The role of theory in science was formulated very brilliantly by Max Planck:

*Experimenters are the striking force of science. The experiment is a question which science puts to nature. The measurement is the registration of nature’s answer. But before the question is put to nature, it must be formulated. Before the measurement result is used, it must be explained, i.e., the answer must be understood correctly. These two problems are obligations of the theoreticians.*

Chemical engineering is an experimental science, but theory permits us to formulate correct experimental conditions and to understand correctly the experimental results. The theoretical methods of chemical engineering for modeling and simulation of industrial processes are surveyed in this book.

Theoretical chemical engineering solves the problems that spring up from the necessity for a quantitative description of the processes in the chemical industry. They are quite different at the different stages of the quantitative description, i.e., a wide circle of theoretical methods are required for their solutions.

Modeling and simulation are a united approach to obtain a quantitative description of the processes and systems in chemical engineering and chemical technology, which is necessary to clarify the process mechanism or for optimal process design, process control, and plant renovation.

Modeling is the creation of the mathematical model, i.e., construction of the mathematical description (on the basis of the process mechanism), calculation of the model parameters (using experimental data), and statistical analysis of the model adequacy.

Simulation is a quantitative description of the processes by means of algorithms and software for the solution of the model equations and numerical (mathematical) experiments.

The processes in chemical engineering are composed of many simple processes, such as hydrodynamic, diffusion, heat conduction, and chemical processes. The models are created in the approximations of continuous media mechanics.

The complex process model is constructed on the basis of the physical mechanism hypothesis. In cases where full information is available, it is possible to create a theoretical type of model. If the information is insufficient (it is not
possible to formulate the hydrodynamic influence on the heat and mass transfer),
the model is pattern theory, diffusion type or similarity criteria type. The absence
of information leads to the regression model.

The theoretical analysis of the models solves qualitative, quantitative, and
stability problems. The qualitative analysis clarifies the process mechanism or
similarity conditions. The quantitative analysis solves the problems related to the
scale-up and model adequacy. The stability analysis explains the increase of the
process efficiency as a result of self-organizing dissipative structures.

All theoretical methods are related to calculation problems. The solutions of the
model equations use analytical and numerical methods. The identification (esti-
mation) of the model parameters leads to the solutions of the inverse problems, but
very often they are incorrect (ill-posed) and need the application of regularization
methods, using a variational or an iterative approach. The solutions of many
chemical engineering problems (especially parameter identification) use minimi-
ization methods.

The book ideology briefly described above addresses the theoretical foundation
of chemical engineering modeling and simulations. It is concerned with building,
developing, and applying the mathematical models that can be applied success-
fully for the solution of chemical engineering problems. Our emphasis is on the
description and evaluation of models and simulations. The theory selected reflects
our own interests and the needs of models employed in chemical and process
engineering. We hope that the problems covered in this book will provide the
readers (Ph.D. students, researchers, and teachers) with the tools to permit the
solution of various problems in modern chemical engineering, applied science, and
other fields through modeling and simulations.

The solutions of the theoretical problems of modeling and simulations employ a
number of mathematical methods (exact, asymptotic, numerical, etc.) whose
adoption by engineers will permit the optimal process design, process control, and
plant renovation.

The modeling and the simulations of chemical systems and plants can be
achieved very often through a hierarchical modeling. This approach uses the
structural analysis of the process systems. The result of the structural analysis is a
quantitative description allowing further optimal process design, process control,
and plant renovation. The effectiveness of the optimal solutions can be enhanced if
they are combined with suitable methods of optimal synthesis. The latter is a
methodical basis and a guide for process system renovations.

The book incorporates a lot of fundamental knowledge, but it is assumed that
the readers are familiar with the mathematics at engineering level of usual uni-
versity courses.

The above comments are the main reasons determining the structure of this
book.

Part 1 concerns model construction problems. The mechanics of the continuum
approach is used for modeling hydrodynamic, diffusion, and heat conduction
processes as basic (elementary) processes in chemical engineering. The modeling
of complex processes in chemical engineering is presented on the basis of the
relation between the process mechanism and the mathematical description. The models are classified in accordance with the knowledge available concerning the process mechanisms. This means a situation when a theoretical model is available, i.e., sufficient knowledge of the process mechanism as well as the opposite situation of knowledge deficiency, which leads to regression models. Theoretical diffusion, dimensionless, and regression types of models are illustrated. The linear, nonlinear, and pattern mass transfer theories are considered too.

**Part 2** focuses on theoretical analysis of chemical engineering process models. The qualitative analysis uses generalized (dimensionless) variables and shows the degree to which the different physical effects participate in a complex process. On this basis, similarity criteria and physical modeling conditions are shown. The quantitative analysis concerns the scale-up problems and statistical analysis of the models. The stability analysis of the models permits the nonlinear mass transfer effects to be obtained and the creation of the self-organizing dissipative structures with very intensive mass transfer.

**Part 3** addresses the calculation problems in modeling and simulation. Different analytical and numerical methods for the solution of differential equations are considered. The estimation of the model parameters is related to the solutions of the ill-posed inverse problems. An iterative method for incorrect problem solutions is presented. Different methods for function minimization are shown for the purposes of process optimization and model parameter identification.

**Part 4** examines modeling and simulation of the chemical plant systems. The simulation of the systems on the basis of structure system analysis is presented. The optimal synthesis of chemical plants is considered in the case of the optimal synthesis of heat recuperation systems. This book can be used as a basis for theoretical and experimental investigations in the field of the chemical engineering. The methods and analyses presented permit theoretical problems to be solved, the experimental conditions to be correctly formulated, and the experimental results to be interpreted correctly.

*The fundamental suggestion in this book is the necessity for full correspondence (direct and inverse) between the separated physical effect in the process and the mathematical (differential) operator in the model equation.*

The main part of this book has a monographic character and the examples are from the author’s papers. The book uses the author’s lectures “Course of modeling and optimization” (subject chemical cybernetics in the Faculty of Chemistry of Sofia University “St. Kliment Ohridski”), “Course of modeling and simulation of chemical plant systems” (Bourgas University “Prof. Asen Zlatarov”), and “Master’s classes of theoretical chemical engineering” (Bourgas University “Prof. Asen Zlatarov”). That is why, as a whole, it is possible for it to be used as teaching material for modeling and simulation. This book proposes an exact formulation and the correct solution of quantitatively described problems in chemical engineering. It may be useful for scientists, Ph.D. students, and undergraduate students.

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