



## Book Review

*Parametric Sensitivity in Chemical Systems*, by Arvind Varma, Massimo Morbidelli and Hua Wu, 1999. Cambridge Series in Chemical Engineering, Cambridge University Press. £60.00/\$90.00, ISBN: 0-521-62171-2.

This is the first textbook to provide a thorough treatment of the concept of parametric sensitivity and the mathematical tool it generated, sensitivity analysis, in chemical systems. The parametric sensitivity is the analysis of how a system responds to changes in the parameters and initial conditions. The book is designed to introduce sensitivity analysis in chemical systems for a senior graduate level specialized course on chemistry, biochemistry or chemical engineering post-graduate programmes. It should appeal to any researcher who is interested in the behaviour of chemical systems and applied mathematicians will find a rich source of interesting problems. The text should be accessible to any reader with some knowledge of calculus, differential equations, and numerical solutions of ordinary differential equations.

*Parametric Sensitivity in Chemical Systems* consists of 10 chapters. The book seems to be divided into three parts. In the first part, Chapter 1 'Introduction' gives a brief introduction and an overview of the topics of the book. In Chapter 2 'Introduction to Sensitivity Analysis', the authors present the basic definition and introduce the mathematical background to obtain the local sensitivity or normalized/relative sensitivity; these are the direct differential method, finite difference method and Green's function method. Attention is drawn to the advantages and disadvantages of the three methods, emphasizing that the Green's function method for estimating the sensitivities can be more convenient when the number of parameters is greater than the equations, while the finite difference method is more efficient for a few parameters. Global sensitivity is introduced to handle stochastic problems, but this method is hardly used in the textbook. Unfortunately, the authors do not introduce enough applications to illustrate the results expected with the methodologies. There are many general comments, but readers learning sensitivity analysis will find it very difficult to understand how a system responds to changes in the parameters with the examples introduced.

The second part of the book, Chapters 3–7, is used to discuss the use of sensitivity to identify the 'sensitive regions' for various types of chemical reactors where either a single or complex reaction occurs. The reactors' studies are presented in the different chapters, 'Thermal Explosion in Batch Reactions' (Chapter 3), 'Runaway in Tubular Reactions' (Chapter 4), 'Parametric Sensitivity in Continuous-Flow Stirred Tank Reactors' (Chapter 5) and 'Runaway in Fixed-Bed Catalytic Reactors' (Chapter 6). In Chapter 7 'Parametric Sensitivity and Ignition Phenomena in Combustion Systems' shows the importance of parametric sensitivity in

combustion chemistry, in particular in the study of radicals and the identification of elementary reactions. The chapters in this part of the book are written for those interested in the application of sensitivity analysis in chemical process engineering, but readers learning sensitivity analysis will find these chapters extremely useful as they are very well-written with extensive references and examples are carefully laid down with full details. The structure of the chapters is very effective from a pedagogical point of view, there are many internal cross-references and comparisons, and continuous references to the basic definitions presented in Chapter 2.

Chapters 8, 9 and 10 comprise the third part of the book illustrating the applications of sensitivity analysis to various chemical systems. This part of the book is of special interest to mathematical biologists. Chapter 8 'Sensitivity Analysis in Mechanistic Study and Model Reduction' focused on one of the fields where sensitivity analysis has been most widely used: (1) the determination of a reduced model (a minimum model) providing the same properties and predictions of the full model and (2) the identification of elementary reactions in a detailed and complex mechanism consisting of a large number of elementary steps. The subject of this chapter is particularly crucial in this post-genomic era when there is a great interest in dissecting the reaction mechanism of a complex biochemical reaction (gene and/or metabolic networks) and solving numerically large and complex models. In Chapter 9 'Sensitivity Analysis in Air Pollution' the applications of sensitivity analysis to air pollution control are shown. The use of parametric analysis to evaluate the influence on model predictions through functional and global sensitivity is discussed. The latter is of particular importance as air pollution processes involve large simulation models characterized by a number of physico-chemical and meteorological parameters with large uncertainties. The concepts of global sensitivity for stochastic problems introduced in Chapter 2 are used to study the relationship between pollutant emission sources and regional air quality, and evaluating the pollutant variations with changes in the parameters. In these problems, the authors try to predict the sensitivity concentration at a particular geographical location to pollution at other points. The models are governed by partial differential equations, but the sensitivities are determined for integrals over different areas. Finally, Chapter 10 'Sensitivity Analysis in Metabolic Processes' is dedicated to metabolic systems. The chapter provides a flavour of the potential of sensitivity analysis in this field. The first applications of sensitivity analysis to metabolism leads to the development of three fundamental theories: metabolic control analysis, biochemical systems theory and flux-oriented theory. The authors develop the chapter along the lines of the metabolic control theory studying the yeast glycolytic pathway and the gluconeogenesis from lactate.

In my opinion, this book can be used as a reference in which it is only necessary to read Chapters 1 and 2 for a short introduction, definition of terms and mathematical background to the subject. Then the reader can study the subject of interest in its corresponding chapter. Each chapter begins with a short introduction giving an overview of the subject. The chemical systems, reactions and problems

are introduced in another section, and the authors always provide references to the basic definitions of Chapter 2. At the end of most of the chapters, a nomenclature table is given and an extensive bibliography. Unfortunately, some chapters lack a glossary of symbols and abbreviations, and exercises are not given in any chapter. In the book, I did not find any reference to principal component analysis, a potentially important supplement to sensitivity analysis. The major issue with sensitivity analysis is that it generates an enormous amount of numerical data from which it may be difficult to extract meaningful kinetic information. It may be very difficult to establish the relative importance of certain kinetic features in very complex mechanisms, particularly since the sensitivity equations are time dependent. The primary purpose of principal component analysis is to provide an absolute measure of significance of the parameters.

This is an extraordinary and remarkable book summarizing a broad field in one volume. The authors have done an admirable job, providing numerous examples for the class. An attractive feature of the book is having this collection of subjects and examples on sensitivity analysis for chemical systems. Moreover, the book is easy to browse and is written in a friendly style. This volume fills a very special niche and deserves a place on the bookshelf of anyone interested in parametric sensitivity analysis.

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