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Book Reviews

Parametric Sensitivity in Chemical Systems

A. Varma, M. Morbidelli, and H. Wu, Cambridge University Press, New York, 1999, 342 pp., $80.00

A major trend in modern engineering research is the exploitation of the enormous computing power readily available to researchers. Complex but mathematically well-posed problems can now be solved and graphed routinely by direct numerical simulations. However, numerical simulations can be performed only when the parameters involved in the problem are given specific numerical values. Therefore, a perennial question for modern researchers is as follows: How sensitive are the computed results to changes or uncertainties of these parameters? As the title indicates, this book focuses on this important question and shows how the chemical systems research community deals with it.

The generic problem is the following. An n-dimensional vector $\boldsymbol{y}$ evolves in time as governed by a system of (nonlinear) ordinary or partial differential equations. The total number of input parameters of the problem is m and is represented by a m-dimensional vector $\boldsymbol{k}$. The question to be addressed is, What happens to the features of interest of the solution $\boldsymbol{y}(t)$ when $\boldsymbol{k}$ is changed? After an overview and introduction chapter, Chapter 2 lays the groundwork for the rest of the book. The concepts of local, objective, and global sensitivity indices, including their appropriate normalized versions, are defined and their method of calculation explained. The obvious strategy to extract sensitivity information is to use brute force: repeat the calculation for other interesting values of $\boldsymbol{k}$ and compare the results. For asymptotically small changes in $\boldsymbol{k}$, one may linearize and all of the small $\Delta\,\boldsymbol{k}$ sensitivity information related to the $\boldsymbol{y}$ vector can be represented by the Jacobian of $\boldsymbol{y}$ with respect to $\boldsymbol{k}$, an $n > m$ time-dependent matrix each element of which is, by definition, a local sensitivity index. When $m \gg n$, the computational effort can be substantially reduced by taking advantage of the methods of Green's function on the linearized equations to be solved. Chapters 3–7 deal with five distinct problems with "runaway" (or ignition) possibilities in chemical systems. All except Chapter 4 are governed by ordinary differential equations; the exception is governed by just algebraic equations. In each case, the existing literature is reviewed, starting with studies that do not use sensitivity indices and ending with studies that do. The major observation is that the sensitivity indices are expected to peak at the runaway boundary in the m-dimensional $\boldsymbol{k}$ space. Hence the runaway boundary can be located by finding the peaks of sensitivity indices using numerical computations. Chapter 8 studies complex chemical kinetics, showing that the elementary reactions that must be kept in a reduced chemistry model (to be able to quantitatively reproduce some user-selected features of interest of the original solution) can be identified by examining the time histories of the normalized local sensitivity indices. Chapter 9 uses the air pollution problem to illustrate the case when the original governing equation is a partial differential equation. Chapter 10 studies metabolic processes governed by ordinary differential equations, the admittedly minor twist here being that the vector representing the parameters is defined in a special way.

This book is a welcome resource to researchers in chemical systems interested in sensitivity analysis. To this reviewer, however, it is a somewhat disappointing book. The authors have limited themselves to reproducing the expositions already in the literature, seldom providing additional insights, refinements, or critiques. In many instances, major claims were echoed without supporting rationalizations (e.g., on page 20, the controversial claim is made that the ordinary equations for the local sensitivity indices may be stiffer than the original equations and are therefore more difficult to compute). Nevertheless, sensitivity analysis is clearly here to stay in the modern age of direct numerical simulations, and this pioneering book fulfills a current need in the chemical system community.

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IUTAM Symposium on Transformation Problems in Composite and Active Materials

Edited by Yehia A. Bahei-El-Din and George J. Dvorak, Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, 317 pp., $143.00

This IUTAM symposium focused attention on new directions in micromechanics research for application to both composite and smart materials. Topics included in the symposium proceedings may be grouped into six topics covered by 23 papers. The first six papers deal with the inelastic behavior of composite materials. Subjects discussed include multiphase composite materials modeling of the micro–macro viscoplastic behavior of single-crystal super alloys and the effect of mechanical stresses leading to morphological changes in the microstructure of materials such as Ni-based superalloys. Other topics include constitutive models for predicting the behavior of two-phase materials, including porous and rigidly reinforced materials, as well as models using transformation strain for predicting the rate-dependent/independent behavior of elastoplastic polycrystals and composite materials. Two of the papers focus on composite laminate construction modeling, one dealing with a method for predicting the failure of continuous-filament metal matrix composites subject to environmental conditioning and the other discussing the inelastic behavior of laminates, including the effects of lamina microgeometry.

The second group of five papers examines issues dealing with understanding and characterizing the behavior of shape memory alloys (SMAs), as exemplified by NiTi. Research areas include shape memory behavior of single crystals and polycrystals, evolution of plastic strains associated with thermally induced cyclic phase transformations, and energy transfer issues accompanying phase changes. Also covered is the role of stress and temperature as they affect the free energy of the SMAs and the development of a macroscopic description for the thermochemical behavior of SMAs based on the principles of the thermodynamics of irreversible processes. One paper in this section reports on approaches to the design of piezocomposites for hydrophone applications.

The third set of four papers deals with the subject of functionally gradient materials (FGMs). Such materials are represented by graded microstructures, and the papers in this section include studies on the effect of through-the-thickness changes of the variable mechanical properties for isotropic, inhomogeneous materials, current thermoelastic models describing the performance of graded microstructures subject to nonuniform loads, modeling of FGMs as a linear thermoelastic composite consisting of a homogeneous matrix with a statistically inhomogeneous set of inclusions, and the effect of thermally induced stresses as effecting cracking in FGMs subject to sudden cooling. The fourth group of three papers deals with transformation problems in composite structures. Included are such topics as the design of isotropic composites using two- and three-phase topology optimization methods; exploring the effects of fiber prestraining, including mandrel stiffness affecting the determination of composite residual stresses; and evaluating the dynamic response of elastic–viscoplastic sandwich beams with asymmetrically arranged thick layers. The fifth series of three papers deals with the subject of adaptive structures. Included in this group of papers are a discussion of a new theory of smart composite structures consisting of servos and actuators and based on a continuum mechanics approach, shape control of smart structures using piezoelectric devices, and SMAs.

The final two papers concentrate on elasticity issues. One examines the development of a variational approach for elastic energy minimization of Martensitic polycrystals, and the other studies optimal cavity shape for minimal energy change for a material without a defined cavity shape to a material with a defined cavity shape. The papers included and reported on in this symposium represent a useful collection of research contributions that merit the attention of researchers active in the cited topical areas.

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