CATALYSIS IN COAL CONVERSION

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tering; new concepts of surface layers; and modern spectroscopic methods for the examination of solid surfaces.

Part III, essentially the second half of the book, reviews the nature of the various coal liquefaction processes and their products. It also covers coal gasification and the synthesis of liquid fuels from carbon monoxide–hydrogen mixtures. In each, the catalytic problems are highlighted, and the potential impact of the recent advances in catalysis and related disciplines on solving these problems are critically evaluated.

Adalbert Farkas
Editor

Preface

One of the major challenges of our time is the solution of the energy problem. The feasibility of the catalytic conversion of coal into liquid and gaseous fuels has been demonstrated, but there is a need for a significant technical breakthrough to make coal conversion an economically attractive process and to permit coal-derived fuels to play an important part in replacing or supplementing our critical oil and gas supplies.

This book marshals the recent advances in catalysis and related disciplines and shows how they might make decisive contributions toward solutions of the catalytic problems of coal conversion.

The book is written primarily for the chemist and chemical engineer engaged in research on some aspect of the conversion of coal into synthetic fuels or of fuel processing. It should also be useful to scientists or technologists concerned with, or interested in, catalysts or catalytic processes in general in view of the wealth of information presented on the preparation, mode of action, and behavior of numerous catalysts, and on the ways their activity, selectivity, and stability can be improved. Teachers of chemistry will find many interesting and instructive examples of practical applications in industrial catalysis for the results of fundamental and theoretical studies.

Part I surveys the advances of catalysis in the past decade or two and covers bimetallic catalysts; the effects of catalyst–support interactions, particle size, and surface morphology; characterization and preparation of catalysts; poisoning and regeneration; and reaction mechanisms relevant to coal conversion.

Part II summarizes the accomplishments of such related disciplines as reactor engineering, inorganic and organometallic chemistry, materials science, and surface science. The topics discussed include catalyst evaluation; novel inorganic, intermetallic, and organometallic compounds of potential catalytic interest; sin-

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Chapter 1

Introduction

The conversion of coal to synthetic fuels encompasses a number of catalytic processes and reactions, the most important of which are summarized in Table 1-1. In addition to various current processes of coal conversion to gaseous and liquid fuels, this list includes many catalytic reactions used in the refining of petroleum. Similar reactions are expected to be applicable for upgrading coal liquids. Therefore, the coal conversion industry is most likely to utilize a significant fraction of presently known catalytic materials, including metals, oxides, solid acids, and sulfides.

Paralleling this projected development of catalyst technology for coal conversion are a number of technical challenges familiar to the catalytic chemist and engineer. These include control of selectivity and activity; minimizing catalyst poisoning, sintering, and mechanical degradation; and the development of efficient regeneration procedures and of reactor designs for optimum heat and mass transfer. Because of the complex nature of coal, these challenges are more difficult than those encountered in the development of petroleum processes, but it is expected that the advances in catalysis during the last decade will play a significant role in solving many of the inherent constraints and problems of coal conversion processes. This book provides a perspective of recent advances in catalysis and related disciplines and analyzes their impact on the current status and future development of the technology of synthetic fuels derived from coal.

TABLE 1-1
CATALYTIC REACTIONS IN COAL CONVERSION

Process	General reactions	Specific reactions/products
Direct liquefaction	Hydrogenation	Aromatic liquids
	Cracking	
	Hydrofining	Hydrodesulfurization (HDS)
		Hydrodenitrogenation (HDN)
CO/H_2 synthesis	Fischer–Tropsch	Methane
		Hydrocarbon liquids
		Alcohols
		Chemicals
Water–gas shift		Hydrogen
Direct gasification	Hydrogasification	Methane
	Oxidative gasification	Synthesis gas
Liquids refining and upgrading	Cracking	Hydrogenation
	Reforming	Dehydrogenation
	Hydroforming	Dehydrocyclization
		Isomerization
		Hydrogenolysis
		Hydrodesulfurization (HDS)
		Hydrodenitrogenation (HDN)

The discussions in Part I cover six broad areas: multimetallic catalysts; effects of catalyst-support interactions, particle size, and surface morphology on catalyst properties; catalyst characterization and preparation; poisoning and regeneration; and reaction mechanisms of importance to catalytic coal conversion. While the emphasis in these areas is on work conducted during the last decade, some relevant information concerning earlier work is included. In addition to a review of the main research topics, the general implications of these topics to coal conversion are outlined.

Part II reviews advances in supporting disciplines related to catalysis under four general subjects: reactor engineering and testing procedures; inorganic and organometallic chemistry of catalysts; certain aspects of material science relevant to supports, sintering, and novel materials; and some concepts of surface science relating to metal catalysis and techniques for materials analysis and characterization.

A summary of the most significant developments discussed in Parts I and II, and their impact on coal conversion technology, is presented in Table 1-2.

Part III is devoted to the detailed review of the specific applications of catalysis to a number of important coal conversion processes. These applications include upgrading of coal liquids derived from the Coalcon, COED, H-Coal, and

TABLE 1-2
ADVANCES OF IMPORTANCE TO THE CATALYTIC CONVERSION OF COAL

Subject	Representative areas of impact
Multimetallic catalysis	Upgrading of coal liquids Methanation Fischer–Tropsch synthesis
Catalyst-support interactions	Thermal and chemical stabilization of catalysts and supports
Catalyst characterization	Improvement of coal liquefaction catalysts Upgrading of coal liquids Determination of catalyst *intrinsic* activity
Catalyst preparation	New catalyst formulations Controlled variation in catalyst properties Higher surface area catalysts
Poisoning and regeneration	Effect of sulfur in coal conversion catalysis Prevention of carbon deposition—removal of carbon
Mechanism and surface chemistry	Better understanding of the important steps in coal conversion Identification of rate limiting processes, directions for process improvement
Reactor engineering and catalyst testing	Development of effective catalyst testing procedures Data interpretation
Inorganic chemistry	New catalytic materials and compositions with improved poison tolerance and activity
Materials science	Novel support materials and structures Novel refractory compounds Understanding of sintering phenomena (catalyst deactivation)
Surface science	New characterization techniques

Synthoil processes; the liquefaction of coal and the conversion of solvent refined coal to boiler fuel low in sulfur and nitrogen; catalytic gasification of coal, shift conversion, and methanation; and the synthesis of diesel fuel, LPG, and selected feedstocks from CO and H_2.

The discussions include a brief review of each process and a summary of the major problems and constraints associated with the catalytic steps. Short- and long-range programs are treated separately, as are developments of fundamental nature.

PART I

SURVEY OF ADVANCES IN CATALYSIS