Parametric sensitivity in chemical systems.

A. Varma, M. Morbidelli, H. Wu. Cambridge University Press, 1999, £50.00 (US\$ 80.00) hardback, pp. 342 ISBN 0521621712.

Parametric sensitivity is a property of a physical or chemical system, where the system responds with a large change in state variables if one or more system parameters are varied only slightly. The interest of both academics and practicing chemical engineers in parametric sensitivity was greatly enhanced already in the mid-1950s, when Bilous and Amundson [1] demonstrated that the hot spot temperature in a homogeneous tubular reactor can increase by almost 100 K when the inlet temperature into the reactor is increased only by 1 or 2°. As such a phenomenon can lead to a runaway of the reactor with possible catastrophic consequences, studies of parametric sensitivity aiming at formulation of various sensitivity indices and/or sufficient criteria for safe ('non-sensitive') operation of reactors and other equipment flourished in the literature, and are documented throughout this book.

The book of Varma, Morbidelli and Wu represents the first comprehensive description of parametric sensitivity in chemical systems. The authors introduce the notions of absolute and normalized (relative) sensitivities in Chapter 2, where they also define the sensitivity indices for state variables with respect to individual parameters (row sensitivity vector) as well as the sensitivity indices for all state variables with respect to the same parameter constituting the column sensitivity vector. The arrangement of row or column sensitivity vectors then forms the sensitivity matrix and the authors discuss various numerical techniques used for computing local sensitivities (evaluation of the sensitivity matrix), particularly the direct differential, finite difference and the Green's function method. Perhaps the connection of the local sensitivity equations with the use of variational equations in the computation of the dependence of a solution of model equation on a parameter used in standard continuation algorithms could have been introduced at this point. The discussions of global sensitivity (the response to simultaneous variations in all relevant parameters) and stochastic sensitivity analysis follow.

In the last 15 years the authors have published a large number of journal articles on the subject of parametric sensitivity in chemical reactors and on ignition in combustion. They use their accumulated experience in the description of sensitivity and identification of sensitive regions of batch, tubular, continuous flow, stirred tank, and fixed bed reactors presented in the next four chapters. These four chapters form, in my opinion, the most useful part of the book. They contain not only a large number of practical examples of real reaction systems in common types of reactors, but also a comparison of sensitivity criteria proposed by various authors, an illustration of the usefulness of such notions as 'normalized objective sensitivity' and plots of sensitive regions for all types of reactors. The following chapter is devoted to an illustration of how the sensitivity concept can be used to analyse explosions in mixtures of hydrogen or hydrocarbons with oxygen. The next chapter describes the possibilities of application of sensitivity analysis to complex reaction kinetic models with the aim of obtaining a robust reduced (minimum) kinetic model. The description of the sensitivity analysis in air pollution reaction-diffusion models explains the methods of global sensitivity analysis and uses the concepts and methods developed mainly in the eighties by Seinfeld and coworkers. In the last chapter the authors use two examples to illustrate possible applications of sensitivity analysis to vast and rapidly developing complex field of kinetic description of metabolic networks.

The book could well serve as a complementary text to graduate courses on chemical reaction engineering and will be also appreciated by practicing chemical engineers, particularly those dealing with reacting systems.

References

 O. Bilous, N.R. Amundson, Chemical reactor stability and sensitivity, II. Effect of parameters in sensitivity of empty tubular reactors, AIChE J. 2 (1956) 117

> Dr. Miloš Marek Department of Chemical Engineering Institute of Chemical Technology Technická, 5 166 28 Prague 6, Czech Republic *Tel.: +420-2-2435-3104/+420-2-2431-0370; fax.: +420-2-311-7335 E-mail address: marek@vscht.cz (M. Marek)

PII: S1385-8947(99)00116-3