

COAL LIQUEFACTION

- A RESEARCH & DEVELOPMENT NEEDS ASSESSMENT

by the

DOE COAL LIQUEFACTION RESEARCH NEEDS

(COLIRN) ASSESSMENT PANEL

Final Report

Volume I

March 1989

Prepared For:

**U.S. Department of Energy
Office of Energy Research
Office of Program Analysis**

Under Contract No. DE-AC01-87ER30110

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Coal Liquefaction

- A Research & Development Needs Assessment

Dr. Harvey D. Schindler*, Dr. Francis P. Burke^a, Dr. K. C. Chao^b, Dr. Burtron H. Davis^c, Dr. Martin L. Gorbaty^d, Dr. Kamil Klier^e, Dr. Carl W. Kruse^f, Dr. John W. Larsen^g, Dr. Robert E. Lumpkin^h, Dr. Michael E. McIlwainⁱ, Dr. Irving Wender^j, Mr. Norman Stewart^k.

- * Energy Technology and Engineering, Science Applications International Corporation, 1710 Goodridge Drive, McLean, VA 22102.
- a. Consolidation Coal Company R&D, 4000 Brownsville Road, Library, PA 15129.
- b. School of Chemical Engineering, Chemical and Metallurgical Engineering Building, Purdue University, West Lafayette, IN 47907.
- c. Kentucky Energy Cabinet Laboratory, P.O. Box 13015, Lexington, KY 40512-3015.
- d. Exxon R&D, Clinton Township, Route 22 East, Annandale, NJ 08801.
- e. Department of Chemistry, Lehigh University, Bethlehem, PA 18015.
- f. Illinois State Geological Survey, 615 East Peabody Drive, Champaign, IL 61820.
- g. Department of Chemistry, Lehigh University, Bethlehem, PA 18015.
- h. AMOCO Corporation, 200 East Randolph Drive, Chicago, IL 60601.
- i. Idaho National Engineering Laboratory, 2151 North Blvd., Idaho Falls, ID 83415.
- j. Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA 15261.
- k. Electric Power Research Institute, 3412 Hillview Avenue, Palo Alto, CA 94303.

*This publication was prepared by the U.S. DOE panel group on research needs assessment for coal liquefaction (COLIRN). The contract sponsor was the DOE Office of Energy Research, Office of Program Analysis. The Director of the Office of Program Analysis was Dr. George Jordy, and the Director of the Research & Technical Assessment Division was Mr. Robert Rader. The DOE technical project officer was Dr. Gilbert Jackson; the DOE Contract Number was DE-AC01-87ER30110. Dr. Harvey D. Schindler of SAIC served as principal investigator and chairman of COLIRN, and other listed authors served as members of COLIRN. In addition, SAIC staff members, Dr. Edward I. Wan, Dr. Malcolm D. Fraser, and Mr. William R. King, participated in developing prioritization methodology and contributed to the preparation of this publication.

The following people, who were not members of the COLIRN panel group, contributed to this publication and are appropriately identified as authors or coauthors of specific chapters or sections.

1. Dr. Christine Curtis, Auburn University
2. Dr. David Gray, MITRE Corporation
3. Mr. Harry Frumkin, Chevron Research Company
4. Dr. Ripudaman Malhotra, SRI International
5. Dr. George Marcelin, University of Pittsburgh
6. Dr. Donald F. McMillen, SRI International
7. Dr. Richard F. Sullivan, Chevron Research Company
8. Mr. Glen Tomlinson, MITRE Corporation
9. Dr. Bary Wilson, Battelle Pacific Northwest Laboratory
10. Mr. Richard A. Winschel, Consolidation Coal Company

TABLE OF CONTENTS

VOLUME I

	<u>Page No.</u>
ABSTRACT	xix
ACKNOWLEDGEMENTS	xx
EXECUTIVE SUMMARY	ES-1
CHAPTER 1 INTRODUCTION	1-1
1.1 BACKGROUND	1-1
1.2 ASSESSMENT OBJECTIVES	1-3
1.3 DEFINITION OF COAL LIQUEFACTION TECHNOLOGIES	1-5
1.4 REPORT ORGANIZATION	1-6
REFERENCE FOR CHAPTER 1	1-7
CHAPTER 2 ASSESSMENT METHODOLOGY	2-1
2.1 TECHNICAL APPROACH	2-1
2.2 SELECTION AND ROLE OF THE COLIRN PANEL	2-3
2.2.1 Selection	2-3
2.2.2 Role	2-4
2.3 SITE VISITS AND OTHER EXPERT INPUTS	2-5
2.4 COLIRN PANEL MEETINGS	2-7
2.4.1 First Panel Meeting	2-7
2.4.2 Second Panel Meeting	2-8
CHAPTER 3 COAL LIQUEFACTION R&D RECOMMENDATIONS	3-1
3.1 SUMMARY	3-1
3.2 RESEARCH NEEDS OF DIRECT LIQUEFACTION	3-9
3.2.1 Current Research Activities and Status	3-9
3.2.2 High-Priority Recommendations in Direct Liquefaction	3-11
3.3 RESEARCH NEEDS OF INDIRECT LIQUEFACTION	3-21
3.3.1 Current Research Activities and Status	3-21
3.3.2 High-Priority Recommendations in Indirect Liquefaction	3-24
3.4 RESEARCH NEEDS IN PYROLYSIS	3-30
3.4.1 Current Research Activities and Status	3-30
3.4.2 High-Priority Recommendations in Pyrolysis	3-31

TABLE OF CONTENTS (Continued)

	<u>Page No.</u>
3.5 RESEARCH NEEDS IN COPROCESSING	3-38
3.5.1 Current Research Activities and Status	3-38
3.5.2 High-Priority Recommendations in Coprocessing	3-39
3.6 RESEARCH NEEDS IN BIOCONVERSION	3-43
3.6.1 Current Research Activities and Status	3-43
3.6.2 High-Priority Recommendation in Bioconversion	3-43
3.7 DIRECT CONVERSION OF METHANE	3-45
3.8 DOE COAL LIQUEFACTION PROGRAM	3-46
3.8.1 Overview	3-46
3.8.2 Advanced Research and Technology Development Program	3-47
3.8.3 Pittsburgh Energy Technology Center Program	3-52
3.9 OTHER CONCLUSIONS AND RECOMMENDATIONS	3-55
3.9.1 Opinions and Comments	3-55
3.9.2 DOE Procedures and Policies	3-56
3.10 PEER REVIEWERS' COMMENTS	3-59
3.10.1 General (Opposing) Comments	3-60
3.10.2 Comments re: Direct Liquefaction	3-60
3.10.3 Comments re: Indirect Liquefaction	3-62
3.10.4 Comments re: Pyrolysis	3-62

TABLE OF CONTENTS (Continued)

VOLUME II

	<u>Page No.</u>
INTRODUCTION TO VOLUME II	xv
CHAPTER 4 REVIEW OF DIRECT LIQUEFACTION	4-1
By Martin L. Gorbaty, Exxon Research and Engineering Company; Donald F. McMillen and Ripudaman Malhotra, SRI International; Burtron H. Davis, Kentucky Energy Cabinet Laboratory; Francis P. Burke, Consolidation Coal Company; Harvey D. Schindler, Science Applications International Corporation; Richard F. Sullivan and Harry Frumkin, Chevron Research Company; David Gray and Glen Tomlinson, MITRE Corporation; and Bary Wilson, Battelle Pacific Northwest Laboratory.	
4.1 INTRODUCTION AND SUMMARY	4-1
4.1.1 Introduction	4-1
4.1.2 Summary	4-4
4.2 FUNDAMENTAL AND APPLIED RESEARCH	4-8
4.2.1 Coal Structure Related to Liquefaction	4-8
4.2.2 Chemistry and Mechanisms of Direct Liquefaction Reactions	4-27
4.2.3 Catalysis of Direct Liquefaction	4-50
4.2.4 Methods for Characterizing Coal Liquids from Direct Coal Liquefaction	4-67
4.3 DIRECT LIQUEFACTION PROCESS DEVELOPMENT	4-76
4.3.1 Overview of Technology Development Status	4-76
4.3.2 Evolution of Direct Liquefaction Technology	4-77
4.3.3 Refining Coal Liquids	4-116
4.3.4 Economics of Coal Liquids	4-139
4.3.5 Environmental Considerations	4-156
REFERENCES FOR CHAPTER 4	4-163
CHAPTER 5 REVIEW OF INDIRECT LIQUEFACTION	5-1
By Irving Wender, University of Pittsburgh, and Kamil Klier, Lehigh University.	
5.1 INTRODUCTION AND SUMMARY	5-1
5.1.1 Introduction	5-1
5.1.2 Summary	5-2
5.2 CONVERSION OF SYNTHESIS GAS TO LIQUID HYDROCARBON FUELS	5-6
5.2.1 Fischer-Tropsch Reactions, Chemistry, and Mechanisms	5-6
5.2.2 Fischer-Tropsch Synthesis Catalysts	5-7
5.2.3 Fischer-Tropsch Processes Not Yet in Commercial Operation	5-9

TABLE OF CONTENTS (Continued)

	<u>Page No.</u>
5.2.4 Fischer-Tropsch Synthesis in the Slurry Phase	5-11
5.2.5 Conversion of Methanol to Gasoline with Zeolite- Containing Catalysts	5-11
5.3 OXYGENATE SYNTHESIS AND PROCESSES	5-19
5.3.1 Methanol Synthesis	5-19
5.3.2 Higher Alcohols	5-61
5.3.3 Water Gas Shift (WGS) Technologies	5-112
5.3.4 The Methyl Tertiary-Butyl Ether (MTBE) and Tertiary- Amyl Methyl Ether (TAME) Technology	5-115
REFERENCES FOR CHAPTER 5	5-123
 CHAPTER 6 REVIEW OF PYROLYSIS	 6-1
By Harvey D. Schindler, Science Applications International Corporation.	
6.1 INTRODUCTION	6-1
6.1.1 Introduction	6-1
6.1.2 Summary	6-2
6.2 FUNDAMENTAL AND APPLIED RESEARCH	6-5
6.2.1 Coal Structure and Physicochemical Properties as Related to Pyrolysis	6-5
6.2.2 Chemistry and Mechanisms of Pyrolysis Reactions	6-13
6.2.3 Catalysis	6-23
6.2.4 Characteristics and Properties of Pyrolysis Products	6-29
6.2.5 Upgrading of Pyrolysis Products and Their Utilization	6-34
6.3 PROCESS DEVELOPMENT	6-44
6.3.1 Descriptions of Advanced Low-Temperature Pyrolysis Processes	6-44
6.3.2 Technology Assessment and Economics	6-57
6.3.3 Environmental Considerations	6-71
REFERENCES FOR CHAPTER 6	6-72
 CHAPTER 7 REVIEW OF COAL/OIL COPROCESSING	 7-1
By Christine W. Curtis, Auburn University, and Richard A. Winschel, Consolidation Coal Company.	
7.1 INTRODUCTION AND SUMMARY	7-1
7.1.1 Introduction	7-1
7.1.2 Summary	7-2

TABLE OF CONTENTS (Continued)

	<u>Page No.</u>
7.2 BACKGROUND OF COPROCESSING	7-4
7.2.1 Early Work	7-4
7.2.2 Advantages of Coprocessing	7-5
7.3 FUNDAMENTAL AND APPLIED RESEARCH	7-8
7.3.1 Chemistry and Mechanisms of Coprocessing Reactions	7-8
7.3.2 Catalytic Coprocessing	7-12
7.4 PROCESS DEVELOPMENT	7-15
7.4.1 Recent Development Work	7-15
7.4.2 Characterization of Coprocessing Products and Their Upgrading	7-25
7.4.3 Economics of Coprocessing	7-25
REFERENCES FOR CHAPTER 7	7-34
 CHAPTER 8 REVIEW OF BIOCONVERSION OF COAL	 8-1
By Michael E. McIlwain, Idaho National Engineering Laboratory.	
8.1 INTRODUCTION AND SUMMARY	8-1
8.1.1 Introduction	8-1
8.1.2 Summary	8-2
8.2 BACKGROUND	8-4
8.2.1 Description of the Bioconversion Concept	8-4
8.2.2 Advantages and Disadvantages of Bioprocessing	8-8
8.3 DIRECT LIQUEFACTION (BIOSOLUBILIZATION)	8-11
8.3.1 Historical Background	8-11
8.3.2 Current Research Agendas and Objectives	8-20
8.3.3 Research and Development Needs	8-22
8.4 INDIRECT LIQUEFACTION	8-25
8.4.1 Historical Background	8-25
8.4.2 Current Research Agendas and Objectives	8-26
8.4.3 Research and Development Needs	8-29
REFERENCES FOR CHAPTER 8	8-32
 CHAPTER 9 LIQUEFACTION DEVELOPMENTS OUTSIDE THE U.S.	 9-1
By Harvey D. Schindler, Science Applications International Corporation.	
9.1 INTRODUCTION AND SUMMARY	9-1

TABLE OF CONTENTS (Continued)

	<u>Page No.</u>
9.1.1 Introduction	9-1
9.1.2 Summary	9-2
9.2 FEDERAL REPUBLIC OF GERMANY	9-4
9.2.1 German Technology	9-4
9.2.2 Pyrosol Process	9-4
9.2.3 High-pressure Hydrogenation	9-9
9.2.4 Coprocessing	9-9
9.3 JAPAN	9-11
9.3.1 Brown Coal Liquefaction	9-11
9.3.2 Bituminous Coal Liquefaction Project	9-11
9.4 CANADA	9-14
9.4.1 Alberta Research Council (ARC)	9-14
9.4.2 CANMET	9-15
9.4.3 Ontario-Ohio Clean Fuels (OOCF)	9-15
9.5 GREAT BRITAIN	9-17
9.5.1 Direct Liquefaction	9-17
9.5.2 Indirect Liquefaction	9-17
9.5.3 Pyrolysis	9-17
9.6 ITALY	9-18
9.7 PEOPLES REPUBLIC OF CHINA (PRC)	9-19
9.7.1 Direct Liquefaction	9-19
9.7.2 Indirect Liquefaction	9-19
REFERENCES FOR CHAPTER 9	9-20
APPENDIX A SUMMARY OF RECOMMENDATIONS FROM THE FERWG-II REPORT .	A-1
APPENDIX B OXIDATIVE COUPLING OF METHANE -- REVIEW	B-1
APPENDIX C MEMBERS OF THE EXPERT PANEL	C-1
APPENDIX D PANEL MEETING REPORTS	D-1
APPENDIX E DEVELOPMENT OF RESEARCH RECOMMENDATION DATABASE . . .	E-1
APPENDIX F PEER REVIEWERS' COMMENTS.	F-1
GLOSSARY	GL-1

LIST OF FIGURES

VOLUME I

	<u>Page No.</u>
CHAPTER 2	
Figure 2-1. Overall Technical Approach for Conducting R&D Needs Assessment in Coal Liquefaction	2-2
CHAPTER 3	
Figure 3-1. U.S. Department of Energy Coal Liquefaction Program	3-48
Figure 3-2. Objectives of the Current DOE Program in Direct Coal Liquefaction	3-49
Figure 3-3. Objectives of the Current DOE Program in Indirect Liquefaction	3-50
Figure 3-4. Objectives of the Current DOE Program in Support Studies/Engineering Evaluations	3-51
Figure 3-5. Research Areas of DOE's Advanced Research and Technology Development Program in Coal Liquefaction	3-53
Figure 3-6. Pittsburgh Energy Technology Center In-House R&D Program in Coal Liquefaction	3-54

LIST OF FIGURES (Continued)

VOLUME IIPage No.

CHAPTER 4

Figure 4-1.	Molecular Structure for a Bituminous Coal	4-16
Figure 4-2.	Distribution of Oxygen Functionality in Coals	4-19
Figure 4-3.	Plot of Fraction of Aromatic Carbon (f_a) Versus Percent Carbon for 63 Coals and Coal Macerals	4-20
Figure 4-4.	Elemental Composition of the Three Main Maceral Groups	4-23
Figure 4-5.	Coal Conversion to Liquids Begins with a Thermolysis	4-25
Figure 4-6.	Proposed Chemistry of Hydrogen Donation	4-25
Figure 4-7.	Some Possible Reactions During Hydrolique- faction	4-28
Figure 4-8.	Liquefaction Mechanisms	4-32
Figure 4-9.	Scission of Strong Bonds Via H-Transfer	4-34
Figure 4-10.	Rationale for Using Additives Rich in Polycyclic Aromatic Hydrocarbons (PCAH)	4-36
Figure 4-11.	Computed Rates for Cleavage by Different Modes	4-37
Figure 4-12.	Replacing Part of Tetrahydrofluoranthene (H-Donor) by Fluoranthene (Non-Donor) Increases Efficiency of H-Utilization and Selectivity to Oils	4-39
Figure 4-13.	Importance of Hydrogen Shuttling in Catalytic Liquefaction	4-40
Figure 4-14.	Intermediates in Liquefaction Reactions	4-42
Figure 4-15.	Ring Closure and Cleavage Rates of 1,1' -Binaphthyl and 1,2'-Dinaphthylmethane	4-45
Figure 4-16.	Electron Loss and Proton Transfer	4-46
Figure 4-17.	Candidate Structures for Study of Retrogressive Reactions	4-49
Figure 4-18.	Asphaltene and Oil Production as a Function of Catalyst Type	4-55
Figure 4-19.	Pore Diffusion Effects in Catalysts	4-56
Figure 4-20.	Catalyst Activity Versus Catalyst Age	4-58
Figure 4-21.	Effective Diffusivities for Spent Catalyst Samples	4-61
Figure 4-22.	H-Coal Ebullated-Bed Reactor	4-79
Figure 4-23.	Block Flow Diagram of NTSL Operation	4-87
Figure 4-24.	Process Flow Diagram of Integrated Two-Stage Liquefaction	4-90

LIST OF FIGURES (Continued)

		<u>Page No.</u>
Figure 4-25.	Block Flow Diagram of Integrated Two-Stage Liquefaction (ITSL)	4-100
Figure 4-26.	Block Flow Diagram of RITSL Operation	4-103
Figure 4-27.	Block Flow Diagram of CC-ITSL Operation at Wilsonville	4-105
Figure 4-28.	HRI Catalytic Two-Stage Unit	4-108
Figure 4-29.	Block Flow Diagram of CTSL Operation with Solids Recycle at Wilsonville	4-112
Figure 4-30.	Distillations of Arabian Crudes and Coal-Derived Oils	4-119
Figure 4-31.	Refining of Coal Syncrude to Transportation Fuels	4-121
Figure 4-32.	Refining of Coal Syncrude to Gasoline	4-122
Figure 4-33.	Effect of Feed End Point on Catalyst Temperature for Hydrodenitrogenation of ITSL Oils with Fresh ICR 106 Catalyst	4-126
Figure 4-34.	Close-Coupled Ash Recycle Configuration	4-141
Figure 4-35.	Yields from Illinois No. 6 Coal	4-144
Figure 4-36.	Yields from Wyoming Coal	4-145
Figure 4-37.	Liquefaction Yields Per Ton of Coal	4-146
Figure 4-38.	Product Quality From Illinois Coal	4-147
CHAPTER 5		
Figure 5-1.	Types of Zeolite Selectivity	5-14
Figure 5-2.	Framework Structure of ZSM-5	5-15
Figure 5-3.	Gibbs Free Energy of Carbon Monoxide Hydrogenation	5-21
Figure 5-4.	ICI Low-Pressure Methanol Synthesis Process	5-25
Figure 5-5.	ICI Methanol Convertor	5-26
Figure 5-6.	Stability of Industrial Cu/ZnO ₃ /Al ₂ O ₃ Catalyst	5-28
Figure 5-7.	Flow Diagram of Lurgi Methanol Synthesis	5-29
Figure 5-8.	Lurgi Boiling-Water Low-Pressure Methanol Reactor	5-30
Figure 5-9.	Simplified Process Flow Sheet for LaPorte PDU	5-33
Figure 5-10.	LaPorte PDU 40-Day Run Performance, May/June 1985	5-35
Figure 5-11.	Yield of Methanol as Function of Water Injection Rate	5-47

LIST OF FIGURES (Continued)

		<u>Page No.</u>
Figure 5-12.	Yield of Methanol as Function of Cs Loading . . .	5-48
Figure 5-13.	MNDO Energy Diagram for Reaction of Carbon Monoxide with Hydroxide to Form Formate	5-53
Figure 5-14.	Infrared Spectra	5-54
Figure 5-15.	Correlation of Specific Methanol Activity as a Function of Normalized Cesium Surface Concentration	5-57
Figure 5-16.	Flow Diagram of MAS Process	5-68
Figure 5-17.	Influence of Composition on the Selectivity of IFP-1 Catalysts	5-71
Figure 5-18.	Block Diagram of the Integrated Natural Gas to Alcohols Complex	5-72
Figure 5-19.	Reactor Section of IFP/Idemitsu Kosan Process . .	5-74
Figure 5-20.	Breakdown of Production Cost of C ₁ -C ₆ Alcohols . .	5-78
Figure 5-21a.	Effect of Cs Content of the MoS ₂ Catalysts on the Product Yield	5-80
Figure 5-21b.	Effect of Cs Content of the MoS ₂ Catalysts on the Total Product Yield as a Function of Temperature	5-81
Figure 5-22.	Flowsheet for the OCTAMIX Synthesis	5-83
Figure 5-23.	Schematic of the Catalytic Testing System	5-87
Figure 5-24.	Chain Growth Reactions	5-92
Figure 5-25.	Integral, Isothermal, Plug-Flow, Fixed-Bed Kinetic Model	5-94
Figure 5-26.	Measured and Predicted Product Yields	5-95
Figure 5-27.	Comparison of Measured and Predicted Yields . . .	5-96
Figure 5-28.	The Roles of Additives for Effective Synthesis of EtOH and AcOH	5-107
Figure 5-29.	Average Forward WGS Rate Constants	5-114
Figure 5-30.	A Schematic Diagram of the Methyl Tertiarybutyl Ether (MTBE) Process	5-118
Figure 5-31.	Variation of Product Yield with Alcohol Mixture Partial Pressure	5-121
CHAPTER 6		
Figure 6-1.	Summary of Coal Structure Information in a Hypothetical Coal Molecule	6-9

LIST OF FIGURES (Continued)

	<u>Page No.</u>
Figure 6-2. Cracking of Hypothetical Coal Molecule During Thermal Decomposition	6-9
Figure 6-3. Effect of ZnCl ₂ on Total Carbon Conversion of MRS and UB Coals at 13.8 MPA H ₂ Pressure	6-26
Figure 6-4. Effect of Acid Washing on MRS Coal with ZnCl ₂ at 467° to 482° Reactor Temperature, 13.8 MPA H ₂ Pressure	6-26
Figure 6-5. Effect of Temperature and Pressure on Catalytic and Noncatalytic Hydropyrolysis	6-28
Figure 6-6. Elemental Compositions of Char and Tar Normalized to the Compositions in the Parent Coal	6-32
Figure 6-7. COED Coal Pyrolysis	6-46
Figure 6-8. Stirred Carbonizer Unit	6-50
Figure 6-9. Effect of Sweep Gas on Yields with Preoxidized Coal	6-51
Figure 6-10. Lurgi Ruhrgas Flash Carbonization Process	6-54
Figure 6-11. Occidental Research Pyrolysis Process Flow Scheme	6-56
Figure 6-12. Demonstration-Scale Pyrolysis Plant	6-60
Figure 6-13. Commercial-Scale Pyrolysis Plant	6-61
Figure 6-14. Breakdown of Capital Costs for Lurgi Plants	6-67
Figure 6-15. Breakdown of Capital Costs for Toscoal Plants	6-67
 CHAPTER 7	
Figure 7-1. Simplified Flow Plan of HRI's Two-Stage Process	7-17
Figure 7-2. Typical Coprocessing Liquid Product Yield Data	7-18
Figure 7-3. Block Flow Diagrams of LCI Coprocessing Concepts	7-22
Figure 7-4. Signal/UOP's Proposed Resid/Coal Processing Scheme	7-23
Figure 7-5. Chemical Composition of Coprocessing Napthas	7-27
Figure 7-6. Coprocessing Product Cost Components	7-33
 CHAPTER 8	
Figure 8-1. Schematic of a Generic Bioprocess	8-5
Figure 8-2a. Mechanism of Lignin Degradation	8-12
Figure 8-2b. Hypothetical Scheme of Cleavage of Ether Bonds by the Enzyme System of <i>Poria subacida</i>	8-12
Figure 8-3a. Arylglycerol- β -aryl etherase	8-13

LIST OF FIGURES (Continued)

	<u>Page No.</u>
Figure 8-3b. 1- β and 4- β Ligninase Reactions	8-13
Figure 8-4. Integrated Gasification, Bioconversion Combined Cycle Processes	8-28
Figure 8-5. Biosolubilized Coal to Methane Processing Plant . .	8-30
 CHAPTER 9	
Figure 9-1. German Technology	9-7
Figure 9-2. Pyrosol Process	9-8
Figure 9-3. High Pressure Hydrogenation	9-10
Figure 9-4. Schematic Flow Diagram of NEDOL Process PDU	9-12
Figure 9-5. CANMET Continuous-Flow Coprocessing Unit	9-16

LIST OF TABLES

VOLUME I

Page No.

EXECUTIVE SUMMARY

Table ES-1.	Summary of High-Priority R&D Recommendations in Coal Liquefaction	ES-10
-------------	--	-------

CHAPTER 3

Table 3-1.	Summary of High-Priority R&D Recommendations	3-3
Table 3-2.	Emerging Indirect Liquefaction R&D Activities	3-23

LIST OF TABLES (Continued)

VOLUME II

	<u>Page No.</u>
CHAPTER 4	
Table 4-1. Properties of Coals of Different Rank	4-11
Table 4-2. Important Process Development and Exploratory Work . .	4-52
Table 4-3. Wilsonville Facility - NTSL (Illinois No. 6 Coal) . .	4-88
Table 4-4. Integrated Two-Stage Liquefaction Process Yields (Lummus SCT Only)	4-92
Table 4-5. Lummus ITSL Product Yields	4-95
Table 4-6. Lummus ITSL Distillate Product Quality (Illinois No. 6)	4-97
Table 4-7. Wilsonville Facility ITSL (Illinois No. 6 Coal) . . .	4-101
Table 4-8. Wilsonville Facility ITSL (Wyodak Subbituminous Coal)	4-106
Table 4-9. CTSL Demonstration Run Comparison with H-Coal (Illinois No. 6 Coal)	4-110
Table 4-10. Wilsonville Facility - CTSL	4-113
Table 4-11. History of Process Development and Performance for Bituminous Coal Liquefaction	4-114
Table 4-12. Coal - Derived Pilot Plant Feeds: Comparison of Properties	4-118
Table 4-13. Hydrotreating Pilot Plant Tests for Coal-Derived Oils 750°F Catalyst Temperature; Fresh ICR 106 Catalyst	4-124
Table 4-14. Summary of Yields and Refining Costs for Coal- Derived Oils	4-131
Table 4-15. Refinery Costs Based on UOP Summary	4-135
Table 4-16. Differential Refining Costs, Dollars per Barrel of Desired Product	4-136
Table 4-17. Conclusions from BRSC/SAIC Economics Study	4-137
Table 4-18. Plant Summaries, Illinois No. 6 Coal	4-148
Table 4-19. Annual Operating Cost Illinois No. 6 Coal	4-150
Table 4-20. Baseline Economic Assumptions	4-152
Table 4-21. Required Selling Price of Products	4-153
Table 4-22. Required Selling Prices from Published Study Designs	4-155
Table 4-23. Summary of Ecological Impacts for A 1-quad Coal Liquefaction Industry and Research Recommendations	4-157

LIST OF TABLES (Continued)

Page No.

CHAPTER 5

Table 5-1.	Typical Process Conditions and Product Yields for MTG Processes	5-17
Table 5-2.	Activities and Selectivities to Oxygenates (Methanol and C ₂ + Alcohols) of Catalysts Based on Copper	5-37
Table 5-3.	Reactivity of Copper Hydride Systems (Soluble Copper Catalyst)	5-43
Table 5-4.	EPA Waivers Granted For Methanol/Cosolvent Alcohol Blends	5-62
Table 5-5.	Acceptable Methanol/Cosolvent Alcohol Blend Under the DuPont Waiver	5-63
Table 5-6.	Comparative Operating Characteristics for Various Alcohol Processes	5-66
Table 5-7.	Typical Composition and Properties of MAS	5-69
Table 5-8.	Performance and Composition of IFP Catalysts	5-75
Table 5-9.	Composition of Fractionated Alcohols from Demonstration Unit	5-76
Table 5-10.	Motor-Fuel Properties of Fractionated Alcohols from Demonstration Unit	5-77
Table 5-11.	OCTAMIX Compositions	5-84
Table 5-12.	Blending Densities of OCTAMIX	5-85
Table 5-13.	Operating Characteristics for Cs-doped Copper-Based Catalytic Processes Obtained at Lehigh University	5-89
Table 5-14.	Comparison of Product Compositions	5-90
Table 5-15.	Effect of Cesium Loading of Catalyst on Selectivity	5-91
Table 5-16.	Activities and Selectivities to Oxygenates (C ₁ -C ₅ Alcohols, Acetic Acid, Esters) of Catalysts Based on Group VIII Metals	5-105
Table 5-17.	Activities and Selectivities to Oxygenates (Methanol and C ₂ + Alcohols) of Catalysts Based on Alkalized MoS ₂	5-109

CHAPTER 6

Table 6-1.	Effect of Additives on Conversion of MRS Coal at 467° to 482°C, 13.8 MPa	6-27
Table 6-2.	Characteristics of Liquids From Coal Pyrolysis Processes	6-30
Table 6-3.	Properties of Feed Coals and Product Chars	6-33
Table 6-4.	Key Properties of Hydrotreated Pyrolysis Liquids	6-39

LIST OF TABLES (Continued)

	<u>Page No.</u>
Table 6-5. Status of Advanced Pyrolysis Developments	6-45
Table 6-6. COED Process Product Distribution	6-48
Table 6-7. Effect of Vapor Residence Time on Tar Yield at 925°F	6-53
Table 6-8. Major Product Yields from the Demonstration-Scale Plants	6-63
Table 6-9. Major Product Yields from the Commercial-Scale Plants	6-64
Table 6-10. Capital Cost Summary	6-66
Table 6-11. Product Unit Prices	6-68
Table 6-12. Annual Operating Cost Summary	6-69

CHAPTER 7

Table 7-1. Product Characterization Overview of Coprocessing Products	7-26
Table 7-2. Product Characterization	7-28
Table 7-3. HRI Economic Screening Studies Summary of Cases . . .	7-31
Table 7-4. HRI Economic Screening Studies Summary of Results . .	7-32

CHAPTER 8

Table 8-1. Fungal Types Examined for Solubilization Activity . .	8-15
--	------

CHAPTER 9

Table 9-1. Direct Liquefaction Processes Under Development Outside the U.S.	9-3
Table 9-2. German Coal Liquefaction Projects	9-5
Table 9-3. German Technology (Ruhrkohle AG) Typical Operating Conditions	9-6