Catalyst Design

Heterogeneous catalysis is widely used in chemical, refinery, and pollutioncontrol processes. For this reason, achieving optimal performance of catalysts is a significant issue for chemical engineers and chemists. This book addresses the question of how catalytic material should be distributed inside a porous support in order to obtain optimal performance. It treats single- and multiple-reaction systems, isothermal and nonisothermal conditions, pellets, monoliths, fixed-bed reactors, and membrane reactors. The effects of physicochemical and operating parameters are analyzed to gain insight into the underlying phenomena governing the performance of optimally designed catalysts. Throughout, the authors offer a balanced treatment of theory and experiment. Particular attention is given to problems of commercial importance. With its thorough treatment of the design, preparation, and utilization of supported catalysts, this book will be a useful resource for graduate students, researchers, and practicing engineers and chemists.

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Catalyst Design

OPTIMAL DISTRIBUTION OF CATALYST IN PELLETS, REACTORS, AND MEMBRANES

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To our teachers and students

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Preface

Heterogeneous catalysis is used widely in chemical, refinery and pollution-control processes. Current worldwide catalyst usage is about 10 billion dollars annually, with ca. 3% annual growth rates. While these numbers are impressive, the economic importance of catalysis is far greater since about \$200–\$1,000 worth of products are manufactured for every \$1 worth of catalyst consumed. Further, a vast majority of pollution-control devices, such as catalytic converters for automobiles, are based on catalysis. Thus, heterogeneous catalysis is critically important for the economic and environmental welfare of society.

In most applications, the catalyst is deposited on a high surface area support of pellet or monolith form. The reactants diffuse from the bulk fluid, within the porous network of the support, react at the active catalytic site, and the products diffuse out. The transport resistance of the porous support alters the concentrations of chemical species at the catalyst site, as compared to the bulk fluid. Similarly, owing to heat effects of reaction, temperature gradients also develop between the bulk fluid and the catalyst. The consequence of these concentration and temperature gradients is that reactions occur at different rates, depending on position of the catalyst site within the porous support. In this context, since the catalytic material is often the most expensive component of the catalyst-support structure, the question naturally arises as to how should it be distributed within the support so that the catalyst performance is optimized? This book addresses this question, both theoretically and experimentally, for supported catalysts used in pellets, reactors and membranes.

In Chapter 2, optimization of catalyst distribution in a single pellet is considered, under both isothermal and nonisothermal conditions. Both single and multiple reaction systems following arbitrary kinetics are discussed. Chapter 3 deals with optimization of catalyst distribution in pellets comprising a fixed-bed reactor, while systems involving catalyst deactivation are addressed in Chapter 4. In Chapter 5, the effect of catalyst distribution on the performance of inorganic membrane reactors is presented, where the catalyst is located either in pellets packed inside an inert tubular membrane or within the membrane itself. Issues related to catalysts of significant commercial importance, including automotive, hydrotreating,

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composite zeolite, biological, and functionalized polymer resin types, are addressed in Chapter 6. The final Chapter 7 considers catalyst preparation by impregnation techniques, where the effects of adsorption, diffusion and drying on obtaining desired nonuniform catalyst distributions within supports are discussed. This book should appeal to all those who are interested in design, preparation and utilization of supported catalysts, including chemical and environmental engineers and chemists. It should also provide a rich source of interesting mathematical problems for applied mathematicians. Finally, we hope that industrial practitioners will find the concepts and results described in this book to be useful for their work.

This book can be used either as text for a senior-graduate level specialized course, or as a supplementary text for existing courses in reaction engineering, industrial chemistry or applied mathematics. It can also be used as a reference for industrial applications.

We thank our departmental colleagues for maintaining an atmosphere conducive to learning. We also thank our families for their encouragement and support, which made this writing possible.

> Massimo Morbidelli Asterios Gavriilidis Arvind Varma