CHEMICAL PROCESS SIMULATION

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FOREWORD

Digital simulation is a relatively new discipline and yet has become very popular in a short span of about two decades. As a matter of fact, it is now considered to be an essential exercise by most design houses and process companies to prepare mathematical models of their prototypes. It enables them to study the effect of variation in the design and operating parameters on the performance of the equipment. Chemical plant design begins with the creation of a process flowsheet. Prerequisite to the generation of an optimal flowsheet is the simulation of the entire process on a computer. In existing plants, the flowsheet exists already and process simulation is carried out to optimize the performance of the plant within the process constraints. There is yet another advantage of this exercise as it provides a better understanding of the process and of the role of engineering parameters in process design. This is of special significance to developing countries like India, since imported technologies must be assimilated and must be improvised indigenously to suit local environment.

Dr. Asghar Husain, Distinguished Scientist at Regional Research Laboratory, Hyderabad has a vast experience in the area of Modelling, Simulation and Optimization. I can not think of a better person to write this exposition. While there are a large number of publications that have appeared in the recent past in the area of chemical process simulation, there are but a few texts available which present a coherent reading of the subject matter. Dr. Husain has not only assimulated the published literature and presented this material in this book admirably but has also blended with it his own contributions and experiences which makes this volume all the more richer. I am sure it will prove to be very valuable addition to the existing literature and will serve well for university teaching as well as for self learning. Only a truly distinguished and committed scientist like Dr. Husain could have completed this mammoth task with such professionalism.

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PREFACE

The last three decades have seen a phenomenal growth in the development and sophistication of electronic computers and their capabilities. This, in turn, has brought new dimensions in the synthesis, design and analysis of systems. Any physical system such as a manufacturing plant, an aircraft, a space vehicle or an abstract economic system can be adequately and realistically represented by its mathematical model for a detailed study, at a fast rate, using a computer. This activity is known as "simulation".

The computer-aided simulation of variety of the systems is catching up very fast and being extensively applied in all fields of human endeavour. One such field is the bulk production of horde of chemicals, petrochemicals, fertilizers, pharmaceuticals, etc. The great importance acquired by simulation in this field is due to the growing complexity of the large chemical plants, high degree of automation required in their control and, often, an improbable situation of experimenting with the real systems. This book is addressed to the particular field of chemical process simulation, which can serve as a highly useful tool in the analysis of a chemical process in order to commercialise it, for studying a running chemical plant to enhance its efficiency and productivity, for locating possible bottlenecks and conserving material and energy resources, for gaining more confidence in upscaling a process from the pilot stage, and for developing improved controls. Various aspects and requirements of such simulation are clearly brought out in the chapters included. Wherever possible, examples and case-studies are given.

The book will, therefore, be of great interest to students, R & D scientists and practising engineers. It can serve as a text book for a full semester graduate course on simulation of the chemical equipment and plants. It contains most up to date material based upon the published and other available information, and an extended bibliography. The main text assumes, on the part of the reader, certain knowledge and acquaintance with the basic information required in modeling a process. However, three appendices are included containing the necessary material.

Appendix I on the "Background information" provides introductory material and concepts in model formulation of various process units. A reader not aware of this can first go to it before start reading the main text. Appendix II on the "Numerical Methods" deals with some of the important techniques used for solving the model equations. For validation of the models and for generating model parameters, very often multivariable function minimization is applied. The important methods used for minimization are discussed in the Appendix III. Each of these topics

warrants a separate book. Numerous texts are already available on each of these subjects; a few of them are listed in the bibliography as a guidance to the reader for a detailed study. However, the inclusion of these appendices enhances the utility of the book and makes it suitable even for the undergraduate teaching.

Appendix IV provides well established correlations for the important properties of some of the common materials, which will be handy for the practising engineers.

The author is grateful to Dr. G. Thyagarajan, Director, Regional Research Laboratory, Hyderabad, for his excellent cooperation in providing all the facilities. The author is thankful to various colleagues who have contributed in different ways; specially to mention are K.V. Reddy, M. Mahmood Ali, K.S. Raghunandanan, C.L.N. Murthy, C.P. Ramulu, B.S.N. Murthy, D.S. Reddy, M. Sriram, P.J. Reddy and P.V.E. Narasimham. Thanks are also due to I.J. Manmadha Rao for his careful typing and to B.G.K. Murthy and B. Rama Rao for drawings.

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CONTENTS

Chapter 1

INTRODUCTION

In future as the energy consumption expands and resources of material and energy become more expensive and less certain, substantial changes are needed in many conventional chemical processing plants. These have to incorporate a high degree of energy integration and achieve greater efficiencies through process modifications, thus conserve material and energy resources. At the same time protection standards are tightening, therefore, lower temperatures and pressures are desired. Higher reaction rates, fewer stages and smaller plants will reduce burden of the material in the process, leading to safer plants. With the growing consciousness about pollution, it is essential to produce less effluents as well as to treat them properly.

For facing all these challenges, larger effort is needed on the part of process engineers in evaluating alternative flowsheets. Fortunately, recent developments in computing procedures combined with increasing capabilities of successive generations of computers enable chemical engineers to tackle the process design problems on a much broader basis.

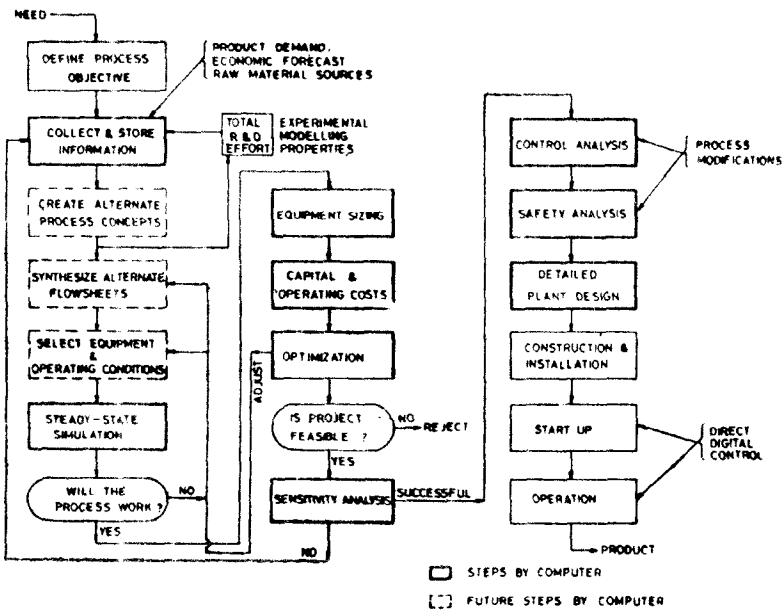


Fig. 1.1. Strategy for Process Engineering.

Figure 1.1 shows a strategy of development from conception to commercialization of a chemical process, [Evans and Seider in (1976)], which thick blocks indicate the steps totally computerised today and constitute elements of modern computer-aided-design (CAD). The broken blocks will eventually be computerised in the course of time.

1.1 PROCESS SYNTHESIS

It is clear from Fig. 1.1 that the total process design effort can be broadly divided into three stages, namely process synthesis, process analysis and optimization. In the first stage (broken blocks), a process concept is generated and a flowsheet structure is primarily chosen with various types of equipment and their interconnections. For this purpose, information from several sources is required, most important being the experience piled up over several years in solving both simple and complex design problems in a certain area of process industry. All this information, along with the knowledge of local conditions, and the facts and relationships that govern behaviour of the processing systems should be put up to the maximum use. The latter usually involve disciplines of chemistry, physics, mathematics and economics.

Process synthesis by and large depends on design heuristics, more so on intuition of the process engineers. This, however, can lead only to that upperbound of efficiency which is inherent to an already synthesised system. On the other hand, there may exist other plausible system structures (i.e. flowsheets) possessing higher upperbounds which should be synthesised in order to achieve maximum benefit. For this reason, during the current years attention is being focussed to develop a general and systematic approach to process synthesis. Though still in a state of infancy, process synthesis will be carried out in future on a more rational basis with the help of computer aids. It is briefly covered in the last chapter.

1.2 PROCESS ANALYSIS

Once a flowsheet is synthesised, an analysis is required to solve material and energy balances for a steady state process, sizing and costing the equipment and evaluating worth of the flowsheet. The area termed as "steady-state simulation" in Fig. 1.1 has seen a phenomenal growth during the last two decades. It has been a subject matter of several extensive reviews, for instance, by Flower and Whitehead (1973), Kehat and Shacham (1973), Husain (1975, 1981), Motard et al (1975), Klemes (1977), Hlavacek (1977), Rosen (1980), and books by Crowe et al (1971), Franks (1972), Ramirez (1976) and Westerberg et al (1979).

Also known as "flowsheeting", chemical process simulation is represented by a mathematical model with an aim to obtain information about response of a plant to various inputs. The model is often applied in the form of a computer program for a continuous steady-state deter-

ministic system simulation. Chapters 2 to 5 describe various features and requirements of general purpose simulation. Chapter 6 outlines an important requirement of any successful simulation, that is, availability of accurate properties of pure chemical species and their mixtures. In a specific purpose simulation study (Chapter 7), the aim is to obtain a much deeper insight of the process response to various inputs; hence, in this situation more detailed and complex modeling is required. Dynamic simulation (Chapter 8) is needed in the analysis of control aspects as well as for studying transient response during startup or shutdown of a plant.

1.3 OPTIMIZATION

Finally, optimization is performed leading to the final flowsheet with its optimal decision variable values. This field has also witnessed tremendous development during the last three decades with numerous techniques perfected for unconstrained and constrained optimization. The functional optimization is required for calculating optimal control policies for implementation of feedforward control through microprocessors and real time computers. Several texts are available describing the theory and practice of optimization, including one by the author [Husain and Gangiah (1976)].

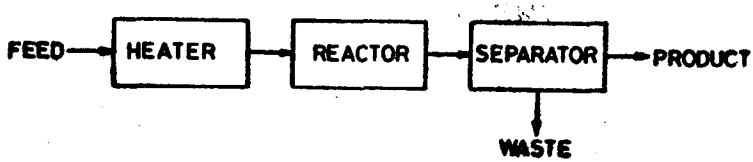
All these interrelated activities should obviously lead to an optimal design and safe operation of a chemical plant. In this endeavour, although the analysis being a small part of the total effort, it is the key starting point, and crucial in determining success of the whole venture. Often special purpose programs, such as for ammonia plants, result into considerable saving in engineering time; the calculations can be set up and run at a fast rate saving several man-weeks of hand calculations. Hence, this book deals with various aspects of process analysis, in other words, process simulation.

Chapter 2

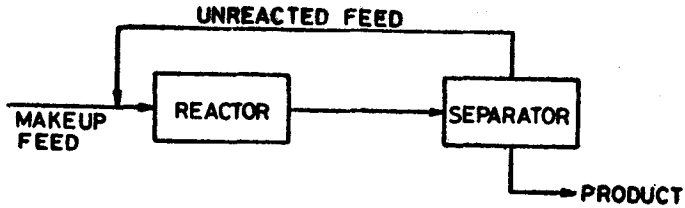
MODULAR APPROACHES TO PROCESS SIMULATION

Among the most tedious and repetitive problems of process design is that of calculating heat and mass balances. During the initial stages of a flowsheet study, whether of a new process or an existing one, simple material balances may alone suffice. At this level, specifications may be set from the plant data if an existing plant is being considered, or from engineering experience or pilot plant data if a new process flowsheet is under development.

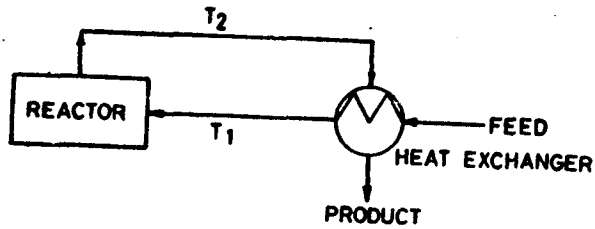
In the later stages of design, however, heat and mass balances must be calculated along with the equilibrium and rate equations, P-V-T relationships and those governing counter current operations. All these



I–Serial Process



II–Recycle of Mass



III–Recycle of Energy

Fig. 2.1. Serial and Recycle Processes.

equations are generally strongly nonlinear. Moreover, in the simplest case if a process is of a sequential configuration, as shown in Fig. 2.1-I, it is easy to proceed from the feed streams until the products are obtained calculating sequentially for one process unit after the other. Unfortunately, majority of the chemical plants are of complex configuration involving recycle of streams, mass (Fig. 2.1-II) or energy (Fig. 2.1-III) or both; they represent interlinked networks of units. In such situations for making calculation procedure sequential, it is essential to decompose the network as discussed in Chapter 4. This, in turn, requires convergence promotion as outlined in Chapter 5.

In the early 1960's, several design organisations started building libraries of computer programs for various unit-operations. It then became evident that many of these could be put into a system enabling one to direct calculations for an entire flowsheet, thus saving considerable engineering time. This resulted into the development of specific purpose programs to simulate a particular plant or part of a plant; these were naturally more detailed in nature but at the same time rigid in structure. On examining these programs, it became clear that a major portion could be common to all types of plants, that is, calculations involved in various unit-operations, methods to compute different physical and thermodynamic properties, decomposition and convergence algorithms, cost information, as well as a library of numerical routines. Furthermore, a common approach to diagnostics might also be beneficial. Ultimately, it gave rise to several general purpose simulation packages; a few typical ones developed earlier by industry, consulting companies and educational institutions are given in Table 2.1.

2.1 ANALYSIS vs. DESIGN MODE

Ideally, with an aim of process simulation to be a design tool, the system inputs and/or design parameters should be calculated from the specified outputs. But such a simulation in a "design mode" (Fig. 2.2-I) is numerically less stable than that in the "analysis or performance mode" (Fig. 2.2-II). The latter is characterized by the fact that all system inputs and design parameters for the units are specified and it calculates outputs using the given information. Thus, the information flow in the analysis mode is in the same direction as the energy and material flow in a chemical plant.

Being numerically more stable, the analysis mode is more often used to perform design calculations iteratively for making case studies. Hence, majority of the application packages are written in this mode of simulation.

2.2 SEQUENTIAL MODULAR APPROACH

The modular viewpoint involves collecting equations and constraints for each process unit into a separate computational subroutine or module as well as the solution procedures for these equations. This

Table 2.1. Major Executive Programs

Name of Program		*Organisation where Developed*
Industry		
CHEOPS	Chemical Engineering Optimization System	Shell Development Co., U.S.A.
CHEVRON	General Heat and Material Balancing System	Chevron Research Co., U.S.A.
NETWORK 67	—	Imperial Chemical Industries, U.K.
SCOPH (66)	Sizing and Costing of Process Equipment	Diamond Shamrock Co., U.S.A.
Consulting Co's		
FLEXIBLE FLOWSHEET		M.W. Kellog Co., U.S.A.
PACER-245	Process and Case Evaluator Routine	Digital Systems Corpn., U.S.A.
Educational Institutions		
CHESS	Chemical Egineering System Simulator	U. of Houston, U.S.A.
GEMICS	General Engineering and Management Computer System	McMaster University, Canada
PACER	Process and Case Evaluator Routine	Dartmouth College, U.S.A.
SPEED-UP	Simulation Program for the Economic Evaluation and Design of Unsteady State Process	Imperial College, London

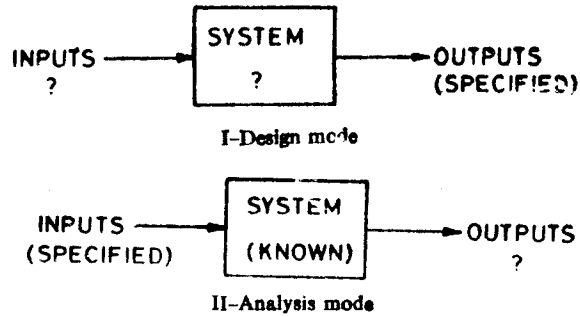


Fig. 2.2. Design vs. Analysis Mode.

concept is parallel to that of a unit-operation, hence termed as a "unit-computation". Thus each module calculates values pertaining to the output streams for the given input conditions and parameters for that process unit or equipment, irrespective of the source of input information or the sink of output information. A typical module embedded in a flowsheet network simulation program is shown in Fig. 2.3. Using such a concept, it is thus possible to evolve a library of modules and use them to simulate variety of flowsheets in a building block approach.

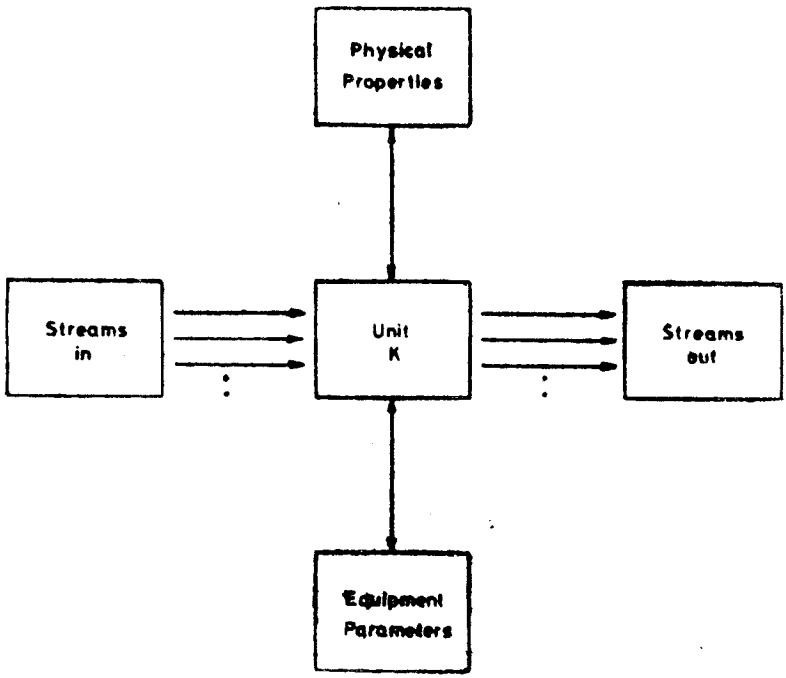


Fig. 2.3. Unit Computation Module.

The sequential part of the approach involves carrying out calculations from module to module, starting with the feed streams until products are obtained. In order to make it totally sequential, it is then necessary to identify recycle loops of units in a given flowsheet and to "tear" certain streams (Chapter 4), in other words, assume values of the variables associated with these streams and adopt an iterative procedure which should converge on the assumed values. For instance, tearing streams 2 and 7 in the network of modules shown in Fig. 2.4, the whole procedure becomes sequential in the order of modules (1), (4), (3), (5) and (2).

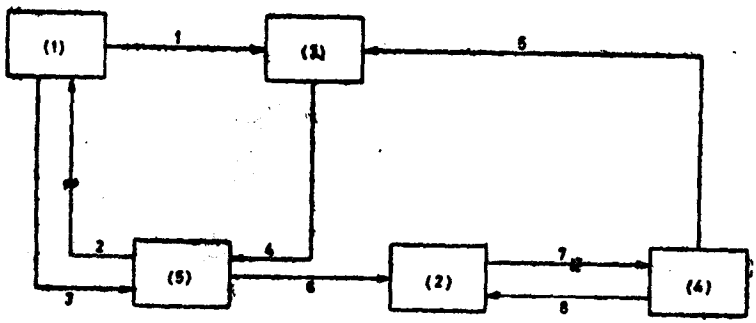


Fig. 2.4. Network of Modules with Tear Streams.

A general purpose sequential modular program has the following structural components:

(i) A store of physical and thermodynamic properties for pure chemical species and their mixtures.

(ii) A system working data base derived from the data obtained from the store as well as the problem input.

(iii) Individual module data base derived from the working data base.

(iv) Modules or subroutines for individual process units, computational procedures including input/output for each module and internally iterated variables, if any.

(v) Flowsheet topology to be used by the system executive to order computation sequence. This is usually defined by a "process matrix", which specifies standard unit modules for use in simulation of a particular process along with identification numbers, positive for input streams and negative for the output. For example, process matrix for the network of Fig. 2.4 will be as shown on next page.

(vi) Routines for recycle calculations and convergence analysis.

(vii) Other mathematical service routines.

Module Identification Number	*Module Standard Name*	*Streams*
(1)	...	2 —1 —3
(2)	...	6 8 —7
(3)	...	1 5 —4
(4)	...	7 —5 —8
(5)	...	3 4 —2 —6

An exhaustive list of simulation packages with programming languages and computers used has been compiled by Klemes (1977). A few typical packages, all written in FORTRAN, along with their significant features and applications made are listed in Table 2.2. The features of one such package, i.e. PROSIM (PROcess SIMulation) are described in the next section.

2.3 PROSIM

PROSIM [Husain & Ali (1977)] is a simulation package designed to work in the analysis mode. Its structural features are shown in Fig. 2.5. It is a fixed structure program which means that the program executive remains the same no matter which flowsheet is being simulated. The executive is a collection of subroutines which receive user input and problem description, decide order of the calculation, decompose recycle loops, check data consistency at various stages of simulation, do all book keeping and execute the whole process of flowsheeting right through. Four main phases in the simulation are as follows:

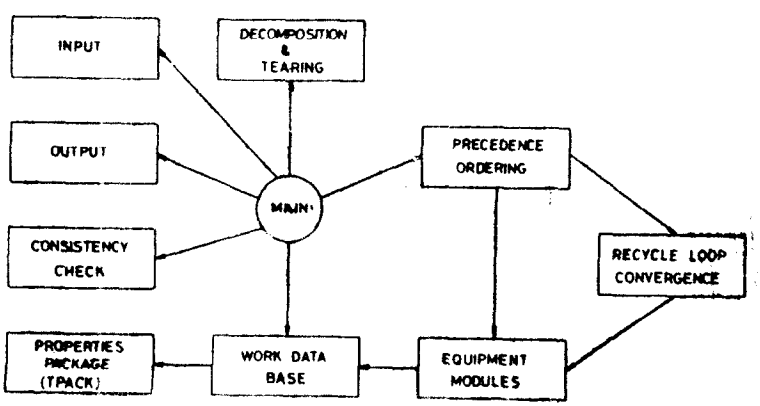


Fig. 2.5. Structure of PROSIM.