Mathematical Modelling and Simulation in Chemical Engineering

In order to model systems, understanding the basic principles and governing laws is essential for making suitable assumptions required to reduce the complexity of a system. Mathematical modelling and simulation tools provide a solid foundation for upgraded system performance. This book bridges the gap by elaborating the essential concepts, including differential equation models and development of model equations, useful for improved system functioning.

The analytical and numerical techniques for solving various mathematical model equations, including nonlinear algebraic equations, initial value ordinary differential equations (ODEs) and boundary value ODEs are discussed here. There is a detailed discussion on optimization methods and sensitivity analysis. In addition, numerous MATLAB/ Scilab applications are interspersed throughout the text and several case studies involving full details of simulation are presented. The accompanying website will host additional MATLAB/ Scilab problems, model question papers, simulation exercises, tutorials and projects. This book will be useful for students of chemical engineering, mechanical engineering, instrumentation engineering and mathematics.

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Preface

This course book on mathematical modelling and simulation has been structured for undergraduate and postgraduate students of Chemical Engineering. It can also be used as a reference book for Instrumentation and Control Engineering, Mechanical Engineering, and Mathematics.

The requirements for modelling a system are: first, an understanding of the underlying physics of the systems and the laws governing it; second, an ability to make suitable assumptions to analyze the system while retaining the valid and realistic description of its behaviour. The aim of this text is to provide readers such practice through several simple examples for setting up model equations followed by their solutions by either analytical or numerical techniques. Wherever possible, analytical methods are provided. For the numerical solution, Matlab/Scilab routines are used.

The first chapter introduces the basic steps in mathematical modelling. Chapter 2 presents the development of mathematical models for simple systems. It provides discussions through several examples making use of mass balance, energy balance or momentum balance equations. In addition, one example for a transport reactor is also given to analyze the problem in detail. The development of partial differential equation with the associated boundary conditions is given for an isothermal tubular reactor with the axial dispersion model.

Chapter 3 provides several examples illustrating the modelling of systems with complex behaviour. Systems exhibiting output multiplicity behaviour, input multiplicity behaviour, and oscillatory behaviour, etc., are discussed.

Chapter 4 presents commonly occurring linear differential equation models and the analytical solution of such equations. The series solutions are given for variable coefficient linear ODEs. Application of the Laplace transform method to solve linear partial differential equation is presented. The solution of a linear partial differential equation (PDE), by the method of separation variable, is also discussed with examples.

Chapter 5 presents the basics of the numerical solution of nonlinear algebraic equations, IVP nonlinear ODEs, BVP nonlinear ODEs, and nonlinear PDE model equations with examples.

Chapter 6 provides case studies involving variable coefficient ODEs, and PDEs with the details on the simulation of such systems.

Chapter 7 poses the problem of discriminating model equations for systems. The use of the periodic operation, to discriminate the model equations, is proposed with the simulation results.

Chapter 8 elucidates the sensitivity analysis of model equations. The direct differentiation method and the finite difference method are discussed.

Chapter 9 provides an overview of optimization methods by analytical methods and numerical methods. Several examples are given for the optimization problems. An introduction is given to the multi-objective optimization methods and the random search optimization method. The importance of estimating model parameters from the output of the system is brought out with examples.

In Chapter 10, the use of Matlab and Scilab routines is discussed to solve the mathematical model equations with several examples.

Chapter 11 provides an introduction to transfer function models, the development of simple model equations and the mathematical methods required to design PI/PID controllers for stable and unstable systems with examples.

Chapters 1, 2, 4, 5, a part of chapter 8, and a part of chapter 10 can be used for an undergraduate level course in any engineering discipline, and Chapters 3, 5, 7, 9 and 11 can be used for a post graduate level course in the Chemical Engineering program. Chapters 2, 3, 5, 9 and 11 can be considered at the postgraduate level for students from Mechanical Engineering, Instrumentation and Control Engineering, and Mathematics. For all the above disciplines, Chapter 10 can be marked for self-study, with two hours for demonstrating the simulation examples.

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