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MATHEMATICAL MODELING OF CHEMICAL-TECHNOLOGICAL PROCESSES, DATA PROCESSING.

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Annotation: The article describes the mathematical modeling of chemical-technological processes and the scientific-methodological processes carried out in this regard.
Key Words: Simulation, experiments, optimization, mathematical,methods.

Introduction

The aim of this textbook is to give the reader insight and skill in the formulation, construction, simplification, evaluation/interpretation, and use of mathematical models in chemical engineering. It is not a book about the solution of mathematical models, even though an overview of solution methods for typical classes of models is given.

Models of different types and complexities find more and more use in chemical engineering, e.g. for the design, scale-up/down, optimization, and operation of reactors, separators, and heat exchangers. Mathematical models are also used in the planning and evaluation of experiments and for developing mechanistic understanding of complex systems. Examples include balance models in differential or integral form, and algebraic models, such as equilibrium models.

Main Part

The book includes model formulation, i.e. how to describe a physical/chemical reality in mathematical language, and how to choose the type and degree of sophistication of a model. It is emphasized that this is an iterative procedure where models are gradually refined or rejected in confrontation with experiments. Model reduction and approximate methods, such as dimensional analysis, time constant analysis, and asymptotic methods, are treated. An overview of solution methods for typical classes of models is given. Parameter estimation and model validation and assessment, as final steps, in model building are discussed. The question "What model should be used for a given situation?" is answered.

The book is accompanied by problems, tutorials, and projects. The projects, in smaller teams, include model formulation at different levels, analysis, parameter estimation, and numerical solution.

The book is aimed at chemical engineering students, and a knowledge basic chemical engineering, in particular transport phenomena, will be assumed. Basic mathematics, statistics, and programming skills are also required.

Using the book (course) the reader should be able to construct, solve, and apply mathematical models for chemical engineering problems. In particular:

- construct models using balances on differential or macroscopic control volumes for momentum, heat, mass, and numbers (population balances);
- construct models by simplification of general model equations;
- understand and use methods for model simplification;

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- understand differences between models;
- understand and use numerical solution methods:
- understand and perform parameter estimation;
- use model assessment techniques to be able to judge if a model is good enough.
- Mathematical modeling has always been an important activity in science and engineering. The formulation of qualitative questions about an observed phenomenon as mathematical problems was the motivation for and an integral part of the development of mathematics from the very beginning.

Although problem solving has been practised for a very long time, the use of math- ematics as a very effective tool in problem solving has gained prominence in the last 50 years, mainly due to rapid developments in computing. Computational power is par- ticularly important in modeling chemical engineering systems, as the physical and chem- ical laws governing these processes are complex. Besides heat, mass, and momentum transfer, these processes may also include chemical reactions, reaction heat, adsorption, desorption, phase transition, multiphase flow, etc. This makes modeling challenging but also necessary to understand complex interactions.

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