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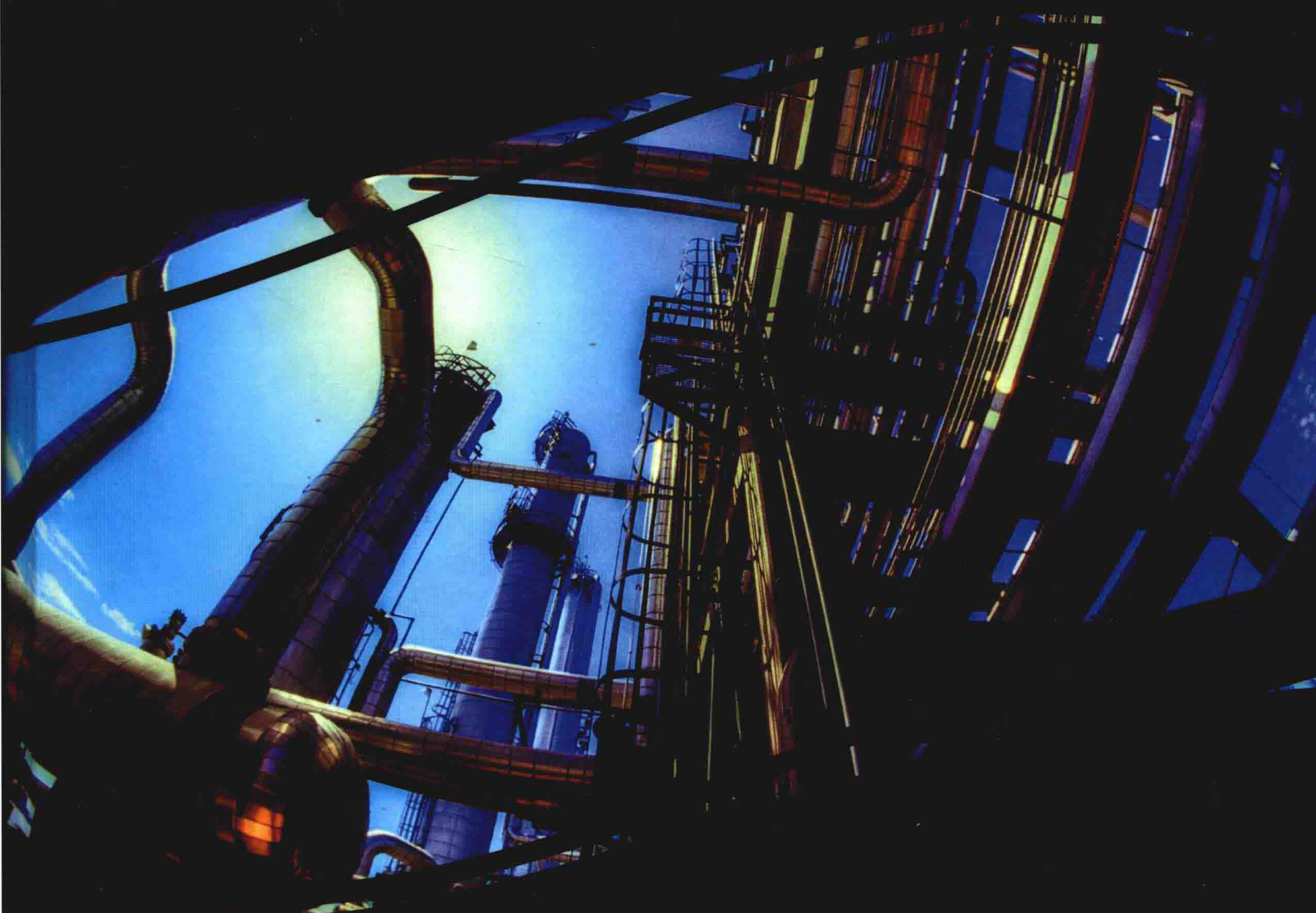

Hamid Al-Megren and Tiancun Xiao

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Petrochemical Catalyst Materials, Processes, and Emerging Technologies

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A volume in the Advances in Chemical and Materials Engineering (ACME) Book Series

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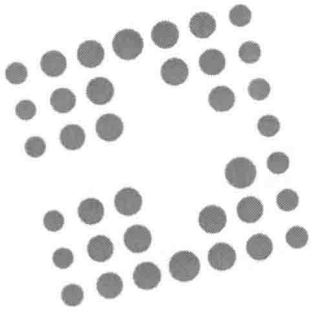

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Detailed Table of Contents

Indeed, these technologies well fit the principles of this design philosophy and this is testified by the various applications of membranes in chemical and petrochemical industry and many are the successful examples of processes that have moved from lab-scale to pilot plant up to a demonstration unit in refinery. The main aim of this chapter is to show the main applications of membrane technology in the petrochemical industry and the related current research trends, focusing on the impact that membrane technology can have on the process sustainability.

Chapter 6

The petrochemical industry has a substantial impact on the environment through the use of large quantities of natural resources (mass and energy) and discharge of wastes into the environment. Process integration offers a powerful framework for the sustainable development of the petrochemical through conservation of mass and energy and synergism among the different building blocks in the supply chain. The chapter provides an overview of process integration basics and tools that can be used to enhance the performance of the petrochemical industry. The chapter also describes the key building blocks of the petrochemical supply chain and how they may be integrated. Finally, the chapter describes key drivers and opportunities of process integration within individual petrochemical plants, among various petrochemical facilities, and the relationship to the existing refining infrastructure.

Chapter 7

Liquefaction of natural gas helps in transporting it over long distances by sea vessels. It is then regasified and transported through pipelines to the consumer. Due to large energy density of Liquefied Natural Gas (LNG), and associated flammability issues, the LNG terminal involves high risk. Consequently, safety is an important factor in the operation of LNG terminals. Although a substantial amount of time money and effort has been put in this area, there is always some possibility of improving the process so that less risk is involved. Rapid advancement in process simulation software like Aspen Plus and Aspen HYSYS, has led to the convenience of experimenting the various control methodologies on the computer offline from the actual plant operation, before they are implemented in real time. In this chapter, main hazards associated with LNG terminal operation will be highlighted. Further, recent advancements in research for safety enhancement and efficiency enhancement in the liquefaction and regasification processes will also be included.

Hydrodesulphurization (HDS) is a standard process for removing sulphur compounds in fuel oils in industry. HDS is effective to remove simple aliphatic sulphur compounds while less effective to remove thiophenes, dibenzothiophenes, and their derivatives because of sterically hindered adsorption on catalyst surface. Application of ionic liquids (ILs, a new class of compounds) substituting for traditional volatile organic solvents in extractive desulphurization (EDS) or oxidative desulphurization (ODS), have been being studied intensively in the latest decades, and many very promising results have been obtained, showing a good prospect as complement method to HDS. In this chapter, these fresh research results of EDS and ODS using ILs are summarized along with comprehensive discussions on diversified desulphurization factors along with some potential problems. It can be inferred that ILs are a class of potential ideal solvents to realize clean fuel oil in future although some problems come too.

There has been still a growing interest in ionic liquids (ILs) for catalysis, in particular considering their tremendous success made over the past decades. Indeed, ILs for catalysis has been a main subject in chemistry and technology, and a rough estimate is that more than 6000 publications involving IL catalysis have been reported in the past fifteen years. Since there have been a large number of excellent reviews and books concerning the catalysis in ILs, in this chapter the authors mainly focus on the IL immobilized nano- or super-fine metal particles for catalysis, which could bridge or fill the gap between homogeneous and heterogeneous catalysis. Detailed IL-immobilized catalyst preparation, characterization and their application in hydrogenation, C-C coupling, oxidation, etc. will be discussed.

Kinetic models were developed to account for the partial contributions of intermediates in complex parallel–consecutive reactions. The models allow precise estimation of the apparent rate constants of all steps in such a reaction network. The hydrodesulfurization (HDS) of dibenzothiophene (DBT) over CoMo-based alumina and carbon catalysts, and over an unsupported molybdenum sulfide catalyst, were investigated in a batch reactor and used to represent this type of reaction. The HDS reactions proceeded

through two parallel–consecutive reaction pathways, i.e., direct desulfurization (DDS) and hydrogenation (HYD), in which two main intermediates, namely biphenyl and partially hydrogenated DBT, were involved. Different selectivities in terms of yield fraction (percentage ratio of HYD/DDS) were observed for these catalysts. The results are discussed in the context of proposed HDS reaction networks. Use of these models enables more accurate assessment of differences among the performances of different catalysts.

The selective transformation of biomass-derived compounds to useful fine chemicals and fuels has developed rapidly in recent years, and biomass compounds will soon become one of the main resource contributors for the production of chemicals. In the near future, it is expected that biomass derived compounds will contribute substantially to global chemical production along with fossil-based analogues. Although, there is still debate about the sustainability of the usage of biomass-derived molecules, it is important to emphasise that effort has been made to use biomass in the most efficient way, and that the biomass resources used are not suitable for food purposes. In this review we will focus to present selected examples on the transformation of glycerol in three distinct areas; (i) glycerol oxidation, (ii) glycerol hydrogenolysis and (iii) glycerol aqueous reforming, using supported metal nanoparticles as the chosen catalysts.

The Mixed Ionic and Electronic Conducting (MIEC) membrane reactors are of interest because they have the potential to produce high purity oxygen from air at lower costs and provide a continuous oxygen supply to reactions or/and industrial processes. The study of the dual role oxygen flux and catalytic performance of the unmodified and Ni-coated La0.6Sr0.4Co0.2Fe0.8O3-δ hollow fibre membranes (LSCF6428 HFM) in the methane oxidation reactions (i.e., partial oxidation of methane and methane combustion) by using air on lumen side and methane on shell side are shown in this chapter. The LSCF6428 HFM participates not only in the oxygen flux but also in the methane conversion to C2. A Ni-coated LSCF6428 HFM under lean O2/CH4 gradient (i.e., 0.5) showed the production of syngas, carbon dioxide and C2 products in agreement with the thermodynamic calculation. At rich O2/CH4 gradient (i.e., 1.0), the formation of carbon dioxide was facilitated. The main catalytic pathway at lean O2/CH4 gradient and H2 reduction treatment was partial oxidation of methane to C2 and syngas.

Hydrodesulfurization (HDS) is an important technology to produce clean fuels, in which the nickel phosphide catalysts exhibit excellent catalytic performances. In this work, a series of NixP/SBA-15 catalysts with various P/Ni molar ratios were prepared using the mesoporous molecular sieve SBA-15 as the support. The structure and surface properties of the catalysts were characterized by X-ray diffraction (XRD), N2 sorption analysis, transmission electron microscopy (TEM), Fourier transform infrared spectrometry (FTIR), and in situ diffuse reflectance infrared Fourier transfer spectroscopy (DRIFTS). The catalytic performances for the HDS of dibenzothiophene (DBT) were evaluated. The results demonstrated that the NixP/SBA-15 catalysts possessed high specific surface area and the mesoporous structures, which benefited the elimination of the internal diffusion limitation in the HDS reactions. Both Ni2P and Ni12P5 phases showed catalytic activity in HDS reactions while Ni2P was more active. The optimal P/Ni molar ratio was about 0.75. The DBT conversion can reach 95.8% under the reaction condition of pressure at 3.0 MPa, H2:oil=600, WHSV at 26.7 h-1, and temperature at 340oC. In situ DRIFTS spectra indicated that the coordinative unsaturated Niδ+ (0<δ<1) species on the catalysts surface were the active sites for the HDS of DBT.

Preface

Dear Readers,

It is our great honor to present this IGI Global Series book on the "Petrochemical Catalyst Materials, Processes, and Emerging Technologies". As we know that Petrochemical Industry is a technology-intensive sector, where any small changes in the technology could lead to a big improvement. The development and understanding of chemical processes relies on knowledge of various disciplines, from raw materials, reaction mechanism, process parameters and the target materials. In the modern information age, lots of changes are happening every day in petrochemical industry, such as new materials discovery and application, process modification and automation, market and demand changes, thus leading to new and emerging technologies.

This IGI Global book is to address the latest development in the petrochemical technologies, especially focusing on the core technologies such as catalyst materials for fuel upgrading, especially on sulfur removal, syngas conversion, alkane and oxygen activation, functionization of polymer. Of course safety is always the top priority in petrochemical industry, so we also cover these topics for the expanding LNG industry. The chapters cover research from mechanism study to the industry catalysts development, from homogenous catalysis to the heterogeneous catalyst and from small molecules activation to the heavy oil upgrading. This book also includes both the conventional process like supported catalysts, and latest catalytic process and materials in ionic liquid, the chemicals resources include fossil fuel, syngas as well as the glycerol, the renewable resources. These will be helpful for the academic researchers and the industrial engineers for them to have a quick view on the latest development in these areas.

Compilation of a professional book is a trivial job, which takes us 15 months. However, we are encouraged by the very enthusiastic authors from various countries, they actively responded for the call for chapters and we initially have received more than 50 plans for chapters. We screened down to 26 chapters for full writing, and after submission and extensive reviewing, we are very pleased to include 15 chapters in this book.

Here we would like to express our sincere thanks to these contributors for their hard and serious working, also we like to thanks our reviewers for their constructive input. Last but not least, thanks are due to IGI Global for giving us the chance to edit the book. We hope readers would enjoy the reading and feel free to point any errors or mistakes which we may not be spotted. Your comments and suggestions are highly appreciated.

Yours sincerely,

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