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Modelling Techniques for Catalyst Development

Computer-Aided Design of Catalysts

EDITED BY E. ROBERT BECKER AND CAMO J. PEREIRA, Marcel Dekker Inc., New York, 1993, 640 pages, ISBN 0–8247–9003–0, U.S.$195.00

This book is the 51st in an occasionally excellent series on the chemical industries, and while it has its limitations it is nevertheless a valuable addition to the collection. The series consists of assembled chapters on a theme contributed by distinguished professionals. As such the volumes often lack coherence and stand or fall on the excellence of the contributions and the timeliness of the theme. This book is certainly timely as the use of computing methods in catalysis is growing rapidly. Computer aided design can mean different things; here the editors define it as "the process of selecting catalyst properties that ..... optimise the reactor performance". The emphasis on choosing catalyst properties means that there is very little on the design of new catalysts in this book. Rather the chapters deal with the methods for the measurement and modelling of catalyst parameters and the application of these methods in various industrial processes. Also missing is any attempt to discuss the modelling and economics of entire processes and plants; the emphasis is firmly on the performance of the reactor section.

The early chapters deal with modelling methods, such as: selectivity patterns in methane partial oxidation; modelling complex mixtures in catalytic cracking using carbon centre methods; Monte Carlo simulations for complex hydrotreating mixtures; pore diffusion models; catalyst pellet impregnation profiles and catalyst wetting effects on multiphase reactions. Later chapters concentrate on particular applications, such as Fischer-Tropsch catalysts, automobile catalysts including transient behaviour in monolith reactors; polymerisation catalysts; membrane reactors and petroleum refining. Platinum group metals feature here most directly, particularly platinum, palladium and ruthenium.

The chapter on the design of Fischer-Tropsch catalysts by E. Iglesia, S. C. Reyes and S. L. Soled, compares cobalt and ruthenium catalysts in the context of models which combine transport processes and elementary kinetics, and concludes that selectivity is dominated by the transport processes rather than by the nature of the active sites.

Chapters on modelling for automotive emission control by S. H. Oh, and design of monolithic catalysts for improved transient reactor performance by K. Zygourakis, use platinum catalysts as the basis for a discussion of modelling in car exhaust systems. Oh reviews his outstanding work and shows that even with many simplifying assumptions useful predictions as to catalyst loadings and performance may be obtained. The application of this approach to heated catalysts was discussed at the recent North American Catalysis Society meeting. The importance of 2-dimensional modelling for problems such as flow maldistribution and other transient effects is dealt with at greater length by Zygourakis.

Palladium features most extensively in a chapter on catalytic membrane reactors by T. T. Tsotsis, R. G. Minet, A. M. Champagnie and P. K. T. Liu. This topic has a long history and remains popular due to the inherent elegance of controlling reactant addition or product removal by a selective membrane. However large scale applications await the development of membranes that are thin enough and robust enough for the demanding conditions of most petrochemical processes.

This book is a useful contribution to bridging the gap between chemical engineers and chemists in the field of catalyst and reactor design. While individual chapters may disappoint specialists on any given topic, together they provide a valuable introduction to the area and can be read profitably by non specialists; the book will be of use in advanced education. J.C.F.