Process Modelling and Simulation in Chemical, Biochemical and Environmental Engineering

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Dedicated to my wife, Geeta Verma,

and sons, Anurag Srivastava and Anupam Srivastava.

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Preface

The quest for understanding various phenomena is human nature, and the development of science and engineering is based on it. Observation, searching for a trend in it, is followed by invention. Theoretical knowledge helps in predicting possible phenomena without carrying out an experiment. Chemical engineers are involved in the safe and economic design and operation of process plants and in increasing the productivity of existing process plants.

Today, simulation is an accepted way of studying various process industries. It may be carried out to study the behaviour of unit operations or a plant without fabricating any equipment, or to study the entire plant without any real loss or damage to the real equipment or environment. However, simulation requires a process model, which is a mathematical representation of a simplified picture of the process. Simulation studies are carried out by experimenting with the model. Thus, modelling and simulation both exist together.

The engineering of process systems was initially qualitative in nature. At present, it is founded on engineering sciences, computer-aided tools and the system-theoretical methodologies. The use of simulation has helped in developing an integrated approach to process design. The effects of environmental issues, choice of the controller, process safety and so forth on the economic design of the process plant can now be considered.

Earlier modelling efforts focused on developing analytical models. Various mathematical techniques were applied to obtain analytical solutions of various chemical engineering problems. Later, various numerical techniques were also applied to solve more rigorous problems. The books on modelling during those days covered these topics comprehensively. At present, many of these techniques such as estimation of the inverse of a matrix, solution of non-linear equations, numerical integration and so on are available with many types of software. The focus on modelling is now to understand the process in more detail and represent it in mathematical form. This book is written with this aim. It attempts to explain the simplification of a complicated process at various levels with the help of a 'model sketch' and to proceed in a systematic manner.

The models have been divided into four categories. The simple models are those which are based on simple laws such as Fick's law. The next category of models consists of generalised equations such as equations of motion. These deterministic models do not have any random phenomena and consider all variables as continuous variables. The next category covers discrete-event models and stochastic models which consider at least one variable as a discrete variable. The models based on population balance have also been covered with it. The boundary between these models is not sharp; however, they certainly reflect increasing levels of difficulty and require different approaches.

The dynamic models have no separate treatment as many good books on dynamic modelling and process control are already available. Computational fluid dynamics has been purposefully left out due to the different nature of the modelling. It is not possible to cover everything related to modelling and simulation in this volume. The field of modelling and simulation is rapidly advancing. However, I hope that the concepts discussed here will be useful in future also.

Most of the software have their own syntax and semantics. Therefore, choosing a software was not an easy task. Finally, it was decided that the examples will be solved in MATLAB®. The code is short, and more attention can be given to the representation of process in mathematical form. The code also runs on open-source SCILAB, with minor modifications if no specific toolbox was used.

The vector notation of laws of conservation has been avoided because it is not intended to illustrate the derivation of the analytical solution. The Nomenclature does not provide unit as empirical correlations are not used in this book. The model equations are independent of units.

Chapter 1 introduces the complex nature of chemical processes and an introduction to the terms 'modelling' and 'simulation'. The advantages of simulation and the role of modelling in simulation have been studied.

Chapter 2 describes steps in simulation, various types of models, the approach to modelling, types of model equations, solution strategies, sources of equations and some of the common assumptions that are made to simplify the complexity of the process.

The few simple models that are still useful have been described in Chapter 3. The equation of state, Newton's law, Fourier's law, Ficks' law, Henry's law, Arrhenius law and adsorption isotherms, film model were discussed and their application was illustrated in few simple problems. In Chapter 4, the models based on laws of conservation of momentum, mass and heat transfer have been described. These models are applicable to systems involving a single phase only. Chapters 5 and 6 cover the models based on laws of conservation in multiphase systems without and with chemical reactions. The examples include the stationary dispersed phase (packed beds) and moving dispersed phase (fluidised beds and bubble columns).

Models based on population balance, discrete-event models and stochastic models have been covered in Chapter 7. These models generally involve random variables to describe discrete or even continuous variables. The simulation strategy is different in the sense that no analytical or numerical solution is sought as in the case of deterministic models.

The artificial neural network (ANN)–based models follow a black-box approach. They relate the data through a network of nodes and have a different nature. Feedforward-type ANNs and hybrid-type ANNs, which combine the advantage of the first principle model, have been described in Chapter 8.

A model has to be validated for either experimental observations or benchmark problems. After validation, the model is acceptable for simulation purposes. The procedures for model validation and parametric sensitivity analysis have been presented in Chapter 9.

To illustrate the model development methodology, four case studies have been presented in Chapter 10: an analytical model, a numerical model, a stochastic model and an ANN-based model. The detailed reasoning while making assumptions, the development of model equations and simulation methodology are discussed. The second example of a numerical model, the breaking of a model into several sub-models during model development, was discussed. The complete MATLAB code is given in Appendix B.

The last chapter, Chapter 11, discusses the various approaches used for simulation of a large plant. The methodology needed to break down a large problem into sub-problems, the handling of recycle streams and other topics are discussed. A brief discussion on the nature of the problem related to batch process scheduling is included.

The techniques for solving model equations are outside of the scope of the book. Hence, various topics on solving differential equations, optimisation, genetic algorithms and so on have not been included.

It was not possible to include every good model in this book. Only those models were chosen which I could access and for which I found a fit at a right place in the manuscript.

I hope that this book will be helpful to senior undergraduate and postgraduate students and fulfil the expectations of its readers.

Ashok Kumar Verma