FUNDAMENTAL DATA NEEDS FOR COAL CONVERSION
TECHNOLOGY

Six-Month Progress Report, August 15, 1976—February 15, 1977

February 28, 1977

Work Performed Under Contract No. EY-76-C-02-4059

Recon Systems, Incorporated
Princeton, New Jersey

MASTER

U. S. DEPARTMENT OF ENERGY

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SIX MONTH PROGRESS REPORT
August 15, 1976 - February 15, 1976²⁷

Contract No. EY-76-C-02-4059

FUNDAMENTAL DATA NEEDS FOR
COAL CONVERSION TECHNOLOGY

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February 28, 1977

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FUNDAMENTAL DATA NEEDS FOR
COAL CONVERSION TECHNOLOGY

Contract No. EY-76-C-02-4059

Six Month Progress Report

August 15, 1976 - February 15, 1977

INTRODUCTION

A thirteen month study (including final report preparation) of fundamental data needs for coal conversion technology was undertaken by RECON SYSTEMS, INC. of Princeton, N.J. in August 1976. The study has been conducted under the technical guidance of Dr. Roland H. Harrison, Technical Project Officer, of the Bartlesville Energy Research Center.

The work has been designed to meeting the following objectives:

- Phase I The Contractor shall identify the important processes or plants, pilot or demonstration, where thermodynamic research can be applied to effect a more efficient conversion of coal.
- Phase II The Contractor shall make a detailed study of the items identified in Phase I and determine where additional thermodynamic design information is needed or would be desirable.
- Phase III The Contractor and Consultants shall study the problem areas and identify all of these areas where new or improved thermodynamic data are needed and make specific recommendations for research.

Phase I work, which has been completed, and Phase II work, which is underway, will be discussed in this six month progress report.

PHASE I

Objective: The Contractor shall identify the important processes or plants, pilot or demonstration, where thermodynamic research can be applied to effect a more efficient conversion of coal.

Study of coal conversion literature and contacts with organizations known to be active in coal conversion were used to formulate a list of processes identified as being potentially important in coal conversion technology. Contacts made are listed in Table 1, and a compilation of processes are provided in Table 2. In Table 3, further detail is provided on twenty-five processes considered to be of current importance because at least pilot plant scale operations have been conducted.

With the aid of the Technical Project Officer, the twenty-five processes described in Table 3 were narrowed down to eleven processes for further study of fundamental data needs. The selection was based upon potential importance, state of development, desire to examine all basic process types, and availability of sufficient information. The process selection and reasoning are provided in Table 4.

TABLE 1
LIST OF ORGANIZATIONS CONTACTED

<u>Organization</u>	<u>Type of Contact*</u>	<u>Notes</u>
1. U.S. Energy Research and Development Administration	M, T, V	Visit to Pittsburgh Energy Research Center
2. Bituminous Coal Research, Inc.	M, T, V	Visit to Homer City, Pa.
3. Electric Power Research Institute	M, T	
4. American Gas Association	M, T	
5. Institute of Gas Technology	M, T	
6. Fluor Engineers & Constructors, Inc.	M, T, V	Visit to Irvine, Calif.
7. C. F. Braun Co.	M, T, V	Visit to Alhambra, Calif.
8. Combustion Engineering	M, T	
9. General Electric Company	M, T	
10. Stone & Webster	M, T, V	Visit to Boston, Mass
11. Ralph M. Parsons Co.	M, T, V	Visit to Pasadena, Calif.
12. Babcock & Wilcox Co.	M, T	
13. Westinghouse Research Laboratories	M, T, V	Visit to Pittsburgh, Pa.

* M = Mail; T = Telephone; V = Visit

TABLE 1 (Continued)

<u>Organization</u>	<u>Type of Contact*</u>	<u>Notes</u>
14. Consolidation Coal Company	M, T, V	Visit to Library, Pa.
15. Phillips Petroleum Company	T, V	Visit to Homer City, Pa.
16. Hydrocarbon Research, Incorporated	M, T, V	Visit to Trenton, N.J.
17. Rockwell Corporation	M, T, V	Visit to Canoga Park, Calif.
18. Gulf Mineral Resources Company	M, T, V	Visit to Denver, Col.
19. National Technical Information Services	M, T	
20. Coalcon, Inc.	M, T	
21. Continental Oil Company	M	
22. M. W. Kellogg Co., Inc.	M	
23. FMC Corporation	M, T	
24. Exxon Research & Development Co.	M, T	
25. Foster Wheeler Corporation	M	
26. Lummus Corporation	M	
27. U. S. Bureau of Mines	M, T	
28. Gulf General Atomics Company	M	
29. Pittsburgh & Midway Coal Mining Company	M	
30. Union Carbide Corporation	M	
31. Occidental Research & Development Corporation	M, T	
32. Battelle Memorial Institute	M, T	
33. Chemico	M	

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TABLE 2
COAL CONVERSION PROCESSES REVIEWED

<u>PRODUCTION OF SOLID, LIQUID AND GASEOUS PRODUCTS</u>		
<u>PROCESS</u>	<u>TYPE</u>	<u>T/D</u>
CCL (GULF)	1b	1
CLEAN-COKE (U.S. STEEL)	2+1b	$\frac{1}{2}$
COALCON (UCC/CHEMICO)	5+4b	20
COED (FMC)	2	36
COG (PAMCO)	1b+3b	?
COGAS (FMC/JV)	2+4b	50
CSF (CONSOL. COAL)	1b+2	70 (SD)
EXXON LIQUEFACTION	1a+3	1
F-T SYNTHESIS (KELLOGG et al.)	3b+6b	C (6600)
OCCID. PYROLYSIS	2	3
H-COAL (HRI)	1b	3 (600 TPD UC)
INTERMEDIATE HYDROG. (UNIV. OF UTAH)	5	$\frac{1}{2}$
LURGI-RUHRGAS	2	C
SRL (UNIV. OF NORTH DAKOTA)	1b	$\frac{1}{2}$
CRE SOLVENT EXTRACTION	1a	$\frac{1}{2}$
OLD BEN SRC	1	?
MITSUI SRC	1	5
PAMCO SRC	1b	50
SYNTHOIL (B of M)	1b	$\frac{1}{2}$ (10 TPD UC)

TABLE 2 (Continued)

COAL CONVERSION PROCESSES REVIEWED

PRODUCTION OF SOLID, LIQUID
AND GASEOUS PRODUCTS (Continued)

<u>PROCESS</u>	<u>TYPE</u>	<u>T/D</u>
TOSCOAL (OIL SHALE CORP)	2	25
CFFC (C-E LUMMUS)	1b	?
SRC (SOUTHERN SERVICES, INC.)	1b	6
<u>PRODUCTION OF HIGH BTU GAS</u>		
AGGLOMERATING ASH (BATTELLE/UCC/CHEMICO)	4b*	25
PATGAS (ATC)	3b*	?
ATGAS (ATC)	3b+6a	?
BI-GAS (BCR)	3b+6a	120
CO ₂ ACCEPTOR (CONSOL. COAL)	4b+6a	30
EXXON GASIF.	4b*	$\frac{1}{2}$
OCCID. COAL GASIF.	2	-
GEGAS (GE)	4b* (?)	$\frac{1}{2}$
HYDRANE (B of M)	5*	$\frac{1}{4}$ (24 PLANNED)
HYGAS (IGT)	5*, +	75
KOPPERS-TOTZEK	3b*	C (850)
LPM (CHEM SYSTEMS)	6a	-
LURGI PRES. GASIF.	3a or 3b*	C (1000)
MOLTEN SALT GASIF. (KELLOGG)	3b*	?

TABLE 2 (Continued)

COAL CONVERSION PROCESSES REVIEWED

PRODUCTION OF HIGH
BTU GAS (Continued)

<u>PROCESS</u>	<u>TYPE</u>	<u>T/D</u>
SOLUTION GASIF. (S & W/GULF)	5 [†]	(2) [†]
SYNTHANE (B of M)	3b*	70
TEXACO GASIF.	3b*	?
WELLMAN-GALUSHA (McDOWELL-WELLMAN)	3a or 3b*	C
WINKLER (DAVY POWERGAS)	3a or 3b*	C (100)
LURGI RECYCLE METHANATION	6a	-
RM PROCESS (PARSONS/TEXACO)	6a	-

OTHER COAL GASIFICATION
PROCESSES

B & W-DUPONT	3b	400
CE ENTRAINED FUEL PROCESS	3a	120
COMBINED CYCLE B & W (B&W/GE)	3a	60
COMBINED CYCLE F-W (F-W/PAMCO)	3a	?
OCCID. GASIF.	2, 4b	½
IFE TWO-STAGE	3a	C
IGI TWO-STAGE (W-D)	4a	C
KERPELY PRODUCER (B of M)	3a or 3b	?
MARISCHKA	3a ?	C
MULTIPLE FLUIDIZED BED (BCR)	3a	1

TABLE 2 (Continued)

COAL CONVERSION PROCESSES REVIEWED

OTHER COAL GASIFICATION
PROCESSES (Continued)

<u>PROCESS</u>	<u>TYPE</u>	<u>T/D</u>
PINTSCH HILLEBRAND	2, 4b	C
POWER-GAS LOW BTU	3a	C
ROCKGAS (ROCKWELL)	3a	1/4 (24 TPD UC)
RUHRGAS VORTEX	3a	C
RUMMEL SLAG BATH (URBK)	3a or 3b	C
STIRRED FIXED-BED (B of M)	3a	18
THYSSEN GALOCSY	3b	C
TWO-STAGE PROCESS (ATC)	3a	?
U-GAS (IGT)	3a or 3b	6
UGI BLUE WATER GAS	4a	C
WESTINGHOUSE LOW-BTU	3a	14
WILPUTTE	3a	C (30)
GE LOW BTU	3a	24
RILEY-MORGAN (RILEY CO.)	3a or 3b	C

Notes:

C Commercial plants have been operated

SD Shutdown

UC Under construction

* Methanation (6a) can be added

† Requires external source of heat for H₂ manuf.,
e.g. nuclear reactor. Bergbau-Forschung has
operated a 2 T/D unit.

TABLE 2 (Continued)

KEY TO PROCESS TYPES

Type

1. Solvent extraction of coal (for demineralization and depolymerization).
 - a. H_2 donor solvent
 - b. H_2 + process derived solvent
2. Pyrolysis (thermal decomposition in the absence of oxygen to produce gases, liquids, and solids).
3. Partial oxidation (reaction of coal with air or oxygen, with or without steam, to produce primarily CO and H_2).
 - a. low BTU gas (air oxidation) - 100-200 BTU/SCF
 - b. medium BTU gas (O_2 oxidation) - 250-500 BTU/SCF
4. Steam gasification (reaction of coal or coke with steam-air oxidation of coal or coke as heat source).
 - a. Two stage, cyclic - 250-350 BTU/SCF
 - b. Two vessel, continuous - 300-400 BTU/SCF
 - c. External heat source
5. Hydrogasifier
6. Synthesis
 - a. Methanation
 - b. Fischer-Tropsch
 - c. Methanol
7. Steam-Iron Process for H_2 manufacture

TABLE 2 (Continued)

KEY TO ORGANIZATIONS

AGA	American Gas Association
ATC	Applied Technology Corp (subsidiary of International Systems and Controls Corp.)
B of M	U.S. Bureau of Mines
B & W	Babcock & Wilcox Co., Ltd.
BATTELLE	Battelle Memorial Institute
BCR	Bituminous Coal Research, Inc.
CE	Combustion Engineering, Inc.
CHEMICO	Chemical Construction Corp.
CHEM SYSTEMS-	Chen Systems, Inc.
CONSOL. COAL	Consolidation Coal Co. (subsidiary of Continental Oil Co.)
CRE	Coal Research Establishment (U.K.)
DUPONT	E. I. duPont de Nemours & Co.
EXXON	Exxon Research and Engineering Co.
FMC	FMC Corp.
F-W	Foster-Wheeler Corp.
GE	General Electric Co.
GULF	Gulf Oil Corp.
HRI	Hydrocarbon Research, Inc. (subsidiary of Dynalectron Corp.)
IFE	International Furnace Equipment Co. Ltd.
IGI	Il Gaz Integrale (Italy) (subsidiary of B&W)
IGT	Institute of Gas Technology
MCDOWELL-WELLMAN	McDowell-Wellman Engineering Co.
JV	joint venture of two or more companies
KELLOGG	M. W. Kellogg Co. (subsidiary of Pullman, Inc.)
KOPPERS	Heinrich Koppers GmbH

TABLE 2 (Continued)

KEY TO ORGANIZATIONS

LUMMUS	The C-E Lummus Co. (subsidiary of CE)
LURGI	Lurgi GmbH (subsidiary of Metallgesellschaft AG)
MITSUI	Mitsui Group of Companies (Japan)
OCCID.	Occidental Research and Development Co. (subsidiary of Occidental Petroleum Corp.)
OLD BEN	Old Ben Coal Co. (subsidiary of Standard Oil of Ohio)
PAMCO	Pittsburgh and Midway Mining Co. (subsidiary of Gulf)
PARSONS	The Ralph M. Parsons Co.
POWER-GAS	Power-Gas Co.
ROCKWELL	Rockwell International Corp.
RUHRGAS	Ruhrgas AG
S & W	Stone & Webster Engineering Corp.
TEXACO	Texaco Development Co.
UCC	Union Carbide Corp.
UGI	UGI Corp.
URBK	Union Rheinische Braunkohlen Kraftstoff AG
U.S. STEEL	United States Steel Corp.
W-D	Woodall-Duckham Ltd. (subsidiary of B&W)
WESTINGHOUSE	Westinghouse Electric Corp.

TABLE 3. PRELIMINARY PROCESS SELECTION

<u>PROCESS</u>	<u>TYPE</u>	<u>PRODUCTS</u>	<u>STATUS</u>
1. COALCON (UCC/CHEMICO)	Fluidized Bed Hydrogasifier (1040°F/540 psig) + Partial Oxidation (O ₂) Char Slurry Gasifier (?/585 psig) (AAG - see 7. below - and other types of char gasification can be used)	SNG + LPG + Light Fuel Oil + Heavy Fuel Oil	25 TPD pilot plant (now shut down); large scale pilot plant being considered with ERDA funding
2. COGAS (FMC/JV)	Multi-Stage Fluidized Bed Pyrolysis (600-1500°F, 5-10 psig) + Two Stage Continuous Char-Steam Gasifier (1500-1700°F, 0-30 psig)	Fuel Gas + Oil	50 TPD pilot plant operated in England; ERDA funding being sought
3. EXXON LIQUEFACTION	Extraction With H ₂ Donor Solvent (800°F/2000 psig) + Partial Oxidation (O ₂)	Fuel Gas + Oil	1 TPD pilot plant (ERDA support since June 1976); seeking funding for 200 TPD unit
4. FISCHER-TROPSCH SYNTHESIS (KELLOGG et al)	Lurgi Moving Bed Partial Oxidation (O ₂) (1140-1400°F/350-450 psig) + Synthesis (620°F/330 psig)	Fuel Gas + Oil + Gasoline	Commercial 6600 TPD plant in South Africa
5. OCCIDENTAL PYROLYSIS	Flash Pyrolysis (1100°F/1 atm. + Char Heater at 1200-1600°F/1 atm.)	Tar + Char + Fuel Gas (700 BTU/SCF)	3.6 TPD pilot plant (ERDA support since July 1976)
6. PAMCO SRC	Extraction With Process Derived Solvent (815°F, 1000 psig)	SRC + Fuel Gas (or Fuel Oil + Fuel Gas in SRC-II)	6 TPD pilot plant in Wilsonville, Ala (sponsored by EPRI & others); 50 TPD pilot plant in Ft. Lewis, Wash (ERDA)
7. AAG (BATTELLE/UCC/CHEMICO)	Continuous Agglomerating Ash Coal-Steam Gasifier (AAG) (1800°F/100 psig + Char Heater at 2000-2100°F/100 psig) (+ Methanation for SNG)	Fuel Gas (300 BTU/SCF)	25 TPD pilot plant (AGA and ERDA funding)
8. BI-GAS (BCR)	Upper Stage Coal-Steam Gasifier (1400-1700°F/1000-1500 psig) + Lower Stage Partial Oxidation (O ₂) (2800°F/1000-1500 psig) + Methanation	SNG (378 BTU/SCF)	120 TPD pilot plant (AGA and ERDA funding)

TABLE 3. PRELIMINARY PROCESS SELECTION (Continued)

<u>PROCESS</u>	<u>TYPE</u>	<u>PRODUCTS</u>	<u>STATUS</u>
9. CO ₂ ACCEPTOR (CONSOL. COAL)	Continuous Fluidized Bed Coal-Steam-CaO Gasifier (1500°F/150-300 psig) + Char-Air-Dolomite Regenerator (1900°F/150-300 psig) + Methanation	SNG (400 BTU/SCF)	30 TPD pilot plant (ERDA funding)
10. HYDRANE (B of M)	Dilute Phase/Fluidized Bed Hydrogasifier (1650°F/1000 psig) + Partial Oxidation (1800-1900°F/1000 psig) + Methanation (partial in situ methanation)	SNG (826 BTU/SCF)	1/4 TPD pilot plant (24 TPD planned) (ERDA funding)
11. HYGAS (IGT)	Fluidized Bed Hydrogasifier (1300-1800°F/ 1000-1500 psig) + H ₂ From Partial Oxidation (1800-1900°F/1000-1500 psig) or Steam/Iron (2000°F/1200 psig) + Methanation (partial in situ methanation)	SNG	75 TPD pilot plant (AGA and ERDA funding)
12. SOLUTION-GASIFICATION (S&W/GULF)	Hydrogasifier (+ H ₂ From External Source or hi pressure Steam Reforming of Product SNG) (in situ methanation)	SNG	2 TPD pilot plant in Germany (external heat) (some ERDA funding)
13. SYNTHANE (B of M)	Fluidized Bed Partial Oxidation (O ₂) (1800°F/1000 psig) + Methanation	SNG (or SNG + Methanol) (405 BTU/SCF)	70 TPD pilot plant (ERDA funding)
14. CE ENTRAINED FUEL	Partial Oxidation (Air) (3300-3400°F/1 atm.)	Fuel Gas (125 BTU/SCF)	120 TPD pilot plant (ERDA and EPRI funding)
15. COMBINED CYCLE B&W (B&W/GE)	Partial Oxidation (Air) (900°F/high pressure gasifier; 1600°F/95 psig combustor)	Steam and/or Electric Power	60 TPD pilot plant (EPRI funding of design work)
16. ROCKGAS (ROCKWELL)	Partial Oxidation (Air) (Molten Sodium Carbonate, 1800°F/75-150 psig) (S & Ash Removal from salt)	Low BTU Fuel Gas	Tested in 2.4 TPD unit. ERDA Contract for 120 TPD pilot plant
17. SYNTHOIL (B of M)	Catalytic Fixed Bed Liquefaction With Process Derived Solvent (850°F/2000-4000 psig)	Fuel Gas + Oil	Tested in 1/2 TPD unit 10 TPD pilot plant in 1976 (ERDA funding)

TABLE 3. PRELIMINARY PROCESS SELECTION (Continued)

<u>PROCESS</u>	<u>TYPE</u>	<u>PRODUCTS</u>	<u>STATUS</u>
18. B of M LOW BTU/ COMBINED CYCLE	Moving Bed Partial Oxidation (Air) (1300°F/120 psig) + Combustor (1950°F/105 psig)	Steam and/or Electric Power	
19. WESTINGHOUSE LOW BTU	Fluidized Bed Partial Oxidation (Air) (1600°F/250 psig)	Fuel Gas (135 BTU/SCF)	14 TPD pilot plant (partial ERDA funding)
20. SUSPENSION-FIRED GASIFIER (B&W)	Partial Oxidation (O ₂) (1800°F after waste heat boilers/48-1500 psig) peak temperature near 2800°F	Fuel Gas (300 BTU/SCF)	120 TPD (1100-1500 psig) unit supplied to Bi-Gas (Process No. 8) Earlier units up to 400 TPD in 1950's for duPont and B of M
21. COED (FMC)	Fluidized Bed Pyrolysis (600-1500°F/ 5-10 psig) + Catalytic Fixed Bed Hydrotreat (750°F/2500-3100 psig)	Synthetic Crude + Fuel Gas	36 TPD (ERDA and EPRI funding)
22. H-COAL (HRI)	Catalytic Ebullated Bed Hydrogenation of a Coal/Oil Slurry (850°F/2250-2700 psig)	Synthetic Crude + Fuel Gas	3 TPD (ERDA support for 600 TPD pilot plant)
23. LURGI	Moving Bed Partial Oxidation (O ₂) (1140-1400°F/350-450 psig)	Fuel Gas (450 BTU/SCF)	Commercial plants in South Africa and elsewhere
24. CSF (CONSOL. COAL)	Stirred Reactor Extractor (765°F, 150- 400 psig) + Carbonizer (925°F, 10 psig)	Fuel Oil and Fuel Gas (820 BTU/SCF)	13 TPD pilot plant in Cresap, W. Va. being modified and reactivated for startup in 1977 by Fluor
24. TEXACO	Partial Oxidation (O ₂) (greater than 2000°F/300 + psig) + Shift to make H ₂ or Methanation for SNG	Fuel Gas (CO + H ₂)	Pilot plant in Montebello, Calif.

TABLE 4

COAL CONVERSION PROCESSES SELECTED
FOR FURTHER STUDY

<u>PROCESS (ERDA Project Officer or Program Manager)</u>	<u>Selected for Further Study</u>	<u>Reasons</u>
1. COALCON (M. A. Christensen)	Yes	- Potential commercial importance; liquids produced
2. COGAS	No	- Insufficient information available - Pyrolysis step covered by COED
3. EXXON LIQUEFACTION (J. Farley)	No	- Insufficient information
4. FISCHER-TROPSCH	No	- Already commercialized with Lurgi gasifiers in 6600 T/D South African plant
5. OCCIDENTAL PYROLYSIS (D. Hart)	No	- Insufficient information
6. PAMCO SRC (Martin Neuwirth)	Yes	- Major ERDA project
7. AAG (L. Jablansky)	No	- Insufficient information
8. BI-GAS	Yes	- Major ERDA project
9. CO ₂ ACCEPTOR	Yes	- Major ERDA project
10. HYDRANE (Dr. Gilmore)	No	- Insufficient information; conditions similar to Synthane and Hygas
11. HYGAS (B. C. Almula)	Yes	- Major ERDA project
12. SOLUTION-GASIFICATION	No	- Insufficient information
13. SYNTHANE (E. L. Clark)	Yes	- Major ERDA project
14. CE ENTRAINED FUEL	No	- Gaseous products at low pressure where thermodynamic data already available

TABLE 4 (Continued)

PROCESS (ERDA Project Officer or Program Manager)	Selected for Further Study	Reasons
15. COMBINED CYCLE B&W	No	- Insufficient information; similar process by Westinghouse
16. ROCKGAS	Yes	- Recirculation of molten sodium carbonate distinguishes ROCKGAS process from others
17. SYNTHOIL (William C. Morel)	Yes	- Major ERDA project
18. B. of M LOW BTU	No	- Insufficient information; similar process by Westinghouse; no major program underway
19. WESTINGHOUSE LOW BTU	Yes	- High pressure partial oxidation with air distinguishes WESTINGHOUSE process from lower pressure operations
20. SUSPENSION-FIRED GASIFIER	No	- Included in BI-GAS
21. COED (John Morris)	Yes	- Low pressure pyrolysis distinguishes COED process from others; covers wide range of temperature
22. H-COAL	Yes	- Major ERDA project
23. LURGI	No	- Process already commercial; conditions similar to those in other processes to be studied

TABLE 4 (Continued)

<u>ERDA (ERDA Project Officer or Program Manager)</u>	<u>Selected for Further Study</u>	<u>Reasons</u>
24. CSF (CONSOL. COAL)	No	- Limited information available; conditions similar to other liquefaction processes
25. TEXACO PARTIAL OXIDATION	No	- Limited information available; some form of partial oxidation to make H ₂ is an integral part of most hydrogenation processes to be studied

PHASE II

Objective: The Contractor shall make a detailed study of the items identified in Phase I and determine where additional thermodynamic design information is needed or would be desirable.

Process flow diagrams for the eleven selected processes follow as Figures 1-11. Temperature and pressure conditions are provided on the flow diagram for each major subsystem.

Reports for each of the ten processes which have been investigated follow as Tables 6-15. Followup for the Coalcon Process has not yet been completed. Fundamental data need areas identified by process developers and designers are compiled in Tables 6-15 and keyed to a general description of data types shown in Table 5. This raw tabulation will be evaluated and shaped into a specific R&D program with the aid of information forthcoming from the computer-aided sensitivity analysis.

The Chemshare computer simulation system has been chosen as the basis of heat and material balance models for each of the selected processes. At the present time, a terminal at the University of Pennsylvania is being used with the UCS computer in Springfield, N.J., but a Texas Instruments Model 733 ASR Send-Receive Terminal with dual tape cassettes and built-in acoustic coupler has been ordered for installation in RECON's offices to expedite the modeling work.

The Hygas Process has been simulated, as shown in Figures 12-15 and Table 16. The H-Coal process has been selected for the second simulation because of its current importance, and because it is a liquefaction process as contrasted to the Hygas high BTU process.

SRC PROCESS SCHEMATIC

Figure 1

SYNTHOIL PROCESS SCHEMATIC

Figure 2

H-COAL PROCESS SCHEMATIC

Figure 3

COALCON HYDROCARBONIZATION PROCESS

Figure 4

COED PROCESS SCHEMATIC

Figure 5

HYGAS PROCESS SCHEMATIC

Figure 7

SYNTHANE PROCESS SCHEMATIC

Figure 8

BI-GAS PROCESS SCHEMATIC

Figure 9

**SCHEMATIC OF ADVANCED COAL GASIFICATION SYSTEM
FOR ELECTRIC POWER GENERATION
(WESTINGHOUSE)**

Figure 10

MOLTEN SALT COMBUSTION AND GASIFICATION PROCESS SCHEMATIC

Figure 11

TABLE 5

KEY TO FUNDAMENTAL DATA NEEDS*

A. Physical Properties

1. Density of solids
2. Density of liquids
3. Density of slurries
4. PVT relationship of gases
5. Boiling points
6. Melting points

B. Thermodynamic Properties

1. True critical points and pseudocritical constants
2. Vapor pressures and vapor-liquid equilibria
3. Solubility of gases in liquids and slurries
4. Solubility of solids in liquids
5. Solid/liquid equilibria
6. Heat capacity of solids
7. Heat capacities of liquids
8. Heat capacity of slurries
9. Heat capacity of gases
10. Enthalpy of fusion
11. Enthalpy of vaporization
12. Enthalpy of solution
13. Standard heat of formation and heat of reaction
14. Standard free energy of formation and equilibrium constants
15. Joule-Thompson inversion point
16. Liquid/liquid equilibria

C. Chemical Properties

1. Elemental composition
2. Pure component composition or composition by type (aromaticity, polynuclear content, branching, olefins, etc.)
3. Molecular weight
4. Reactions between materials of construction/reactants/products

*These data needs are designated by letters and numbers on Tables 6-15.

TABLE 5 (Continued)

D. Transport Properties

1. Viscosity of liquids
2. Viscosity of slurries
3. Viscosity of gases
4. Thermal conductivity
5. Diffusivity

E. Engineering Data

1. Properties of fluidized gas/solids systems
2. Slurry flow characteristics
3. Slurry characterization and stability
4. Foam characterization and stability
5. Characteristics of two and three phase flow thru reactors
6. Adsorption equilibria
7. Characterization of gases, liquids, solids, obtained by devolatilization of coal
8. Characterization of ash agglomeration
9. Product compatibility information, including solubility, flammability, stability
10. Solids-liquid separation problems
11. Flammability data
12. Reactivities of solids with O_2 , CO_2 , H_2O , etc.

TABLE 6

SYNTHOIL PROCESS

Primary Sources of Information:

- Visit with Dr. Sayeed Akhtar, PERC, 12/13/76
- References 1-4

Status:

- 1/2 T/D (coal slurry) pilot plant in operation at PERC (lacks gas purification facilities)
- 10 T/D (coal) pilot plant under construction at PERC; startup early in 1978

Heat and Material Balance Information:

- Reference 2 (incomplete)

Fundamental Data Need Areas Identified:

- B.8.13.14;
D.2.; E.3. - Oil/coal slurry properties (viscosity and stability vs temperature, oil and coal properties; heat of formation; specific heat; free energy of formation)
- B.2.3. - Solubility of gaseous components in oil/coal slurry (primarily H₂, but also CO, CO₂, NH₃, and other minor components) and vapor-liquid equilibria
- C.2. - Properties of ammonium polysulfides found in recycle gas
- B.13.; C.2. - Variation of reactor thermal properties with position in reactor (to answer question of optimum position for interstage reactor cooling)
- B.14.; C.1. - Equilibrium information for amine absorber includes H₂S, but especially minor constituents of gas--some of which may not yet have been identified)
- E.4. - Foaming mechanism in amine absorber
- C.1.2. - Properties of product to char deoiler (pyrolysis?)
- E.5. - Flow thru fixed bed reactor
- Needs for O₂ gasifier to be discussed elsewhere

TABLE 6 (Continued)

Miscellaneous:

- Characterization studies of the centrifuged liquid and solid products have been made (reference 1, p. 2-20)
- Argonne National Laboratory is investigating heat of reaction of H_2 with coal slurries. Specifications for the calorimetric pressure vessel are 135-270 atm, up to 885°F. (reference 1, p. 2-20)
- Work being done by Battelle Memorial Institute involves measuring viscosity, density, electrical resistivity, and the dielectric constant of Synthoil liquids (intermediate and product at 1-270 atm, 75-840°F). (reference 1, p. 2-21)
- Work done by Exxon Research and Engineering Company to determine the chemical properties of Synthoil products and feed (mass spectrometry, gas chromatography, nuclear magnetic resonance) (reference 1, p. 2-21)
- Some work has been done in Bartlesville on Synthoil composition.

TABLE 7

SYNTHANE PROCESS

Primary Sources of Information:

- Visit with Mr. William Haynes and Mr. Joseph Strakey, PERC, 12/13/76
- References 1, 5-8

Status:

- 72 TPD Pilot Plant in shakedown phase at PERC

Heat and Material Balance Information:

- Reference 2 (incomplete)
- Synthane Pilot Plant Information from Lummus

Fundamental Data Need Areas Identified:

- B.13. - Coal and pretreated coal heat of formation (Dulong and Petit correlation is used)
- D.3. - Distribution coefficients of gaseous components between gas and water phases, including tar components (e.g. phenolics), NH_3 , CO_2 , H_2S , trace components (e.g. thiocyanates, HCN , thiophenes), etc.
- E.4. - Foaming mechanism in tar scrubber and decanter
- B.13.; C.1.2. - Char properties (experimental chemical composition and heat of combustion have been done; have used Lee's correlation for specific heat vs volatile content)
- A.2.6.; C.1.2. - Tar properties
- E.6. - Adsorption equilibria on char used for premethanation purification (Exxon has contract in this area of work)
- B.2. - Glycol drier equilibria
- B.1.13.14. - Equilibria in Benfield hot carbonate process (e.g. COS to $\text{H}_2\text{S} + \text{CO}_2$ hydrolysis), but may be available on a proprietary basis
- B.2.3. - Information for water treatment systems for NH_3 , CO_2 , H_2S , HCN , trace component elimination or recovery (e.g. see reference 7, Figure 6)
- B.2. - Vapor-liquid equilibrium for various stages of product gas cooling

TABLE 8

WESTINGHOUSE LOW BTU GAS PROCESS

Primary Sources of Information:

- Visit with Dr. D. L. Keairns and Dr. D. Archer, Westinghouse Research Laboratories, Pittsburgh, Pa., 12/14/76
- References 1, 6, 9-12

Status:

- 15 T/D process development unit near Pittsburgh, Pa. (Waltz Mill)
- Next stage of scaleup not yet determined

Heat and Material Balance Information:

- References 8 and 9

Fundamental Data Need Areas Identified:

- B.13; E.7. - Characterization of gases, liquids, and solids obtained by devolatilization of coals at various temperatures, times, and particle size (Westinghouse devolatilization at about 1500-1600°F, 225 psig.-- other processes at different conditions)
- B.5.13.14 - Gas/solid free energy and thermal data for dolomite-sulfur systems including regeneration by

and

and effect of impurities in forming eutectics.

- B.5.13.14 - Gas/solid free energy and thermal data for Fe/O/S systems (see Morgantown work by Oldaker)
- B.13 - Heats of formation for chars made by devolatilization and used in gasifier
- C.1.2; B.6 - Characterization of trace inorganic species and their role in ash agglomeration

TABLE 8 (Continued)

- C.1.2.; B.5. - Characterization of Na, K, Cl and other inorganic species and their role in turbine blade degradation
- A.4. - Gas properties required for expansion calculations
- C.1.2.; B.5. - Vapor pressure and other characterization of trace elements and their compounds released during gasification (under reducing conditions in Westinghouse process)

TABLE 9

CO₂ ACCEPTOR PROCESS

Primary Sources of Information:

- Visit with Mr. George P. Curran, Consolidation Coal Company, Library, Pa., 12/15/76
- References 1, 6, 13-16

Status:

- 40 T/D pilot plant in Rapid City, South Dakota

Heat and Material Balance Information:

- Reference 13

Fundamental Data Need Areas Identified:

- B.5.13.14. - Distribution of sulfur compounds from the gasifier and regenerator, including CaS, CaSO₄, SO₂, H₂S, S, COS
- B.6.10. - Phase diagrams for coal ash, including all impurities (liquid formation temperatures much more important than heats of fusion)
- B.3.14. - H₂O/H₂S/NH₃/CO₂ system data for quench tower (150-250°F, approx. 150 psig) (summary of data for this system underway by IGT, but not yet reported)
- B.3.4.13.14 - Thermodynamic data for Chance reaction (CO₂ + H₂O + CaS = CaCO₃ + H₂S) (150-200°F)

Miscellaneous:

- Considerable work on thermodynamic properties done by Consolidation Coal Company prior to major development work (e.g. references 14-16)
- IGT work on a coal conversion systems technical data book (reference 19) meets at least some important needs including char properties.
- Radian Corp. has a \$400,000 contract to measure and identify sulfur emissions on Rapid City, South Dakota pilot plant. Work is now underway.
- Diethylene glycol system used for SNG in this and other processes. Considerable experience available from commercial natural gas plants.

TABLE 9 (Continued)

- Optimum position for compression (before or after methanation) not yet established, but compression properties for gases produced are available.
- Thermodynamic data developed by Kelley (Bureau of Mines) should be reviewed and updated by literature and experimental work.
- Dr. Jack Redden of the South Dakota School of Mines is studying "Phase Relationships in the CaCO_3 - CaSO_4 - CaS System" under OCR Prime Contract No. 14-01-0001405(3).

TABLE 10

BI-GAS PROCESS

Primary Sources of Information:

- Visit with Donald E. Hull and John M. Miles of Phillips Petroleum Company in Homer City, Pa., 12/15/76
- References 1, 6, 17, 18

Status:

- 120 T/D pilot plant being started up in Homer City, Pa.

Heat and Material Balance Information:

- Reference 17

Fundamental Data Need Areas Identified:

- B.13.14.C.1.2 - Coal properties, including free energy
- C.2. - Coal trace element analyses
- B.5. - Phase diagrams for trace components and fluxes (under reducing conditions). Examples of fluxes of interest are sand, blast furnace slag, and limestone.
- B.14. - Sulfur distribution equilibria, e.g. between ash components and gas
 - Data on COS hydrolysis
- B.4. - Distribution of coal impurities between coal and water in slurries ("leachability")
- B.13.14. - $\text{NH}_3/\text{CO}_2/\text{H}_2\text{O}/\text{H}_2\text{S}$ equilibria in water wash system
- B.3.12. - Selexol absorber data
- C.2., E.6. - Data on Ni-COS system (COS poisons nickel methanation catalysts)

TABLE 11

HYGAS PROCESS

Primary Sources of Information:

- Telephone conversation with Dr. Bernard Lee, IGT, Chicago, Ill., 12/1/76
- References 1, 6, 19, 20

Status:

- Pilot plant in Chicago designed to convert 75 T/d of coal to 1.5 million SCFD of clean high BTU gas. Sustained operations have been attained at various feed rates. A steam-iron pilot plant for H₂ generation has been built at the same site for comparison with the steam-oxygen and electrothermal techniques.

Heat and Material Balance Information:

- Reference 20 (includes steam-oxygen process)

Fundamental Data Need Areas Identified:

- BTX - gas separation with water present (BTX = benzene/toluene/xylene mixture) (100-400°F, approximately 1150 psig)
- see Bi-Gas, CO₂ Acceptor, Synthane, Westinghouse processes.

Miscellaneous:

- B.2. - In Dr. Lee's opinion the Hygas Process has no thermodynamic data needs because essentially only gas phase reactions take place, for which data is available.
- B.13; C.1.2 - Some data requirements on coal, char, etc. are provided in the data book being prepared by IGT (reference 19)

TABLE 12

H-COAL PROCESS

Primary Sources of Information:

- Visits with Al Comolli and Edwin Johanson, Hydrocarbon Research, Incorporated (HRI), Trenton, N.J., 1/6/77 and E. Edwards, Fluor Engineers and Constructors, Inc., Irvine, Calif., 1/13/77; telephone conversations with H. Stottler, HRI, Morristown, N.J.
- References 1, 21-24

Status:

- 3 T/D PDU at Trenton, N.J.; 600 T/D pilot plant under construction in Catlettsburg, Kentucky scheduled for completion in 1978.

Heat and Material Balance Information:

- Reference 23

Fundamental Data Need Areas Identified:

- B.2.5.11;
C.1.2. - Information on the nature of water contained in coals, including form of water present and vapor pressure at temperatures up to 200°F (drier operation), and also at temperatures and pressures up to 700°F and 3000 psig (oil slurry). This information is very important because drying affects liquefiability of lignite and insufficient drying leads to foaming in oil slurry.
- B.2. - Vapor-liquid equilibrium data for vapor and liquid streams leaving H-Coal reactor at about 850°F, 3000 psig, and 1800 psig H₂ partial pressure. Pilot plant data apparently indicates greater volatility than Chao-Seader correlations. Some lab work is being done by Dr. Chao under EPRI sponsorship.
- C.1.2. - Residual oil produced contains about 3% oxygen and 1.5% nitrogen. These levels are lower in lighter products.
- B.4. - Data on solubilization of coal and product chars in various types of oil up to 700°F.
- B.6.13. - Heats of formation and specific heats for coal and products for better estimation of heat of reaction.

TABLE 12 (Continued)

H-COAL PROCESS (Continued)

- E.2.3. - Flow properties for slurries and oils up to 700°F, 3000 psig. Oscillating disc methods? Work to date has been with Brookfield Viscometer at atmospheric pressure up to 550°F.
- A.4. - H₂ compressibility data up to 3000 psig.
- B.3.14. - H₂S/NH₃/CO₂/H₂O equilibrium data.
- B.2.3. - Data on "K" values for absorption of vent gas streams, e.g. by aromatic oils which are available as products.
- B.2.14; C.2. - Information on forms of sulfur and equilibria in vapor streams.
- C.1.2. - Chemistry of metallic components in coal, e.g. titanium, iron, sodium, calcium. Porphyrin and other organic compounds. These questions are related to catalyst activity.
- C.1.2; E.6. - Chemistry of metallic compounds in catalyst, and other forms of deactivation.
- E.10. - Properties related to hydroclone design for solids separation, e.g. viscosity, density, particle size.
- E.10. - Mechanism of anti-solvent action where light oils are used to precipitate residual oils from product slurry.
- E.9. - Data on product compatibility with H-coal products.

TABLE 13

PAMCO SRC

Primary Sources of Information:

- Visits with B. K. Schmid, Gulf Mineral Resources Co., Denver, Colorado, 1/14/77 and J. B. O'Hara, A. Bela, and D. G. Reynolds, The Ralph M. Parsons Co., Pasadena, Calif., 1/12/77
- References 1, 24-29

Status:

- 50 T/D pilot plant in operation at Ft. Lewis Washington on both SRC-I (primarily solid fuel product) and SRC-II processes (primarily liquid fuel product); 1 lb/hr bench scale unit in Merriam, Kansas primarily on SRC-II; 6 T/D developmental unit at Wilsonville, Alabama on SRC-I.

Heat and Material Balance Information:

- Reference 25 (hybrid demonstration plant with elements of SRC-I and SRC-II)

Fundamental Data Need Areas Identified:

- B.8.13; D.2.- Fundamental data on slurry formulation and preheating would be useful to understand viscosity and gelling effects. Gelling is endothermic. Slurry formulation at high temperature is important in SRC-II process to conserve heat. Expect to design for about 450°F, 40-50% solids (1.5-2.5 lbs. slurry per lb. coal).
- E.3. - Study of flow phenomena under slurry preheater conditions (450-750°F, 1000-2500 psig) is an important area for engineering research. Pressure drop appears to be lower than anticipated, possibly because of low viscosity flow near tube walls with gel sliding through.
- B.7.8.13. - Heats of formation and heat capacities of feed and products to dissolver (reactor). Reaction is very exothermic.
- B.2; C.1.2.- Vapor-liquid equilibria for separation steps over full range of pressures and temperatures from reaction conditions (about 850°F) to atmospheric conditions. Vapor from first stage of separation remains at relatively high pressure (about 500 psi or above) for purification and recycle. Liquids are reduced in pressure and temperature. Good data base would help in optimization of the vapor-liquid separation system.

TABLE 13 (Continued)

PAMCO SRC (Continued)

- D.2.; E.2.3. - Viscosity and flow information on product slurry under reducing conditions. Slurries contain up to 50% solids (very fine particles). Important in flow design and vacuum distillation.
- B.2.3.; C.1.2. - Absorption equilibrium for scrubbing vapor with coal-derived-naphtha at high pressure. Test data results are different than expected. Coal-derived-naphtha very aromatic with appreciable oxygen and nitrogen compounds.
- B.2.3.; C.1.2. - Vapor-liquid equilibrium for high pressure cryogenic system to purify vapor. This is one alternative purification system, but data lacking for reliable design.
- B.2.7.9.; D.1.3.5. - Vapor-liquid equilibria, enthalpy, heat capacity, viscosity, and thermal conductivity data all lacking for design of product oil fractionators.
- B.5.7.8.13. - Design of gasifier would be aided by further characterization of feed (60 wt % 850°F+ oil, 11% undissolved organics, 29% ash from SRC-II) with regard to heat of formation and heat capacity, and phase diagrams for inorganic materials. Although a gasifier would be required in final design, there is none in the Ft. Lewis pilot plant. Gasifier pressure depends on process chosen and design optimization.
- B.16. - Distribution of phenols, creosols, etc. between oil and water phases under various conditions of water separation. Phenols present to the extent of about 0.5-1% of water.
- A.2.5.6.; B.1.2.7.10.11.; C.1.2.3.; D.1.4. - Generalized correlations for properties of coal-derived-liquids would be very useful, including density, composition, viscosity, specific heat, vapor pressure, etc. Gulf is beginning to compile data available from SRC development programs, most of which appears in progress reports.

PAMCO SRC (Continued)

Miscellaneous:

- There are several major versions of the SRC Process:

SRC-I makes primarily solid fuel product, using an all-distillate recycle "coal solvent" (reference 27)

SRC-II makes primarily low-sulfur distillate fuel oil, using a product slurry "coal solvent" (avoids filtration) (reference 26)

Hybrid versions which contain features of both SRC-I and SRC-II (reference 25)

- About 3000 tons of SRC solid has been made and sent to Southern Services in Georgia for combustion tests.
- Ft. Lewis pilot plant is being revamped for SRC-II, to be ready by Spring 1977.
- Coal preparation presents no particular problems. Normally dry to 1% water at Ft. Lewis; expect to dry to 3% in commercial operation.

TABLE 14

ROCKGAS PROCESS

(Molten Salt Coal Gasification Process)

Primary Sources of Information:

- Visit with C. A. Trilling and A. L. Kohl, Atomics International Div., Rockwell International, Canoga Park, Calif., 1/12/77
- References 1, 30

Status:

- Detailed design and procurement of equipment for 24 T/D PDU to be located at Santa Susana, Calif. now underway, under ERDA sponsorship.
- Test reactor with about 500 lb/hr capability in operation.

Heat and Material Balance Information:

- Detailed heat and material balance information not available.

Fundamental Data Need Areas Identified:

- E.11. - Combustibility information on coal conveying with air at high pressure. Normal NFPA codes would require extraordinarily thick walls for piping and vessels.
- B.2.5.13.14. - Partition of inorganic materials (e.g. sulfur, sodium, nitrogen, silica) and carbon among gas, liquid, and solids in molten salt reactor under reaction conditions (1750-1800°F, 150-300 psi, reducing conditions). Available data on two and three phase systems have limited value.
- B.13. - Heats of reaction in melt phase in reactor.
- D.1. - Viscosity of melt at reaction conditions to quench conditions (320-350°F).
- B.3.4. - Partition of gaseous components and inorganic materials between water and gas phases in scrubber (about 150-200°F, 150-300 psi)

TABLE 14 (Continued)

ROCKGAS PROCESS (Continued)

- B.5. - Partition of various melt components between liquid and solid phases in quench tank (320-350°F), including sodium carbonate, sulfite, silicate, aluminate, iron, carbon, etc. (recycle liquor almost saturated in NaHCO_3 is used to enhance silica precipitation).
- B.2.14. - Equilibrium data for green liquor slurry flash (300 psig to below atmospheric pressure).
- B.4.14. - Equilibrium data in the carbonation system (175°F, atmospheric) where CO_2 causes precipitation and allows H_2S stripping.
- B.4.14. - Equilibrium data on $\text{H}_2\text{O}/\text{CO}_2/\text{Na}_2\text{CO}_3/\text{NaHCO}_3/\text{H}_2\text{S}$ system (180°F, subatmospheric) for H_2S stripper (steam or CO_2 can be used).
- B.13.14. - Reaction heat (exothermic) and equilibrium data for NaHCO_3 precipitation using CO_2 (120°F, 1 atm).
- B.3.14. - High pressure data on CO_2 scrubbing using plant liquor ($\text{Na}_2\text{CO}_3/\text{NaHCO}_3/\text{CO}_2$).
- B.14. - Equilibrium data for $\text{NaHCO}_3/\text{Na}_2\text{CO}_3/\text{H}_2\text{O}/\text{CO}_2$ in calcination and drying at 350°F.
- C.4. - Refractory interactions with melt (hi purity alumina refractory appears resistant even though sodium aluminate would be present at equilibrium in the presence of molten sodium carbonate).

Miscellaneous:

- Atomics International has relied on JANAF tables for thermodynamic data. Discrepancies and gaps include iron sulfide and sodium sulfide, for example discrepancy in sodium sulfide melting point. This and Kelly work should be reviewed by RECON for usefulness.
- Gas cleanup not part of present ERDA program on this process.

TABLE 15

COED PROCESS

Primary Sources of Information:

- Visit with J. B. O'Hara, A. Bela, and D. Reynolds, The Ralph M. Parsons Company, Pasadena, Calif., 1/12/77
- References 1, 31, 32

Status:

- A 36 T/D pilot plant, operated intermittently from 1970-1975 by FMC Corp. in Princeton, N.J. is now shut down.
- The Cogas Development Company of Princeton, N.J., a joint-venture partnership including FMC, is developing the COGAS Process to produce synthetic crude oil and synthesis gas. The COGAS process is based on the COED pyrolysis development plus char gasification and oil hydrotreating steps.

Heat and Material Balance Information:

- Reference 31

Fundamental Data Need Areas Identified:

- B.6.9.11. - Data on heat effects in coal drying, including water vaporization and heat capacity of coal (dryer uses sensible heat of low-BTU gas in entrained flow driers 200-600°F gas, 2-5 psig).
- B.6.7.9.14.;
C.1.2.3.;
D.1. - Thermal data for pyrolysis, including heat of pyrolysis, heat capacities, and physical and chemical characterization of coal feed and products (575-1050°F, 15 psig).
- B.6.7.9.11. - Heat capacities and heats of vaporization for pyrolysis product streams to be used in condenser designs.
- B.2.6.7.9.11.;
D.1.3. - Vapor-liquid equilibria, thermal, and viscosity data for oil recovery tower.
- D.2. - Viscosity data for liquids containing residual solids to be used in flow and filtration designs.

TABLE 15 (Continued)

COED PROCESS (Continued)

- B.1.2.3.14, C.1.2.3. - Equilibrium and other thermodynamic data for pyrolysis oil hydrotreater design, including saturate/unsaturate equilibrium and solubility data for NH_3 , H_2S , and H_2O in product liquid (650-750°F, 2000-3000 psig).
- B.2. - Vapor-liquid equilibrium data for post-hydrotreater separators (to 100°F, 100 psig).
- B.2.3.13.14. - Equilibrium and thermal data for DGA (diethylene glycol amine) $\text{H}_2\text{S}/\text{CO}_2$ scrubbing from pyrolysis gas (approx. 100°F, 50 psig contactor; 263°F, 16 psig regenerator) and for alternative solvents such as alcohols.
- E.12. - Fundamental data on reactivities and other properties of pyrolysis chars for gasifier design (1600°F, 15 psig)
- B.1.2.3.14., C.1.2.3. - Pyrolysis equilibria and heats of reaction at high pressure, up to 500 psig, a condition which could significantly decrease capital cost (according to Parsons).

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IGT PROCESS FLOWSHEET
(MONTANA COAL)

Figure 12

PROCESS SIMULATION BLOCK DIAGRAM FOR
DUST REMOVAL SECTION OF IGT HYGAS PROCESS

Figure 13

STEAM NUMBER KEY
IGT = INSTITUTE OF GAS TECH
RSI = RECON SYSTEMS, INC.
COMPUTER SIMULATION

DUST REMOVAL AND SHIFT CONVERTER COMPUTER BLOCK DIAGRAM

IGT HYGAS PROCESS

B-T-X RECOVERY COMPUTER BLOCK DIAGRAM

Figure 15

TABLE 16

COMPARISON OF IGT PROCESS HEAT & MATERIAL BALANCE⁽³⁾ WITH COMPUTER SIMULATION

Stream Designation	Feed From Hydrogasifier		Gas From Venturi Scrubber		Feed To Shift Converter		Gas From Shift Converter		Gas Feed To Scrubber		Gas Feed To Activated Carbon	
	IGT No.	RECON No.	IGT No.	RECON No.	IGT No.	RECON No.	IGT No.	RECON No.	IGT No.	RECON No.	IGT No.	RECON No.
	<u>1</u>	<u>1</u>	<u>2</u>	<u>7</u>	<u>3</u>	<u>9</u>	<u>4</u>	<u>10</u>	<u>5</u>	<u>36</u>	<u>6</u>	<u>21</u>
Temp °F	600	600	300 ⁽¹⁾	466	550	550	692	550 ⁽²⁾	125	125	125	130
Pressure °F	1155	1155	-	1144	-	1140	1125	1140	-	1110	1100	1110
Component												
CO	12.93	12.93	13.04	13.88	13.04	13.88	3.40	3.61	12.05	11.73	12.08	11.87
CO ₂	11.98	11.98	12.08	12.85	12.08	12.86	21.72	23.13	31.40	32.89	31.34	32.68
H ₂	15.20	15.20	15.34	16.31	15.34	16.31	24.98	26.58	39.75	38.66	39.87	39.22
H ₂ O	50.43	50.43	49.99	46.80	49.99	46.80	40.35	36.53	0.17	0.17	0.17	0.0
CH ₄	8.26	8.26	8.33	8.87	8.33	8.87	8.33	8.87	15.18	14.80	15.22	14.85
C ₂ H ₆	0.63	0.63	0.64	0.68	0.64	0.68	0.64	0.68	1.16	1.13	1.15	1.10
B-T-X	0.19	0.19	0.19	0.20	0.19	0.20	0.19	0.19	0.13	0.33	0.01	0.0
NH ₃	0.22	0.22	0.22	0.24	0.22	0.24	0.22	0.24	0.0	0.0	0.0	0.0
H ₂ S	0.12	0.12	0.13	0.13	0.13	0.13	0.13	0.13	0.08	0.21	0.08	0.20
N ₂	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.08	0.07	0.08	0.07
SUM	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	99.99	100.0	99.99
MM of SCFH	60.952	60.952	60.43	56.79	40.287	37.88	40.287	37.88	33.065	34.03	32.962	33.42

(1) Apparent imbalance in IGT flowsheet

(2) Single stage shift conversion simulated. May add intercooler which would correct.

(3) From ERDA Report 76-47, Montana Coal Seam, Figure 1.

FUTURE PROGRAM

1. Computer studies

- a. Close heat and material balances as required manually or with computer model.
- b. Compare computer results with results available in reports.
- c. Account for discrepancies, if any.
- d. Calculate thermodynamic efficiencies.
- e. Conduct sensitivity analyses to detect the effect of uncertainties in thermodynamic data. These will be noted as variations in temperature, pressure, composition, and efficiency.

2. Other calculations

- a. Where data are available, calculate reaction equilibrium constants and compare with information based on compositions used in heat and material balances.
- b. Make similar checks, if possible, for phase equilibria.
- c. Note discrepancies and data deficiencies.

3. Complete work on Phase III program related to specific recommendations for research.