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Catalysis Today 53 (1999) 159

CATALYSIS TODAY

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Preface

This issue of Catalysis Today focuses on the microkinetic modelling of catalytic reactions. The purpose of this issue is two-fold. Firstly, to present specific examples of recent work on the development of microkinetic models and, secondly, to introduce new theoretical ideas for extending microkinetic models to consider reactions on heterogeneous surfaces.

Specific applications of the microkinetic method in heterogeneous catalysis are presented in the first set of papers. Ammonia synthesis over iron and the water-gas shift reaction over copper are discussed by Waugh. Further developments in ammonia synthesis, catalysed by supported ruthenium, are then presented by Hinrichsen. The inclusion of diffusion in microkinetic models is discussed by Nijhuis et al. with respect to zeolite catalysis.

Despite the advances that have been made in acquiring kinetic data for the individual steps of catalytic reactions, the mathematical methods used to incorporate these data into kinetic models are often over-simplified. In the second set of papers, on modelling theory, recent ideas on applying fractal geometry and numerical simulation to model catalytic reactions are presented.

The application of fractal concepts to develop models of transport and reaction within porous catalysts is discussed in a pair of papers. In the first of these papers, Rigby presents an analysis of diffusion on the surface of amorphous catalyst supports. The second paper on this subject, by Coppens, discusses molecular transport and reaction within the fractal pores of alumina catalyst supports. These two papers are followed by a more general discussion on modelling transport and reaction in catalyst pellets by Keil.

Frequently, kinetic models of catalytic reactions assume that the catalyst surface is uniform. While it is acknowledged that this is a serious deficiency, the incorporation of information from catalyst characterisation studies in kinetic models is a demanding task. Monte Carlo simulation, however, provides a powerful numerical framework by which the influence of the catalyst surface structure on the reaction kinetics can be accounted for. The final set of three papers by Persson et al., Jansen et al., and McLeod discuss the application of Monte Carlo simulation to modelling catalytic reactions. In these three examples, an emphasis has been placed on supported-metal catalysis.

The Editor would like to thank both the authors and the referees for their contributions to this issue. It is hoped that this collection of papers will introduce new numerical tools to those engaged in experimental catalysis and will encourage their use in applied catalysis.

Alistair S. McLeod
University of Cambridge
Department of Chemical Engineering
Pembroke Street
Cambridge, CB2 3RA, UK
Present address
School of Chemical Engineering
University of Edinburgh, Kings' Buildings
Mayfield Road, Edinburgh EH9 3JL
UK

PII: S0920-5861(99)00113-3