Tanase G. Dobre and
José G. Sanchez Marcano

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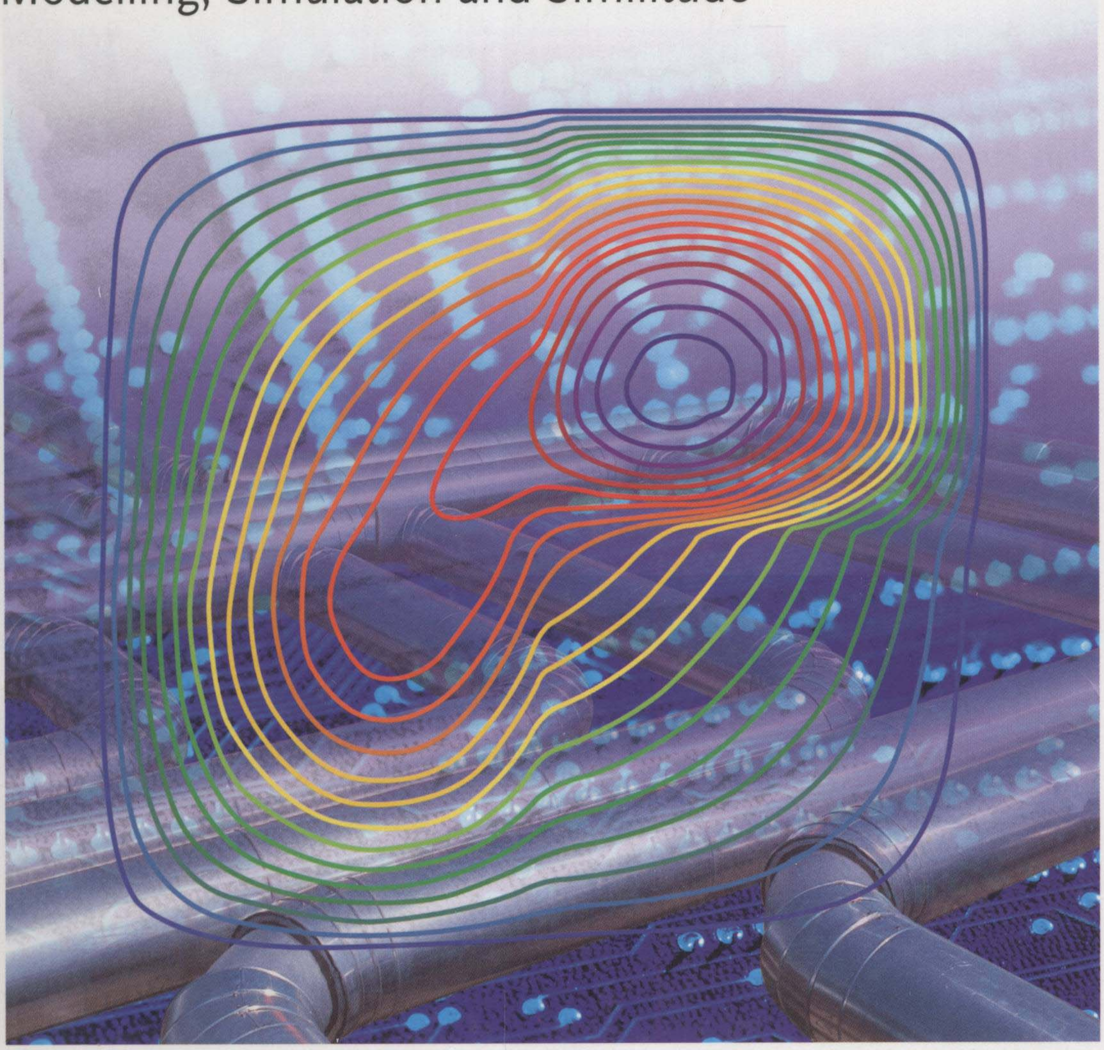
Chemical Engineering

Modelling, Simulation and Similitude



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To Christine, Laura, Benjamin and Anaïs, for their love and ongoing support
To Marie, Raluca, Diana and Fineta for their confidence and love

Preface

Scientific research is a systematic investigation, which establishes facts, and develops understanding in many sciences such as mathematics, physics, chemistry and biology. In addition to these fundamental goals, scientific research can also create development in engineering. During all systematic investigation, modelling is essential in order to understand and to analyze the various steps of experimentation, data analysis, process development, and engineering design. This book is devoted to the development and use of the different types of mathematical models which can be applied for processes and data analysis.

Modelling, simulation and similitude of chemical engineering processes has attracted the attention of scientists and engineers for many decades and is still today a subject of major importance for the knowledge of unitary processes of transport and kinetics as well as a fundamental key in design and scale-up. A fundamental knowledge of the mathematics of modelling as well as its theoretical basis and software practice are essential for its correct application, not only in chemical engineering but also in many other domains like materials science, bioengineering, chemistry, physics, etc. In so far as modelling simulation and similitude are essential in the development of chemical engineering processes, it will continue to progress in parallel with new processes such as micro-fluidics, nanotechnologies, environmentally-friendly chemistry processes and devices for non-conventional energy production such as fuel cells. Indeed, this subject will keep on attracting substantial worldwide research and development efforts.

This book is completely dedicated to the topic of modelling, simulation and similitude in chemical engineering. It first introduces the topic, and then aims to give the fundamentals of mathematics as well as the different approaches of modelling in order to be used as a reference manual by a wide audience of scientists and engineers.

The book is divided into six chapters, each covering a different aspect of the topic. Chapter 1 provides a short introduction to the key concepts and some pertinent basic concepts and definitions, including processes and process modelling definitions, division of processes and models into basic steps or components, as well as a general methodology for modelling and simulation including the modes of model use for all the stages of the life-cycle processes: simulation, design, parameter estimation and optimization. Chapter 2 is dedicated to the difficult task of

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classifying the numerous types of models used in chemical engineering. This classification is made in terms of the theoretical base used for the development or the mathematical complexity of the process model. In this chapter, in addition to the traditional modelling procedures or computer-aided process engineering, other modelling and simulation fields have also been introduced. They include molecular modelling and computational chemistry, computational fluid dynamics, artificial intelligence and neural networks etc.

Chapter 3 concerns the topic of mathematical models based on transport phenomena. The particularizations of the property conservation equation for mass, energy and physical species are developed. They include the usual flow, heat and species transport equations, which give the basic mathematical relations of these models. Then, the general methodology to establish a process model is described step by step – from the division of the descriptive model into basic parts to its numerical development. In this chapter, other models are also described, including chemical engineering flow models, the distribution function and dispersion flow models as well as the application of computational fluid dynamics. The identification of parameters is approached through various methods such as the Lagrange multiplicators, the gradient and Gauss-Newton, the maximum likelihood and the Kalman Filter Equations. These methods are explained with several examples including batch adsorption, stirred and plug flow reactors, filtration of liquids and gas permeation with membranes, zone refining, heat transfer in a composite medium etc.

Chapter 4 is devoted to the description of stochastic mathematical modelling and the methods used to solve these models such as analytical, asymptotic or numerical methods. The evolution of processes is then analyzed by using different concepts, theories and methods. The concept of Markov chains or of complete connected chains, probability balance, the similarity between the Fokker–Plank–Kolmogorov equation and the property transport equation, and the stochastic differential equation systems are presented as the basic elements of stochastic process modelling. Mathematical models of the application of continuous and discrete polystochastic processes to chemical engineering processes are discussed. They include liquid and gas flow in a column with a mobile packed bed, mechanical stirring of a liquid in a tank, solid motion in a liquid fluidized bed, species movement and transfer in a porous media. Deep bed filtration and heat exchanger dynamics are also analyzed.

In Chapter 5, a survey of statistical models in chemical engineering is presented, including the characteristics of the statistical selection, the distribution of frequently used random variables as well as the intervals and limits for confidence methods such as linear, multiple linear, parabolic and transcendental regression, etc. A large part of this chapter is devoted to experimental design methods and their geometric interpretation. Starting with a discussion on the investigation of the great curvature domain of a process response surface, we introduce sequential experimental planning, the second order orthogonal or complete plan and the use of the simplex regular plan for experimental research as well as the analysis of variances and interaction of factors. In the last part of this chapter, a short review of the application in the chemical engineering field of artificial neural networks is given. Throughout this chapter, the discussion is illustrated by some numerical applications, which include the relationships between the reactant conversion and the input concentration for a continuously stirred reactor and liquid–solid extraction in a batch reactor.

Chapter 6 presents dimensional analysis in chemical engineering. The Vaschy–Buckingham Pi theorem is described here and a methodology for the identification and determination of Pi groups is discussed. After this introduction, the dimensional analysis is particularized for chemical engineering problems and illustrated by two examples: mass transfer by natural convection in a finite space and the mixing of liquids in a stirred vessel. This chapter also explains how the selection of variables is imposed in a system by its geometry, the properties of the materials and the dynamic internal and external effects. The dimensional analysis is completed with a synthetic presentation of the dimensionless groups commonly used in chemical engineering, their physical significance and their relationships. This chapter finishes with a discussion of physical models, similitude and design aspects. Throughout this chapter, some examples exemplify the analysis carried out; they include heat transfer by natural convection from a plate to an infinite medium, a catalytic membrane reactor and the heat loss in a rectification column.

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Why Modelling?

Analysis of the cognition methods which have been used since early times reveals that the general methods created in order to investigate life phenomena could be divided into two groups: (i) the application of similitude, modelling and simulation, (ii) experimental research which also uses physical models. These methods have always been applied to all branches of human activity all around the world and consequently belong to the universal patrimony of human knowledge. The two short stories told below aim to explain the fundamental characteristics of these cognition methods.

First story. When, by chance, men were confronted by natural fire, its heat may have strongly affected them. As a result of these ancient repeated encounters on cold days, men began to feel the agreeable effect of fire and then wondered how they could proceed to carry this fire into their cold caves where they spent their nights. The precise answer to this question is not known, but it is true that fire has been taken into men's houses. Nevertheless, it is clear that men tried to elaborate a scheme to transport this natural fire from outside into their caves. We therefore realize that during the old times men began to exercise their minds in order to plan a specific action. This cognition process can be considered as one of the oldest examples of the use of modelling research on life.

So we can hold in mind that the use of modelling research on life is a method used to analyze a phenomenon based on qualitative and quantitative cognition where only mental exercises are used.

Second Story. The invention of the bow resulted in a new lifestyle because it led to an increase in men's hunting capacity. After using the bow for the first time, men began to wonder how they could make it stronger and more efficient. Such improvements were repeated continually until the effect of these changes began to be analysed. This example of human progress illustrates a cognition process based on experimentation in which a physical model (the bow) was used.

In accordance with the example described above, we can deduce that research based on a physical model results from linking the causes and effects that characterize an investigated phenomenon. With reference to the relationships existing between different investigation methods, we can conclude that, before modifying

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the physical model used, modelling research has to be carried out. The modelling can then suggest various strategies but a single one has to be chosen. At the same time, the physical model used determines the conditions required to measure the effect of the adopted strategy. Further improvement of the physical model may also imply additional investigation.

If we investigate the scientific and technical evolution for a random selected domain, we can see that research by modelling or experimentation is fundamental. The evolution of research by modelling and/or experimentation (i.e. based on a physical model) has known an important particularization in each basic domain of science and techniques. Research by modelling, by simulation and similitude as well as experimental research, have become fundamental methods in each basic scientific domain (such as, in this book, chemical engineering). However, they tend to be considered as interdisciplinary activities. In the case of modelling simulation and similitude in chemical engineering, the interdisciplinary state is shown by coupling the phenomena studied with mathematics and computing science.

1.1
Process and Process Modelling

In chemical engineering, as well as in other scientific and technical domains, where one or more materials are physically or chemically transformed, a process is represented in its abstract form as in Fig. 1.1(a). The global process could be characterized by considering the inputs and outputs. As input variables (also called "independent process variables", "process command variables", "process factors" or "simple factors"), we have deterministic and random components. From a physical viewpoint, these variables concern materials, energy and state parameters, and of these, the most commonly used are pressure and temperature. The deterministic process input variables, contain all the process variables that strongly influence the process exits and that can be measured and controlled so as to obtain a designed process output.

The random process input variables represent those variables that influence the process evolution, but they can hardly be influenced by any external action. Frequently, the random input variables are associated with deterministic input variables when the latter are considered to be in fact normal randomly distributed variables with mean $\bar{x}_j,\ j = 1, N$ ("mean" expresses the deterministic behaviour of variable x_j) and variance $\sigma_{xj},\ j = 1, N$. So the probability distribution function of the x_j variable can be expressed by the following equation:

$$f(x_j) = \frac{1}{\sqrt{2\pi}\sigma_{xj}} \exp\left(-\frac{(x_j - \bar{x}_j)^2}{2\sigma_{xj}^2}\right) \tag{1.1}$$

The values of $\bar{x}_j,\ j = 1, N$ and $\sigma_{xj},\ j = 1, N$ can be obtained by the observation of each x_j when the investigated process presents a steady state evolution.