THEORETICAL CHEMICAL ENGINEERING

Modeling and Simulation

by

Christo Boyadjiev

Institute of Chemical Engineering, Bulgarian Academy of Science, Sofia

Publisher: Springer, 2010

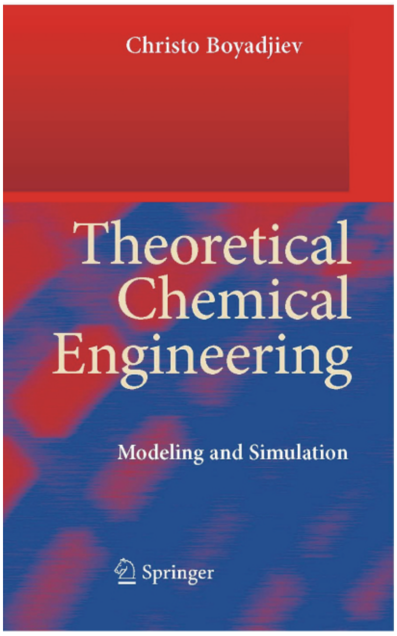
ISBN: 978-3-642-10777-1

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 non-linear 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 non-linear mass transfer problem, non-linear 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, non-stationary 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 non-linear effects, non-stationary absorption mechanisms, and non-stationary 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 non-linear 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.

Prof. Simeon Oka, Ph. D.
Scientific advisor – retired
Belgrade, Serbia