## Catalytic Materials

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## I. Available Knowledge

Coal conversion catalysis has a vast store of empirical information of which the prime contributors are the German World War II activities and research of the Bureau of Mines and many companies and research institutes in the United States and elsewhere. Work of the petroleum industry includes catalysts and processes similar to those of coal conversion, but the petroleum feed stocks are generally very much easier to handle and convert than coal or coal-derived products. The bulk of these studies has not been published. Fundamental studies in catalysis have been reported by both industrial and academic workers.

# II. Knowledge Required

Additional information is needed for some of the catalysis of the hydrogenation of oxides of carbon, for bridging the gap between current petroleum refining practice and coal conversion, and on the fundamental aspects of catalysis. New research tools that have become available in the last decade should enlarge the understanding of catalysis significantly.

# III. Recommendations

The workshop indicated that most of these areas would be continuing problems over the next 20 years, but in some cases,

the priorities may be expected to change. They suggested that priorities of high (H), moderate (M), and low (L) be assigned.

- A. Basic Investigations as a moderate continuing activity Priority: 1984 H, 1994 H
  - 1. Encourage the development of new research tools for studying surfaces and adsorbed molecules.
  - Structure of coal and chars. Also the occurrence of minor elements in coal.
  - Fundamental studies of surfaces and catalysts; electronic structure and its interaction with adsorbed molecules.
  - 4. Chemisorption and poisoning
  - Preparation and characterization of catalysts. New supports and alloys.
  - 6. Action of promoters and supports
  - 7. Kinetics and mechanism of catalytic reactions
  - 8. Catalysis of reactions of CO and CO<sub>2</sub>. These oxides are the unique products of coal gasification.
- B. Methanation on Ni Priority: 1984 H, 1994 H
  - 1. Sulfur-tolerant catalysts, 10 ppm
  - 2. Preparation of catalysts of required gross geometry.
  - 3. Control of carbon deposition and carbide formation.
  - Sulfur poisoning and regeneration. Recovery of Ni.
- C. Liquid-phase coal hydrogenation Priority: 1984 H, 1994 H
  - 1. Improved supported or other catalysts

- C. Liquid-phase coal hydrogenation (cont.)
  - 2. Fouling and poisoning
  - 3. Control of selectivity and hydrogen consumption.
    Nitrogen removal. Hydrogen-transfer processes.
  - 4. Catalysts for lower-pressure operation.
- D. Hydrorefining considered here with respect to hydrogen addition and nitrogen removal.

Priority: 1984 L, 1994 M

- E. Water-Gas Shift Priority: 1984 H
  - Sulfur-resistant catalysts
- F. Fischer-Tropsch Synthesis Priority: 1984 L, 1994 M
  - 1. Highly selective catalysts
  - 2. S-tolerant catalysts (10 ppm)
  - 3. Catalysts for use with low BTU gas
- G. Alcohol syntheses (methanol, isobutanol) Priority: 1984 L, 1994 L

#### NOTE:

- A. In some cases, priorities increase from 1984 to 1994 in the recommendations. Generally, this situation resulted from concern with the operation of currently proposed processes and the possibility of changes in requirements for fuels and chemicals.
- B. Members of the workshop noted that the group present was probably not an adequate sampling of catalysis workers in the United States.