C. Boyadjiev
Theoretical Chemical Engineering

This survey presents the theoretical methods of chemical engineering for modeling and simulation of industrial processes. On this base it is possible to formulate correct experimental conditions and to understand rightly the experimental results.The book uses the mechanics of continuous media approach for modeling of the simple processes as hydrodynamic processes, mass and heat transfer processes. The theory of the scalar, vector and tensor fields permit to create the basic equations and boundary conditions. The problems of rheology, turbulence, turbulent diffusion and turbulent mass transfer are examined too.

The book incorporates a lot of fundamental knowledge, but it is assumed that the readers are familiar with the mathematics at engineering level and that they thought some special topics in usual university courses. It includes examples at the end of all chapters using the author's investigations. Therefore, it is highly valuable for scientists as well as graduate and PhD students.

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Modeling and Simulation

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Abstract

The theoretical methods of chemical engineering for modeling and simulation of industrial processes are surveyed in this book. On this basis it is possible to formulate correct experimental conditions and to understand correctly the experimental results.

The continuous media approach is used for modeling simple processes such as hydrodynamic processes, mass transfer processes, and heat transfer processes. The theory of scalar, vector, and tensor fields permits one to create the basic equations and boundary conditions. Problems of rheology, turbulence, turbulent diffusion, and turbulent mass transfer are examined too.

The chemical processes and adsorption models and especially the stoichiometry, reaction mechanism, reaction route, kinetics of simple and complex chemical reactions, physical and chemical adsorption, and heterogeneous reactions are discussed.

Different types of complex process models are presented depending on the process mechanism. The relation between the mechanism and the mathematical description is shown in the case of physical absorption. Characteristic scales, generalized variables, and dimensionless parameters are used for analysis of the process mechanism. Full information about this mechanism permits the creation of theoretical models. Mass transfer in film flows is an example of such models, where the effects of a chemical reaction and gas motion and absorption of slightly and highly soluble gases are considered.

The very complicated hydrodynamic behavior in column apparatuses is a reason for using diffusion-type models in the cases of mass transfer with a chemical reaction and interphase mass transfer. An average concentration model of an airlift reactor is presented.

Similarity theory models are demonstrated in the case of absorption in packed-bed columns. Generalized (dimensionless) variables and generalized individual cases are used for formulation of the similarity conditions and similarity criteria. The dimension analysis, mathematical structure of the models, and some errors in criteria models are discussed.

Regression models are preferred when there is complete absence of information about the process mechanism and the least-squares method is used for parameter identification.

A theoretical analysis of models of the mass transfer theories is presented in the cases of linear and nonlinear mass transfer. The model theories, boundary layer theory, mass transfer in countercurrent flows, influence of the intensive mass transfer on the hydrodynamics, boundary conditions of the nonlinear mass transfer problem, nonlinear mass transfer in the boundary layer, and the Marangoni effect are examined.

A qualitative theoretical analysis is presented as a generalized analysis. The use of generalized variables permits the analysis of the models of mass transfer with a chemical reaction, nonstationary processes, and stationary processes and the effect of the chemical reaction rate.

The generalized analysis permits the analysis of the mechanism of gas–liquid chemical reactions in the cases of irreversible chemical reactions, homogenous catalytic reactions, and reversible chemical reactions and the relationships between the chemical and physical equilibria during absorption.

A comparative qualitative analysis for process mechanism identification is presented in the cases of different nonlinear effects, nonstationary absorption mechanisms, and nonstationary evaporation kinetics.

A quantitative theoretical analysis is presented for solution of the scale-up problems and statistical analysis of the models. The similarity and scale-up, scale effect and scale effect modeling, scale-up theory and hydrodynamic modeling, and scale effect and scale-up of column apparatuses are discussed. The statistical analysis ranges over basic terms, statistical treatment of experimental data, testing of hypotheses, significance of parameters, and model adequacy of different types of models.

The stability analysis of the models examines the general theory of stability (evolution equations, bifurcation theory), hydrodynamic stability (fundamental equations, power theory, linear theory, stability, bifurcations, and turbulence), the Orr–Sommerfeld equation (parallel flows, almost parallel flows, linear stability, and nonlinear mass transfer), and self-organizing dissipative structures (interphase heat and mass transfer between gas–liquid immovable layers, Oberbeck–Boussinesq equations, gas absorption, and liquid evaporation).

The calculation problems in chemical engineering theory are related to the solutions of differential equations and identification of the model parameters (estimation). Different analytical methods, such as the similarity variables method, Green's functions, Laplace transforms, the Sturm–Liouville problem, the eigenvalue problem, and perturbation methods, are presented. Numerical methods (finite differences method, finite elements method) are examined on the basis of commercial software. Iterative solution methods are considered too.

Parameter estimation methods are discussed in the case of incorrect (ill-posed) inverse problems. An iterative method for parameter identification is presented for solution of correct, incorrect, and essentially incorrect problems. The optimization methods are examined as a basis of the least squares function minimization.

Models of chemical plant systems are presented as a set of process models and the relations between them. An algorithm for simulation of chemical plants is proposed. The methods of optimal synthesis of chemical plants are considered in the case of optimal synthesis of heat recuperation systems. The renovation of chemical plants is formulated as a mathematical model. The main problems are the renovation by optimal synthesis, renovation by introduction of new equipment, and renovation by introduction of new processes.

Examples from the author's investigations are presented at the end of all chapters.

Motto

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.**

Max Planck

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Preface

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 (estimation) 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 minimization 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 successfully 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 university 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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