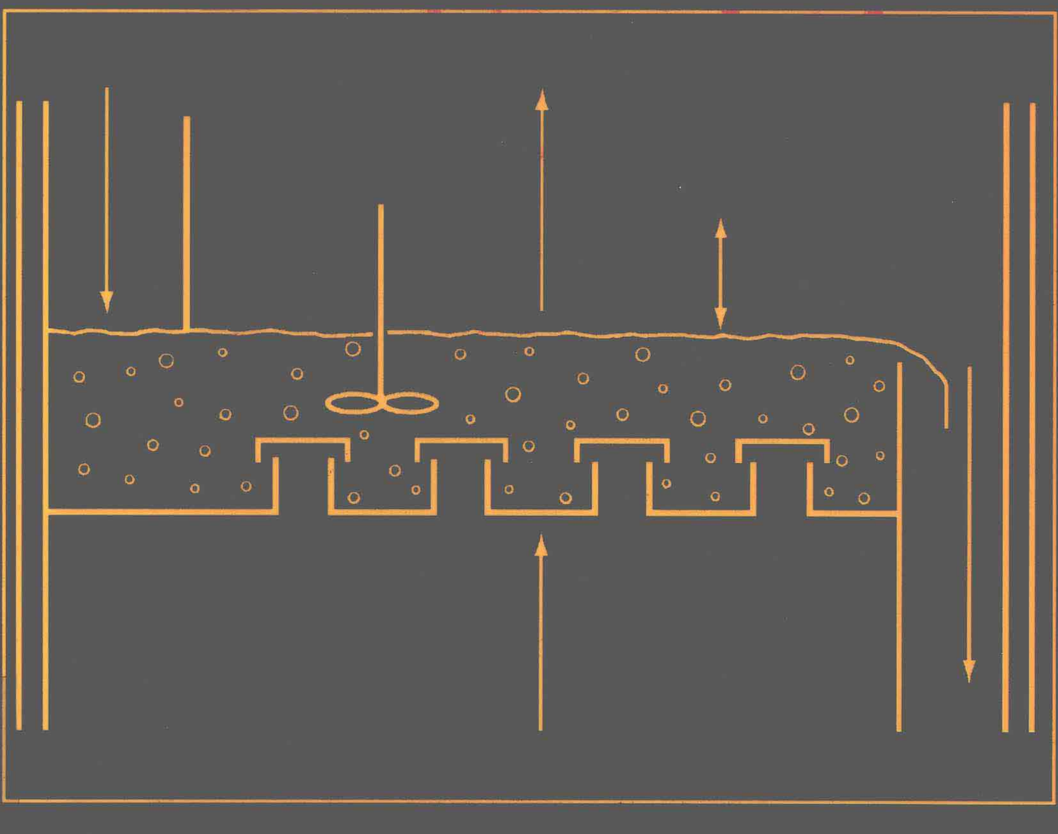
Computational Methods for Process Simulation

W F Ramirez



Second Edition

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PREFACE

The purpose of this book is to present a time domain approach to modern process control. The time domain approach has several advantages including the fact that process models are naturally developed through conservation laws and mechanistic phenomena in the time domain. This approach also allows for the formulation of precise performance objectives that can be extremized. There is a definite need in the process industries for improved control. New hardware and software tools now allow the control engineer to consider the implementation of more sophisticated control strategies that address critical and difficult process control problems. In general, it is necessary to incorporate process knowledge into the control design in order to improve process operation. Advanced control designs require more engineering analysis but can lead to significant improvements in process behavior and profitability.

The reader will notice that I have tried to include practical examples throughout the book in order to illustrate theoretical concepts. This approach also allows the reader to be aware of computational issues of implementation as well as the interpretation of the results of process testing.

Chapter 1 presents basic time domain system concepts that are needed to mathematically describe an advanced process control problem. The important concepts of observability and controllability are introduced. Observability is used in the design of the measurement system, and controllability is important for the specification of the control variables of the system. The software package MATLAB is introduced. It simplifies many of the control design calculations.

Chapter 2 treats the topic of steady-state optimization. Necessary conditions for extrema of functions are derived using variational principles. These steady-state optimization techniques are used for the determination of optimal setpoints for regulators used in supervisory computer control.

Chapter 3 gives the fundamental mathematical principles of the calculus of variations used for the optimization of dynamic systems. Classical results of the Euler equation for functional extrema and those of constrained optimization given by the Euler–Lagrange equation are developed.

Chapter 4 applies variational calculus to problems that include control variables as well as state variables. Optimal control strategies are developed that extremize precise performance criteria. Necessary conditions for optimization are shown to be conveniently expressed in terms of a mathematical function called the Hamiltonian. Pontryagin's maximum principle is developed for systems that have control constraints. Process applications of optimal control are presented.

Chapter 5 considers optimal regulator control problems. The Kalman linear quadratic regulator (LQR) problem is developed, and this optimal multivariable proportional controller is shown to be easily computable using the Riccati matrix differential equation. The regulator problem with unmeasurable load disturbances is shown to lead to an optimal multivariable proportional-integral feedback structure.

Chapter 6 develops model predictive control concepts. This structure allows for the inclusion of predictive feed-forward control into the optimal control problem. We consider design strategies for completely measurable disturbances as well as systems with both measurable and unmeasurable disturbances.

Chapter 7 discusses robust control. This allows for the inclusion of uncertainty of process parameters in the control design. The concept of robustness refers to the preservation of closed-loop stability under allowable variations in system parameters. General stability results and integrity results are given for the LQR problem.

Chapter 8 considers optimal control problems for systems that are either linear or nonlinear in the state variables but are linear in the controls. The solution of this class of problems leads to bang-bang control strategies. The existence of singular or intermediate control must also be investigated. Both time-optimal control and minimum integral square error problems are discussed.

Chapter 9 develops necessary conditions for optimality of discrete time problems. In implementing optimal control problems using digital computers, the control is usually kept constant over a period of time. Problems that were originally described by differential equations defined over a continuous time domain are transformed to problems that are described by a set of discrete algebraic equations. Necessary conditions for optimality are derived for this class of problems and are applied to several process control situations.

Chapter 10 discusses state and parameter identification. Using uncertainty concepts, an optimal estimate of the state for a linear system is obtained based upon available measurements. The result is the Kalman filter. The Kalman filter is extended for nonlinear systems and discrete-time models. Kalman filtering is also shown to be effective for the estimation of model parameters.

Chapter 11 presents the use of sequential least squares techniques for the recursive estimation of uncertain model parameters. There is a statistical advantage in taking this approach to model parameter identification over that of incorporating model parameter estimation directly into Kalman filtering.

Chapter 12 considers the combination of optimal control with state and parameter estimation. The separation principle is developed, which states that the design of a control problem with measurement and model uncertainty can be treated by first performing a Kalman filter estimate of the states and then developing the optimal control law based upon the estimated states. For linear regulator problems, the problem is known as the linear quadratic Gaussian (LQG) problem. The inclusion of model parameter identification results in adaptive control algorithms.

ACKNOWLEDGMENTS

This book is a result of the author's research and teaching career in the area of optimal process control and identification. I gratefully acknowledge the contributions of my research students to the development of many of the ideas contained in this book. I have been fortunate to have had a group of research students who have stimulated new and creative insights into process control. They deserve credit for many of the novel and important ideas found in this work.

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Finally, I want to thank my wife, Marion, who has been my personal inspiration for many years.

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 three decades because of the availability of high–speed computers and computer workstations. In the chemical process industry, large, realistic nonlinear problems are now routinely being solved via computer simulation. Also, the recent trends toward personal computing and specialized, industrial software allow for the expanded use of computers in engineering practice. This means that virtually all engineering computations will shortly be computerized and engineers need to understand the principles behind available software and how to effectively use software to solve pertinent process engineering problems.

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.

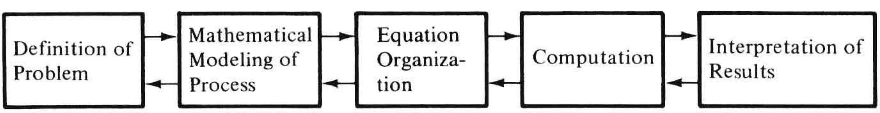
3. Computational skills: Rapid and inexpensive solutions to simulation problems must be obtained. The engineer must be capable of choosing and using the proper computational tool. For realistic problems, the tool of interest is usually a digital computer. The engineer must also be able to evaluate and use correctly available commercial software packages.

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 NAG library, which is available on both personal computers and workstations. Additional software packages are also now available which have excellent graphical capabilities and ease the programming of specific problems. One popular package is Matlab (Math Works, Inc.; Sherborn, MA). This is a special interactive software package developed for use in the solution of algebraic and dynamic response problems. A number of Toolboxes are also available for use in the solution of specific engineering problems such as process control and process identification.

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