MODELING AND SIMULATION IN CHEMICAL ENGINEERING

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PREFACE

The forerunner to this book, published in 1967, was titled *Mathematical Modeling in Chemical Engineering*. It was written at a time (1964–1966) when analog computation in industry was phasing out, to be replaced by digital simulation. Digital computer technology at that time was in an early stage of evolution. Thus, other than a brief description of the MIMIC dynamic simulator, the emphasis of that book was almost entirely on presenting the analytical techniques that lead to models suitable for simulation by either analog, hybrid, or digital computers. During the past seven years, considerable progress has been made in the development of digital programs for the chemical engineering field, and some common procedures are now emerging. Consequently, this book will present two FORTRAN IV computer programs (INT and DYFLO) that are designed for solving sets of differential equations, thereby simulating the dynamic behavior of chemical processes. The primary reason for offering these programs in FORTRAN is that it is the most common language for computers today. The program (developed for the UNIVAC 1108) as listed in this text can be adapted to any computer with FORTRAN with only minor modifications.

This book addresses itself to those chemical engineering systems that, when analysed, lead to models involving ordinary and/or partial differential equations. Consequently, it does not concern itself with steady-state energy and material balance, nor does it cover programs directed to detailed engineering design of process equipment.

In order to make the simulation programs meaningful, they are described in a framework of engineering applications, the various parts of the program being introduced in the chapters throughout the book as each area of chemical engineering is covered. If these programs are to be used effectively a knowledge of elementary numerical methods is recommended. For this reason chapters II and III cover the basic concepts of numerical iteration and integration. This leads to the development of the INT program, which consists of a set of subroutines for solving simultaneous differential equations and associated algebraic equations. The INT program forms the basis of a higher-level set of subroutines (DYFLO) that simulate the dynamic behavior of most of the common unit operations in chemical processes. These are introduced successively in the following chapters and deliberately are designed for simplicity in order to gain execution speed and to facilitate an understanding of the internal computation sequence. It is hoped that this understanding will encourage the reader to develop additional subroutines tailored to his specific needs.

The computer programs provide a ready means for executing the calculations of the mathematical models created in the analytical portions of the text, demonstrating that simulation is a practical approach to complex process problems, typical of present day practice in industry. As in the first book, model formulation methods are stressed. Many engineers have the latent ability to describe physical reality in mathematical symbology. This requires imagination, coupled with experience that is accumulated from frequent practice. Development of these talents leads to greater analytical insights into process systems and a more thorough grasp of fundamentals. This book is intended to stimulate the analytical approach by removing outdated obstacles and presenting a straightforward, unified procedure for constructing mathematical models of complex process systems.

Compared with the complexities of the computer simulations commonly done in industry, and occasionally described in the literature, most of the examples discussed in this book are elementary. For this reason this text should be considered as an introduction to computer simulation. However, most of the general principles inherent in the complex models have been deliberately included in the text examples. The subject matter progresses from lumped systems through staged operations to distributed systems that give rise to partial differential equations. The last chapter shows how nonlinear control problems can be tackled by simulation without detailed knowledge of advanced control theory.

It is assumed that the reader is familiar with the fundamentals of energy and mass transfer, chemical kinetics, and vapor/liquid equilibrium and that he has a working knowledge of FORTRAN. The logical candidates for this book, therefore, are senior undergraduates or first-year graduate students and practicing engineers who have not been exposed to computer modeling.

I am grateful to my colleagues, Mr. R. L. Buchanan, Mr. D. Culver, Mr. T. Keane and Mr. A. Auster for their assistance in the preparation of this text. Mr. D. Culver has been particularly helpful in the development of the DYFLO program. The assistance of Mrs. J. Schweikert and Miss B. Franks in typing the manuscript is gratefully acknowledged.

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CONTENTS

CHAPTER I

INTRODUCTION

Over the last fifteen years in the chemical and petroleum industries there has been a gradual trend toward a more quantitative approach to problems in the design and operation of processes. This trend has been made possible by the increasing use of powerful electronic computers in the solution of complex systems of mathematical equations. This analytical approach to engineering problems allows both considerably wider scope in investigating alternative designs and more efficient operation of commercial batch and continuous processes. In addition, the computerized analytical approach provides a deeper understanding of the internal mechanisms of the processes studied.

Today powerful computers have become almost universally available in both schools and industry. The future promises the rapid expansion of time-sharing and more sophisticated terminal connections, such as graphic displays and automatic plotting equipment. During the period when the analog computer was used to solve process dynamics problems (1955–1965), there existed, by necessity, a specialized staff at each computer installation that performed the programming and computer operation chore for clients with problems to be solved. The analysis of the problem, that is, its definition in mathematical terms, was performed by either the client or the computer specialist, or sometimes both in collaboration. During the middle and late 1960s, the digital computer, because of its increase in speed and size, and the accumulation of library routines, became the favored computer for chemical process simulations. As a result, the analog computer suffered a decline in usage and has now been phased out from most industrial computer installations. The advent of digital simulation with user access to library routines that perform a wide variety of calculations has enabled many analysts to bypass the computer specialist, by constructing their own programs. In other words, it has encouraged the trend to open-shop operation with less reliance by the user on the specialist. One objective of this book is to provide the reader with a set of programs that will enable him to program his own problem with a minimum of effort, specifically in the area of process simulation.

As processes become more complex, incorporating ever-increasing degrees of automation, there will be a greater need for the analytical approach to problems associated with their design and operation. Modern analysis of process problems usually involves some form of mathematical modeling, and, in one sense, this should appeal to chemical engineers because modeling of processes, either on a bench or pilot scale, has long been a favored preliminary to a commercial plant. There are various mathematical models for the same system, each one suited to solve a particular problem associated with the system. The two broad classifications constitute steady-state and dynamic models, and in either type the degree of detail required depends on the problem to be solved as well as the amount of basic data available. A very precise description of a chemical process system will often lead to a large set of unwieldy equations. Although they can be solved, it is advisable for the analyst to use engineering judgment to reduce the equations to a less complex set that for all practical purposes will yield an engineering solution within the accuracy of the basic data provided.

One important aspect of mathematical modeling is the arrangement of the equations. It has been found by experience that if the equations are arranged in a logical or cause-and-effect sequence the computer model is stable. This sequence is termed the "natural" order, for it invariably closely parallels the cause-and-effect sequence found in nature. It will soon be realized that the key to understanding the internal mechanism lies in being able to define this natural cause-and-effect sequence.

The educational background required for modern analysis is an increasing problem, for it is clear that computers have changed the emphasis placed on this subject. Before computer usage became popular, instruction in engineering analysis was (and still is in some places) restricted to simple systems, and most of the effort was devoted to solving the few elementary equations that were derived. These cases were mostly of academic interest and, because of their simplicity, were of little practical value. To this end, a considerable amount of time was devoted to acquiring skills in mathematics, especially to methods of solving differential equations. In fact, most chemical engineers are given courses in differential equations, but experience shows that very little of this knowledge is retained by the engineer after graduation for the simple reason that mathematical methods are not adequate to solving most systems of equations encountered in

Table 1-1. Classification of Mathematical Problems* and Their Ease of Solution by Analytical Methods

	Linear Equations			Nonlinear Equations		
Equation	One Equation	Several Equations	Many Equations	One Equation	Several Equations	Many Equations
Algebraic	Trivial	Easy	Essentially impossible	Very difficult	Very difficult	Impossible
Ordinary differential	Easy	Difficult	Essentially impossible	Very difficult	Impossible	Impossible
Partial differential	Difficult	Essentially impossible	Impossible	Impossible	Impossible	Impossible

* Courtesy of Electronic Associates, Inc.

industry, and any advanced mathematics is forgotten through sheer disuse. Table 1-1 shows the various classes of mathematical equation and the limited class amenable to analytical solution. Most industrial process problems fall into the category of nonlinear differential equations, which can be solved only by a computer. The classes of equation that are amenable to analytic solution are of a trivial nature and restricted to very few cases of industrial interest. The table shows a heavy border that separates the possible from the impossible, and by these standards practical problems defy *analytical* solution or yield extremely cumbersome, essentially useless answers.

The three broad areas that are fertile fields of analytical studies are the following:

1. Research and process development
2. Process design
3. Improvement of process operations

The areas of analysis cover these categories:

1. Fluid flow
2. Mass transfer
3. Heat transfer
4. Kinetics
5. Dynamics and control

The approach to mathematical model building outlined in this book assumes that the student is familiar with the fundamentals of these areas. A model of a typical process will often involve all five categories and the

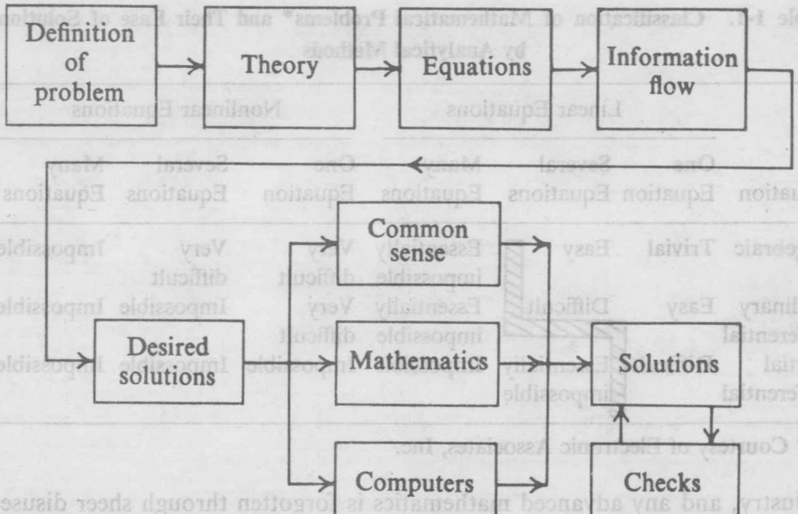

FIG. 1-1. Procedure for Analytical Approach

general procedure for conducting an analytical study can be grouped into seven stages as shown in Figure 1-1

The first step, perhaps the most important one, is that of problem definition, yet it is not possible to establish rules for problem definition that are sufficiently general to be useful. Technical problems are so diverse that it is up to the analyst to state clearly the nature of the individual problem. This will establish a definite objective for the analysis and is invaluable in outlining a path from the problem to the solution.

The second step is a definition of the theory that governs the phenomena of the problem. This theory is usually available from a variety of sources, both published and unpublished, but for those isolated cases in which there is no theory available it is worthwhile to postulate one, or several, and to test its validity later by comparing the solution of the mathematical model with experimental results. One of the advantages of the computerized approach is the facility of rapidly obtaining solutions to various cases; this makes comparisons between alternate theories possible.

Next, the theory, as applied to the problem, is written in mathematical symbology, a necessary step that forces the analyst to a clear unambiguous definition of the problem. The physical systems to be studied in this book are always described by a set of simultaneous algebraic and differential equations, which must be written in the most direct form possible; no manipulations are required at this stage. It is worthwhile at this point however, to simplify the equations, whenever possible, by omitting insignificant terms. Care is needed, though, to ensure that any terms omitted are indeed insignificant during the entire course of the problem run. Often it is possible to eliminate entire equations by merely neglecting minor fluctuations in certain intermediate variables; for example, suppose the specific heat of a multicomponent mixture required for a heat balance varies only 1% of its value because of expected variations in composition; rather than include an equation in the model, to compute a value continuously, an average constant number could be substituted.

When the equations are assembled, a procedural method for solving them as a simultaneous set is required. This is sometimes referred to by mathematicians as "equation ordering" but is called "natural arrangement" in this book and consists of placing each equation in an information-flow block diagram which shows how each equation is to be used, that is, the variable it solves for and the interrelationship between the equations.

This technique is merely an extension of the classical linear transfer function notation to systems of nonlinear equations. Such an arrangement, paralleling the logical cause-and-effect relationship in the physical system, presents a clear picture of the postulated mechanism and sometimes reveals interrelationships between variables that were not apparent during previous stages. A consideration of the solutions required from the model is a necessary step preliminary to the computation phase. A list of the various cases required and the information that is expected in each case will reveal possible redundant situations and will be helpful in the programming of the computation phase.

The computation phase that follows offers several alternate routes to the solution. The method selected depends on the complexity of the equations to be solved. There are three general levels, the most elementary being common sense; that is, the solutions desired can be obtained from the model by inspection if the equations or the solutions required are sufficiently simple. It should be realized that this technique cannot be extrapolated to more complex cases without requiring increasing amounts of pure guesswork. The next level, again restricted to systems of modest complexity, solves the equations by analytical techniques. As pointed out in the preceding discussion, a considerable amount of skill is required to solve even some of the simplest sets of nonlinear equations, and such a level is usually beyond the reach of the average process engineer. Fortunately, the third alternative of automatic computation offers the most fruitful path and is the only expedient method for problems of even fair complexity.

The last phase is the study and verification of the solution obtained from the mathematical model. Any unexpected solution should be rationalized to ensure that no errors have occurred in the computation; also, some of

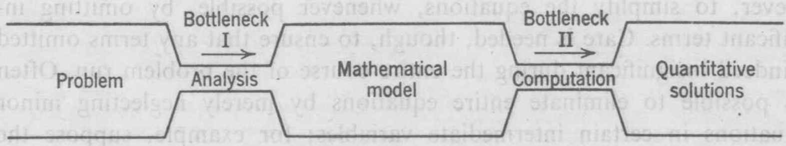

FIG. 1-2. Difficulties of Analytical Approach before Computers

the computer runs should be specifically designed to check the validity of the mathematical model.

The procedure for obtaining quantitative solutions from an analytical approach has changed significantly in recent years. Figure 1-2 is a symbolic representation of the situation that existed before computers became readily available.

Basically, there were two bottlenecks, the analysis of the problem and then the solution of the equations resulting from the analysis. This latter bottleneck was generally impassable, so that efforts made at mathematical modeling were of no practical use since the equations could not be solved anyway. As a result, the effective way to solve technical problems was by laboratory or pilot-plant experimental procedures. The disciplines of the rational/analytical approach were regarded as purely academic and consequently were not practiced as a way of life in industry.

Over the last 15 to 20 years computers became more widely used, and the recent impact of software languages and especially simulation languages has made computers almost completely accessible to the average engineer if he can get past the first bottleneck of analysis. It can be safely stipulated, then, that today the second bottleneck does not exist, as shown in Figure 1-3.

Another purpose of this book, then, is to encourage engineers, having once eliminated their reservations toward computers, to develop their analytical abilities by adopting as a start the simple approach presented in the following pages. It will be helpful for the student to review a few basic concepts in mathematics, covered in the next sections.

1-1 EQUATIONS

Equations can be classified into two broad groups: algebraic and integral/differential equations. Generally, an algebraic equation does not contain

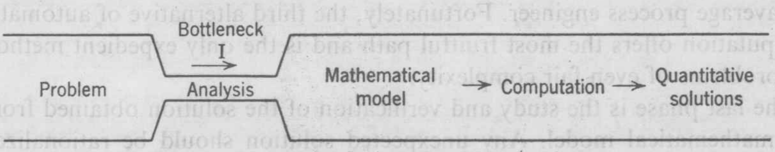

FIG. 1-3. Difficulty of Analytical Approach Today