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Book review

ULLMANN'S
Modeling and Simulation

WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany
ISBN: 978-3-527-31605-2, 2007, XVIII+451 pags.

The book *Ullmann's - Modeling and Simulation*, published in 2007 by Wiley-VCH, is a handbook which includes contributions given by 16 authors, on several subjects concerning mathematical methods in model design and analysis applied in chemical engineering. The main covered topics are:

- mathematics in chemical engineering;
- model reactors and their design equations;
- mathematical modeling;
- molecular modeling;
- molecular dynamics simulation;
- computational fluid dynamics;
- design of experiments;
- microreactors- modeling and simulation.

Frequently encountered problems in engineering such as solving systems of linear or non-linear algebraic equations, handling functions of complex variables, types of ordinary and partial differential equations, integral equations, function approximation and function integration, along with the principal mathematical results concerning these topics are presented in a synopsis in the first part of the book. The principles of analytical and numerical methods used in solving these problems are outlined. The finite difference method, the finite element method and the boundary element methods, widely used in solving partial differential equations (PDE's), as well as numerical methods for solving integral equations, are briefly discussed. Finally, part I (authors: B. Finlayson, L. Biegler, I. Grossmann) discusses optimization methods and elements of probability and statistics.

The second part of the book (authors: V. Hlavacek, J. Puszynski, H. Viljoen, J. Gatica) presents models of the principal types of reactors used in industrial applications and problems connected to this topic. Batch reactors (involving both homogeneous and non-homogeneous systems), continuous stirred-tank reactors and packed-bed reactors are discussed. The physical quantities and laws concerning reactors, such as:

- mass and energy balances;
- definition of reactor parameters: average bed porosity, effective transport coefficients, wall heat transfer coefficient;
- thermo-mechanical effects in the reaction system

are introduced and discussed. Modern topics, such as numerical simulation and optimization of chemical reactors, are also included. Some examples concerning the optimization of batch systems, of continuous systems, of multibed adiabatic reactors with heat exchange between catalytic stages, are presented.

Part III of the book (author H. Bockhorn) presents the principles of mathematical modeling with applications to industrial chemistry and chemical engineering. The construction and classification of mathematical models are introduced. Further on, models based on transport equations for probability density functions are discussed, with emphasis on transport equations for single-point probability density functions. Special attention is given to models based on the laws governing the physicochemical processes (transport phenomena) such as the conservation of momentum, enthalpy and mass.

The fourth part (author D. Boyd) presents a short survey of the main trends in molecular modeling: conformal modeling, quantum mechanical modeling, force field modeling, and statistical modeling.

In the chapter Molecular Dynamics Simulation (authors P. Bopp, J. Buhn, M. Hampe) the types of interaction models (at intramolecular or intermolecular level) are discussed, based on classical Boltzmann statistical thermodynamics.

Part VI, Computational Fluid Dynamics (author A. Paschedag), presents the principal types of partial differential equations describing transport phenomena (the continuity equation, the equation of motion, Navier-Stokes equation, concentration equation, energy equation) and their associated initial and boundary conditions. Transport in multiphase systems or in systems with turbulent flow is considered. The finite volume method used for solving the aforementioned PDE equations is briefly presented.

The next chapter Design of experiments (authors S. Soravia, A. Orth) presents the basic principles for conducting experimental investigations and discusses the factorial designs, response surface designs and optimal designs.

Finally, the chapter Microreactors - Modeling and Simulation (author S. Hardt) discusses flow distributions and heat transfer in straight and curved channel geometries, micro-heat exchangers, mass transfer and chemical kinetics in microreactors.

Each chapter has an up-to-date well documented list of references. Practical examples are discussed and the mathematical, technical or computational solutions are outlined in a ready to use manner.

The book contains many illustrations (some in color) which make the text more comprehensible.

In conclusion, the book *Ulmann's – Modeling and Simulation*, published by Wiley – VCH in 2007, could be recommended to specialists in the field of chemical engineering, working in industry or universities, under or postgraduate students, PhD students and all those interested in topics concerning mathematical modeling in chemical reaction engineering and in transport phenomena.

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