MATHEMATICAL MODELLING: THEORY AND APPLICATIONS

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Concepts and Case Studies

J. Caldwell and Y.M. Ram

Kluwer Academic Publishers

Mathematical Modelling

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VOLUME 6

This series is aimed at publishing work dealing with the definition, development and application of fundamental theory and methodology, computational and algorithmic implementations and comprehensive empirical studies in mathematical modelling. Work on new mathematics inspired by the construction of mathematical models, combining theory and experiment and furthering the understanding of the systems being modelled are particularly welcomed.

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Original monographs, comprehensive surveys as well as edited collections will be considered for publication.

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PREFACE

Over the past decade there has been an increasing demand for suitable material in the area of mathematical modelling as applied to science and engineering. There has been a constant movement in the emphasis from developing proficiency in purely mathematical techniques to an approach which caters for industrial and scientific applications in emerging new technologies. In this textbook we have attempted to present the important fundamental concepts of mathematical modelling and to demonstrate their use in solving certain scientific and engineering problems.

This text, which serves as a general introduction to the area of mathematical modelling, is aimed at advanced undergraduate students in mathematics or closely related disciplines, e.g., students who have some prerequisite knowledge such as one-variable calculus, linear algebra and ordinary differential equations. Some prior knowledge of computer programming would be useful but is not considered essential. The text also contains some more challenging material which could prove attractive to graduate students in engineering or science who are involved in mathematical modelling.

In preparing the text we have tried to use our experience of teaching mathematical modelling to undergraduate students in a wide range of areas including mathematics and computer science and disciplines in engineering and science. An important aspect of the text is the use made of scientific computer software packages such as MAPLE for symbolic algebraic manipulations and MATLAB for numerical simulation.

The book is divided into two main parts. Part I deals with continuous and discrete modelling. The starting point here is the background and fundamental concepts of mathematical modelling. In the formulation of mathematical models (Chapter 1) it is important to understand the mathematical modelling process, the input-output principle, simple rate models, models involving recurrence relations (i.e., discrete models), optimization models and sensitivity analysis.

In Chapter 2 (Compartment Problems) we explore simple linear problems which involve a single compartment (e.g., a room or tank) and the time rate of change of some specified quantity (e.g., heat energy or volume of liquid) within that compartment as it interacts with its environment. The work is extended to deal with multi-compartment problems and mathematical models are developed for problems involving systems of tanks including pollution.

Chapter 3 deals with continuous time models in the important areas of dynamics and vibration. Elementary concepts and principles are introduced and applied in practice by considering several dynamic systems and their mathematical models. The response of single degree of freedom systems is considered and important aspects such as equilibrium, linearisation and stability are dealt with. This work is extended for the more advanced reader to consider both modelling and response of multi-degree-of-freedom systems.

For some applications, e.g., in digital system control, the dynamics of the system is sampled after equal time intervals and so the response of the system involves discrete functions as opposed to continuous functions. So Chapter 4 concentrates on discrete models and includes some essential background material on finite-difference approximations and analytical solutions for linear systems of difference equations. The concept of stability is discussed and examples of discrete time models of dynamic systems are included. This work culminates in the finite-difference model of an eigenvalue problem by considering the problem of an axially vibrating rod.

Chapter 5 deals with numerical techniques for model nonlinear partial differential equations (PDE's) and is aimed primarily at graduate students. The example chosen to illustrate a range of possible numerical techniques for solution of nonlinear PDE's is that of Burgers' equation. The reason for this choice is that Burgers' equation is probably one of the simplest nonlinear PDE's for which it is possible to obtain an exact solution. Also, depending on the magnitude of the various terms in the equation, it behaves as an elliptic, parabolic or hyperbolic PDE. Hence it is very suitable as a model equation for testing and comparing numerical techniques. Such numerical techniques include finite-difference and Fourier methods, the method of lines, finite element methods with both fixed and moving nodes and variational-iterative schemes. Reference is made to past work by Caldwell and other co-researchers where more detailed information can be obtained from the list of bibliography.

The second part of the text, Part II, consists of a number of realistic Case Studies which illustrate the use of the modelling process in the solution of continuous and discrete models. These models are chosen to illustrate the use of the concepts, principles and techniques discussed in Part I.

Case Study A involves the design of biotreatment systems to process the effluent from a steel works. The inspiration here comes from former colleagues Professor Mark Cross, Professor Alfredo Moscardini and Yang, Yiu Wah.

Case Study B involves a deterministic model in the theory of contagious disease. The inspiration here comes from former colleague Dr Colin Creasy and students Andrew Biersterfield and Tse, Hoi Yan.

Case Studies C and D deal with analysis and synthesis of two mechanisms, namely, the cam-follower and the slider-crank. The function of the cam-follower mechanism is to transform rotational motion to linear. The synthesis problem of determining the parametric equations of the contour of the disk cam required to achieve a prescribed follower motion is studied in Case Study C. This essentially geometrical geometry problem involves in real life applications evaluation of some numerical derivatives of first and second order. The phenomenon of catastrophic cancellation associated with numerical differentiation is involved and a least squares smoothing technique is applied to overcome this difficulty.

In Case Study D we determine the position, velocity and acceleration of a slider-crank mechanism, and then evaluate the force applied on the pins connecting the various links. This problem demonstrates analysis of a dynamic system and its application in mechanism design. Both Case Studies C and D are solved via the use of MATLAB.

Each Chapter of Part I ends with a section comprising a number of exercises to be undertaken by students using the text. Challenging problems are also included at the end of each Case Study. To help make the material as clear as possible a number of worked test examples have been included in appropriate parts of the text.

We would like to express our thanks to other authors, former and present modelling colleagues and final year undergraduate students (too numerous to mention by name) who have helped over the past years to give us some of the important modelling ideas contained in this textbook. Finally, we wish to thank Chiu, Chi Keung for his part in the skillful typing of the manuscript.

We hope you find this book both interesting and challenging!

Dr Jim Caldwell
Dr Yitshak Ram

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CONTENTS

Part I

CONTINUOUS & DISCRETE MODELLING

Chapter 1

FORMULATION OF MATHEMATICAL MODELS.

1.1 The Mathematical Modelling Process

The use of mathematics in solving real-world problems is often referred to as 'mathematical modelling'. We could define this as the process of describing a real-world situation using mathematics. However, it must be done in such a way that it helps in the solution of the given problem. The idea of 'modelling' should be emphasized in that it helps to remind us that we must pay attention to things other than mathematics. The following flowchart in Figure 1.1 showing the various stages of the mathematical modelling process is by now well accepted and has been published by many authors of mathematical modelling textbooks.

At stage 1 the modeller has to become familiar with the problem he is trying to solve and to be clear about his objectives. The next stage involves starting to build the model. Here the modeller must decide which features of reality are to be included in the model and which can be neglected. Stage 3 involves formulation of the mathematical problem. This is the crucial stage and often the most difficult one. It involves deciding on symbols for the variables previously chosen at stage 2. Also any information we have about the real situation must be translated into equations or other mathematical statements. It is possible to use a number of techniques to translate the original question (or objective) into a question (or objective) about these equations, e.g., how to recognize and formulate proportionality relations and linear relations between the variables; how to use the 'input-output principle', i.e.

$$\text{Increase} = \text{Input} - \text{Output}$$

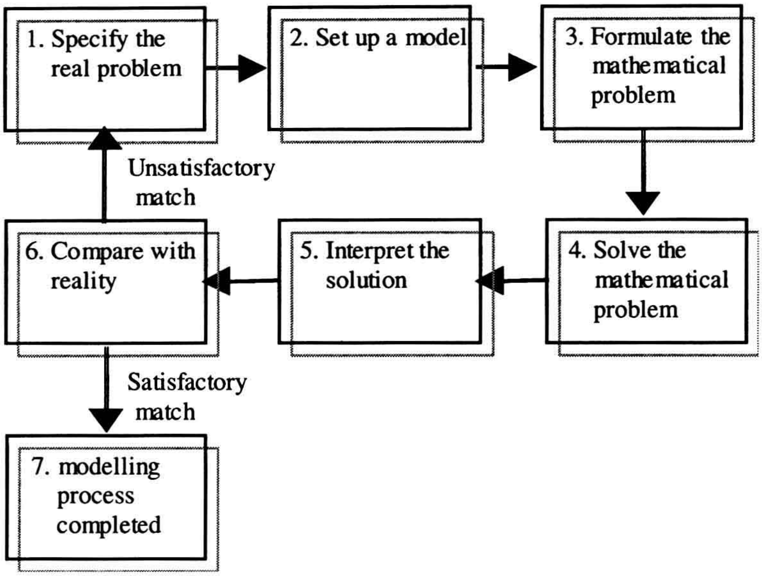

Figure 1.1 A flow-chart showing the various stages of the modelling process.

in formulating differential equations. (This important issue will be discussed in more detail in Section 1.2).

Stage 4 involves the process of solving the mathematical problem. Obviously skill and experience are important qualities here. Decisions need to be made on the method of solution (analytical or numerical) and whether to opt for a simple approximate method of solution or a more complicated accurate method. A detailed check on the mathematics is important.

Stage 5 involves the interpretation of the results of the model. One should consider whether the model behaves reasonably when changes are made to some of the conditions. The accuracy to be expected of the model and the domain of validity are other points to be considered here.

In comparing the model with reality at stage 6 we need to carry out the processes of validation, evaluation and iteration. If we feel that the model can be improved we have the opportunity of returning to stage 1 and going round the loop again. Mathematical modelling can be regarded as an iterative process where we start from a crude model and gradually refine it until it is good enough to solve the original problem.