INSTITUTE OF GAS TECHNOLOGY
IIT CENTER
CHICAGO, ILLINOIS 60616

PREPARATION OF A COAL CONVERSION SYSTEMS TECHNICAL DATA BOOK

OCR Contract No. 14-32-0001-1730
Report No. 2
December 1974

Project 8964 Status Report

for

OFFICE OF COAL RESEARCH

IGT
EDUCATION · RESEARCH
INSTITUTE OF GAS TECHNOLOGY · IIT CENTER · CHICAGO 60616

Project Status Report
For
OFFICE OF COAL RESEARCH

Report For December 1974
OCR Report No. 2

Project Title: Preparation of a Coal Conversion Systems Technical Data Book
OCR Contract No. 14-32-0001-1730

I. Project Objective

The objective of this work is to provide a single, comprehensive source of data on coal conversion systems. This compilation shall be entitled The Coal Conversion Systems Technical Data Book and shall provide up-to-date data and information for the research, development, design, engineering, and construction of coal conversion processes and/or plants. Other concurrent objectives are to identify those areas where data are required and to suggest research programs that will provide the required data.

II. Summary

The scope of work, the general plan of action, and the kind of information to be collected were determined for the various topics assigned high priority in last month's report. These determinations are by no means final and are intended only as a preliminary starting point. The high-priority topics are —

- Liquefaction
- Gasification
- Fluidization
- Combustion
- Coal, char, and oil shale properties.

A tentative data book index has been prepared. This divides the data book into nine volumes, covering specific applicable categories.

A reference file system for the data collected is being set up, and a list of reference sources for the library search has been prepared.

Notice to Readers of Open File

Any comments about the material presented in this report or suggestions about the format and the content of the data book as well as the priorities of the needed data are most welcome. Please direct any communications to Mr. Bipin Almaula of the Office of Coal Research (202/634-6643) or to Dr. Al Talwalkar of the Institute of Gas Technology (312/225-9600, extension 869).

III. Work Accomplished

A. LIQUEFACTION

Scope of Work

We will cover coal liquefaction in the liquid phase at this time. Gas-phase generation of oil by pyrolysis will be covered later.

General Plan

Only data for specific liquefaction processing steps will be considered at this point. Areas of mutual interest to both coal gasification and coal liquefaction, such as coal handling, preparation, and gas cleanup, will be set aside temporarily.

Our overall plan is to provide useful data and not simply a design handbook for particular liquefaction processes. Of course, this general data framework must be built with the data available from the various liquefaction processes now under development or those developed in the past, such as the German work during the 1930's and 1940's. Over the next 2 months, we plan to familiarize ourselves with the scope of liquefaction developments, with the intent of mapping out the type and range of data we should like to include in the liquefaction section of the data book. When this initial "homework" is accomplished, we plan to visit the organizations that have been active in coal liquefaction to discuss data at first hand. This would be done by prior arrangement with the Office of Coal Research (OCR) as would our liaison with the overall coal liquefaction monitor for OCR, the Ralph M. Parsons Co.

A literature search will be carried out concurrently with the above firsthand discussions. Much of the older data may have to be covered by the literature search alone.

At present, we have identified four main liquefaction processing areas in which we will seek data; these are 1) coal dissolution, 2) hydrogenation, 3) solid-liquid separation, and 4) catalysis. A brief outline of the kind of information we anticipate including in each of these areas is given below.

1. Coal Dissolution

   a. Physical and chemical properties of solvents and coal liquids. (These may be included in the properties section.)

   b. Rates of dissolution of various coals in various solvents and solvent combinations as functions of temperature and hydrogen partial pressure. Particle size will also be considered.

   c. Heating of coal-solvent slurries. This requires information on permissible flux and temperature profiles in tubular heaters as well as velocity-erosion data. Viscosity, density, and specific heat and thermal conductivity as functions of temperature and pressure would be required.

   d. Pumping of slurries. The viscosity of slurries entering and leaving the dissolving vessel must be known.

2. Hydrogenation

   a. The degree of hydrogenation achievable with various temperatures and hydrogen partial pressures for various coals

   b. Kinetics of hydrogenation

   c. Effect of hydrogen donor solvent on the above

   d. Hydrogenation of solvents

   e. Control of temperature in the hydrogenator

   f. The effect of residence time on hydrogenation

   g. Heat of reaction for various coals and solvents.

3. Solid-Liquid Separation

   a. Filtration. Specific filtration rates for various coals and solvents at particular temperatures, etc.

   b. Centrifuging. Rates for a particular process and its conditions

   c. Hydroclones. As above

   d. Settling times. Temperature, residence time, and particle size would be considered.

   e. Flotation. Temperature, time, particle size, and wetting agents would be considered.

4. Catalysis

a. Hydrogenation catalyst life studies and the effect of sulfur, nitrogen, and metal contaminants will be considered.

b. Regeneration data would be obtained also.

B. GASIFICATION

Scope of Work

We will initially consider reactions of char with various gases. Coal reactions, including devolatilization and initial rapid-rate reactions, will be covered at a later date.

General Plan

The kinetic equations, developed from the thermobalance data at IGT, will be used in conjunction with suitable assumptions for the fluidized-bed contacting system to describe the various gasification reactors. The integrated solutions, which will be presented in graphical form, will demonstrate the effect of operating variables on the product variables.

Figure 1 is given as an example of the charts that will be developed. It indicates the carbon conversion that can be obtained in a steam-oxygen gasifier as a function of solids residence time for various amounts of steam and oxygen in the feed gas. This model is based on the assumption of plug flow of solids and back-mixed gas flow. Figure 1 gives the results for four reactor temperatures at 70 atm pressure while Figure 2 gives the same data at 15 atmospheres.

Of course, much additional information is needed to completely describe the system. We are preparing it and will present it next month.

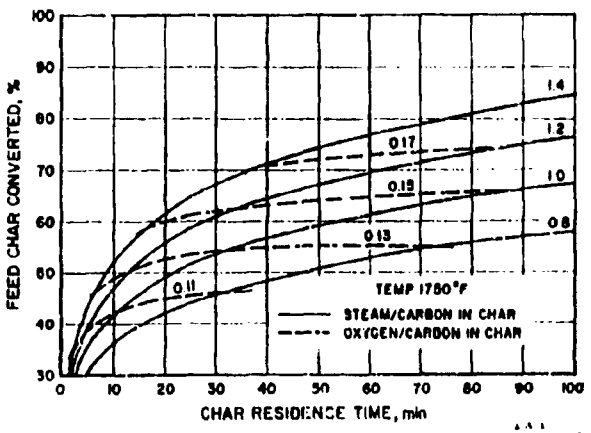
C. FLUIDIZATION

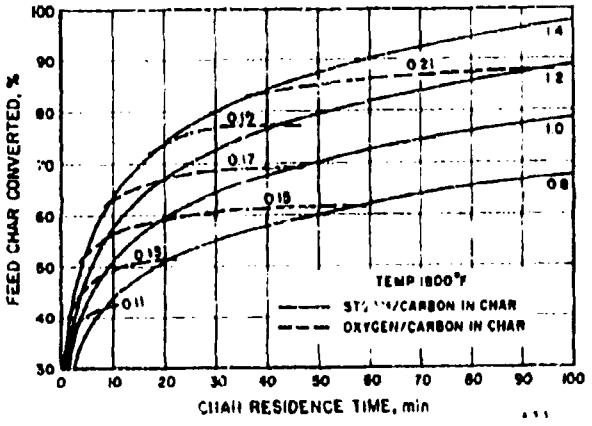
Scope of Work

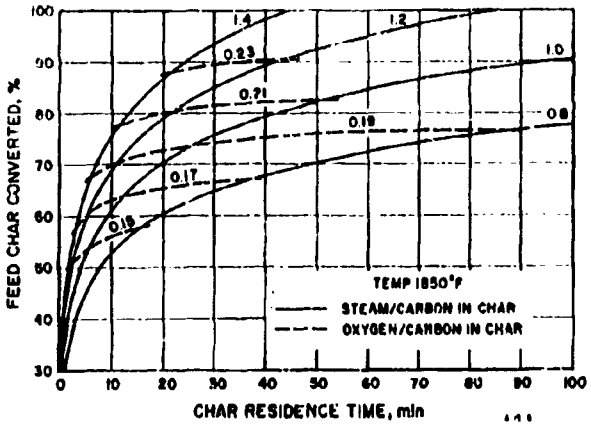
In this section, the correlations relevant to fixed-bed and fluidized-bed operation as well as those pertaining to solids-transport will be covered.

General Plan

Data applicable to fluidization of materials involved in coal conversion systems will be collected. Specific emphasis will be for materials such as







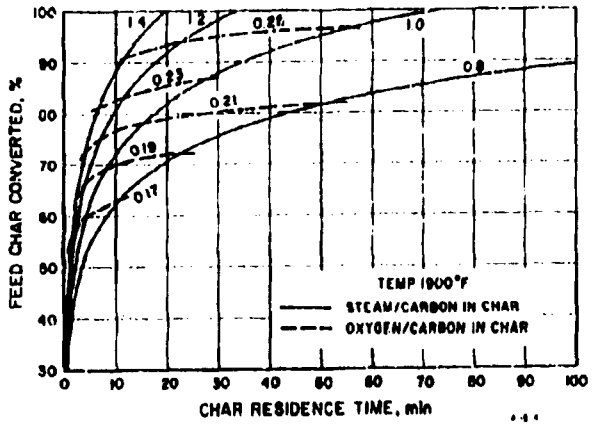
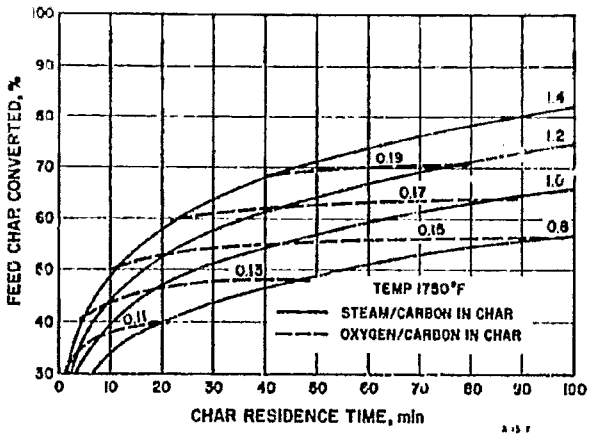
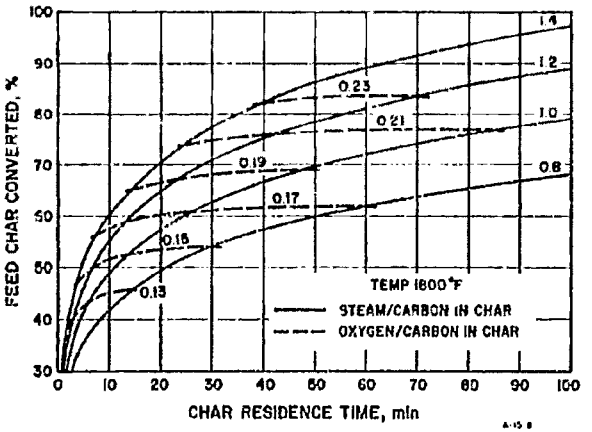
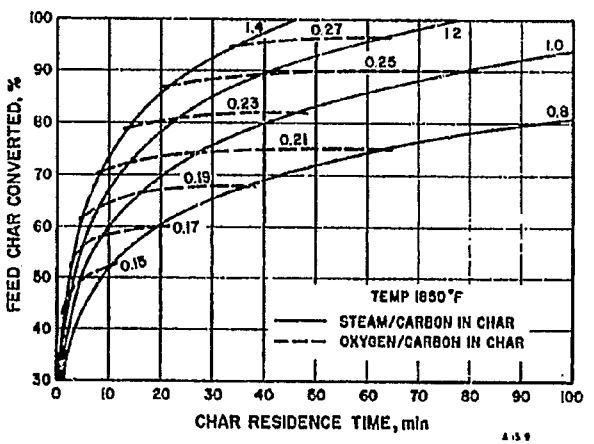


Figure 1. STEAM-OXYGEN GASIFICATION OF DEVOLATILIZED IRELAND MINE CHAR AT VARIOUS TEMPERATURES AND AT 70-atm PRESSURE







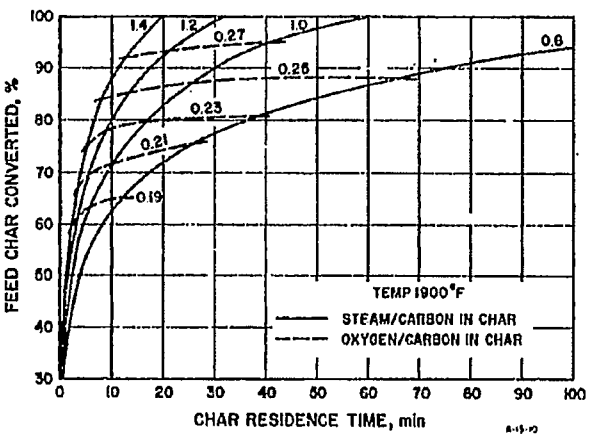


Figure 2. STEAM-OXYGEN GASIFICATION OF DEVOLATILIZED IRELAND MINE CHAR AT VARIOUS TEMPERATURES AND AT 15-atm PRESSURE

coal, char, and solid residues or similar materials. Then applicability of available generalized correlations to accurately describe such data will be determined, and, where necessary, new or modified correlations will be prepared if sufficient data exist. The kind of information that will be collected in the various areas of fluidization is outlined below.

1. Fixed-Bed Operations

   Theoretical and experimental correlations to estimate —

   a. Pressure drop
   b. Heat-transfer coefficient
   c. Diffusion and mass transfer coefficients in isothermal and non-isothermal systems.

2. Fluidized-Bed Operations

   Theoretical and experimental correlations to estimate —

   a. Minimum fluidization velocity
   b. Fluidized-bed densities
   c. Bubble properties
   d. Gas and solids mixing characteristics
   e. Terminal velocity, entrainment, and transport disengagement height
   f. Heat-transfer coefficients between particles and gas and between fluidized beds and surfaces
   g. Selection and design of distributors
   h. Selection and design of fluidized-bed internals.

3. Dilute-Phase Systems

   - Correlations to estimate the physical properties of cocurrent and countercurrent gas-solid systems.

4. Spouting Beds

   Theoretical and experimental correlations to estimate —

   a. Minimum spouting velocity
   b. Spoutable bed depth and average bed density
   c. Gas- and solids-mixing characteristics
   d. Heat-transfer coefficients between particles and gas and between spouting beds and surfaces

5. Gas-Solids Transport Systems

   a. Theoretical and experimental correlations to estimate gas-solid transport characteristics in horizontal, inclined, and vertical pipelines

   b. Design and performance of mechanical and nonmechanical dilute and dense-phase flow control devices.

6. Gas-Solids Separation Systems

   a. Design and performance of cyclones

   b. Design and performance of cyclic filters.

D. COMBUSTION

Low-Temperature (Fluidized-Bed) Combustion

Scope of Work

Data on fluidized-bed combustion (from the literature and OCR reports) will be compiled in this section.

General Plan

The search has been started on available heat-transfer correlations. The fluidization properties needed for necessary calculations will be coordinated with the fluidization section.

Heat Transfer in Fluidized Beds

For possible use in the presentation of heat-transfer estimation procedures, proposed correlations are being evaluated. Particular emphasis is on the adequacy of these for the large particle sizes (>400μm) encountered in fluidized-bed coal-combustion systems. The work and correlations developed by investigations in the U. S. S. R. have been summarized by Gelperin and Einstein.[1] This work is currently being evaluated.

The heat transfer from a fluidized bed to a submerged surface depends on the degree of bed expansion that, in general, is measured at the same time as the heat-transfer rate. For estimation purposes, therefore, bed

---

[1] Gelperin, N. I. and Einstein, V. G., "Heat Transfer in Fluidized Beds," in Davidson, J. F. and Harrison, D., Eds., Fluidization, Chapter 10, 471-540. New York: Academic Press, 1971.

densities as functions of gas velocities must, in general, also be estimated. However, the Soviet workers imply that the maximum heat-transfer coefficient to a given surface is a function only of gas and particle properties. Therefore, estimation of the maximum coefficient will be the first goal; then, estimation at other flow rates will follow when estimation procedures for bed densities are established.

High-Temperature (MHD) Combustion

OCR has initiated work on compilation and evaluation of certain phases of MHD data at the Argonne National Laboratories. The data developed under this effort will be evaluated and coordinated by IGT for inclusion into The Coal Conversion Systems Technical Data Book.

E. COAL, CHAR, AND OIL SHALE PROPERTIES

Data on coal properties were surveyed, and a tentative list for consideration was prepared (Table 1). Three methods of presenting data are being considered:

1. A compilation of basic data on samples from important coal seams that are relevant to conversion processes. Proximate and ultimate analyses, calorific value, and petrographic properties would be included. The Penn State Coal Data Base has tentatively been selected as the main source of such data. The Coal Research Section of the College of Earth and Mineral Sciences, Pennsylvania State University, under contract with OCR, has collected samples of about 250 coals and has obtained (or is obtaining) extensive data on each of them. This can be supplemented by data from other sources. A format with properties tentatively selected for inclusion in the compilation is shown in Table 2.
2. Tabular or other data covering a single property or groups of properties. The amount of data available for a given property varies greatly. For example, tables from the Bureau of Mines Bulletin No. 610, on "Plastic, Agglutinating, and Free-Swelling Properties of American Coals," might be included in toto; for other properties (such as dielectric constant and permeability), only a few data from individual investigators may be available.
3. Correlations, expressed as formulas and graphs. Examples include the Dulong formula for calorific value and variation of true density with carbon and hydrogen content.

Table 1. LIST OF COAL PROPERTIES

- Proximate Analysis
  - Moisture
  - Ash
  - Volatile Matter
  - Fixed Carbon
- Ultimate Analysis
  - Carbon
  - Hydrogen
  - Nitrogen
  - Sulfur
  - Ash
  - Oxygen
- Petrographic Properties
  - Maceral Analysis
    - Vitrinite
    - Exinite
    - Resinite
    - Micrinite
    - Semifusinite
    - Fusinite
  - Vitrinite Reflectance
- Calorific Value
- Forms of Sulfur
  - Pyritic
  - Sulfate
  - Organic
- Chlorine Content
- Rank Classification
  - Rank
  - Fixed Carbon, dry, mm-free
  - Equilibrium Moisture
  - Calorific Value, moist, mm-free
- Structure
  - Porosity
  - Pore-Size Distribution
  - Surface Area
  - True Density
- Mineral Matter Characteristics
  - Elemental Composition
    - SiO_2
    - Al_2O_3
    - Fe_2O_3, etc.
  - Mineralogical Properties
    - Composition
      - Kaolinite
      - Quartz, etc.
    - Size and Shape of Grains

Table 1, Cont. LIST OF COAL PROPERTIES

- Ash-Softening Points
- Trace Elements

Grinding and Handling Characteristics
- Abrasiveness
- Angle of Repose
- Bulk Density
- Apparent (Particle) Density
- Flow Properties
- Friability
- Hardgrove Grindability Index
- Microhardness
- Slacking
- Rate of Oxidation (Spontaneous Combustion)

Miscellaneous Properties
- Compressibility
- Dielectric Constant
- Elasticity
- Electrical Resistivity
- Heat Capacity
- Permeability
- Thermal Conductivity
- Thermal Diffusivity
- Thermal Expansion

Caking and Carbonization Properties
- Free-Swelling Index
- Agglomeration Index
- Gray-King Assay
- Low-Temperature Carbonization Assay (BM) Yield:
  - Char
  - Tar
  - Light Oil
  - Gas
  - Water
- Gieseler Plastometer Test
  - Initial Softening Temperature
  - Fusion Temperature
  - Temperature of Maximum Fluidity
  - Solidification Temperature
- Audibert-Arnu Dilatometer Test

Liquefaction Properties
- Yield by Batch Autoclave Test

Gasification Properties
- Johnson Reactivity Factor

PRELIMINARY
FOR REVIEW ONLY

Table 2. FORMAT FOR COMPILATIO

State	Seam	Mine	County	Proximate Analysis, wt %				Ultimate Analysis, wt %							Calorific Value, Btu/lb, dry basis	Forms of Sul	
					Dry Basis			Dry Basis									
				Moisture	Volatile Matter	Fixed Carbon	Ash	Carbon	Hydrogen	Nitrogen	Chlorine	Sulfur	Ash	Oxygen (difference)		Pyritic	Sulfate
AL	Pratt	Concord	Jefferson	0.76	24.23	71.18	4.58	85.29	4.55	1.45	0.00	0.96	4.58	3.16	14,872	0.32	0.03

Alphabetized by State

BLANK PAGE

ARY
ONLY

MPILATION OF DATA ON COALS

Forms of Sulfur, %			Maceral Analysis, vol %									Reflectance of Vitrinite, %	Rank Classification: Fixed Carbon, dry, mm-free	Equilibrium Moisture	Calorific Value, Moist, mm-free		Hardgrove Grindability Index
Pyritic	Sulfate	Organic	Vitrinite	Pseudo-vitrinite	Fusinite	Semi-fusinite	Massive Micrinite	Granular Micrinite	Exinite	Resinite	Other					Rank	
0.32	0.05	0.61	75.5	3.1	9.5	4.4	3.9	3.6	0.0	0.0	0.0	1.29	75.15	--	--	mvb	112.8

E-15-51

2

F. MISCELLANEOUS

1. Filing System

A central filing system will be established where all the reviewed information will be stored. A card index with cross-references will also be prepared.

2. Library Search

The following sources will be searched for related information:

a. Chemical Abstracts
b. Engineering Index
c. Government Report Index (NTIS)
d. Superintendent of Documents Annual Index
e. Bureau of Mines' Index
f. Air Pollution Index
g. ACS Fuel Division Reprints
h. Geological Surveys of State

3. Data Book Index

An outline of the contents of the data book has been prepared. It divides the data book into nine volumes. (See the Appendix.)

This is a preliminary outline and subject to change. Subsections of some of the volumes have been identified in detail, although the breakdown of others has not yet been considered. This is only a starting point for the data book index. Eventually, a logical decimal index would be developed that would be uniformly applicable to the whole data book.

IV. Patent Status

The work performed during December is not considered patentable.

V. Future Work

The work will be continued on the selected high-priority topics in preparation for meetings with OCR monitors and contractors active in these areas.

Approved W. W. Bodle
W. W. Bodle, Director
Process Analysis

Signed A. Talwalkar
A. Talwalkar, Coordinator
Process Data

APPENDIX. Data Book Outline

Volume 1. Properties of Raw Materials, Intermediates, and Products

A. Properties of Coals, Coal Chars, and Oil Shales

- Proximate Analysis
  - Moisture
  - Ash
  - Volatile Matter
  - Fixed Carbon
- Ultimate Analysis
  - Carbon
  - Hydrogen
  - Nitrogen
  - Sulfur
  - Ash
  - Oxygen
- Petrographic Properties
  - Maceral Analysis
    - Vitrinite
    - Exinite
    - Resinite
    - Micrinite
    - Semifusinite
    - Fusinite
  - Vitrinite Reflectance
- Calorific Value
- Forms of Sulfur
  - Pyritic
  - Sulfate
  - Organic
  - Chlorine Content
- Rank Classification
  - Rank
  - Fixed Carbon, Dry, mm-Free
  - Equilibrium Moisture
  - Calorific Value, Moist, mm-Free

- Structure
  - Porosity
  - Pore-Size Distribution
  - Surface Area
  - True Density
- Mineral Matter Characteristics
  - Elemental Composition
    - SiO_2
    - Al_2O_3
    - Fe_2O_3, etc.
  - Mineralogical Properties
    - Composition
      - Kaolinite
      - Quartz, etc.
    - Size and Shape of Grains
  - Ash-Softening Points
  - Trace Elements
- Grinding and Handling Characteristics
  - Abrasiveness
  - Angle of Repose
  - Bulk Density
  - Apparent (Particle) Density
  - Flow Properties
  - Friability
  - Hardgrove Grindability Index
  - Microhardness
  - Slacking
  - Rate of Oxidation (Spontaneous Combustion)
- Miscellaneous Properties
  - Compressibility
  - Dielectric Constant
  - Elasticity
  - Electrical Resistivity
  - Heat Capacity
  - Permeability
  - Thermal Conductivity

- Thermal Diffusivity
- Thermal Expansion
- Caking and Carbonization Properties
  - Free-Swelling Index
  - Agglomeration Index
  - Gray-King Assay
  - Low-Temperature Carbonization Assay (BM) Yield:
    - Char
    - Tar
    - Light Oil
    - Gas
    - Water
- Geiseler Plastometer Test
  - Initial Softening Temperature
  - Fusion Temperature
  - Temperature of Maximum Fluidity
  - Solidification Temperature
- Audibert-Arnu Dilatometer Test
- Liquefaction Properties
  - Yield by Batch Autoclave Test
- Gasification Properties
  - Johnson Reactivity Factor

B. Properties of Conversion Products

- General Properties
  - Molecular Weight
  - Melting Point
  - Boiling Point
  - Temperature of Transformations
  - Density or Specific Gravity
    - True
    - Bulk
  - Thermal Expansion Coefficient
  - Solubilities
  - Surface Tension
  - Critical Properties

Transport Properties

- Heat Capacity
- Viscosity
- Thermal Conductivity
- Diffusivity
- C_p / C_v
- Prandtl No.
- Diffusion Coefficient
- Electrical Conductivity
- Emissivity
- Absorptivity
- Permeability

Thermodynamic Properties

- Heat of Formation
- Enthalpy
- Free Energy of Formation
- Equilibrium Constant of Formation
- Heat of Fusion
- Heat of Vaporization
- Heat of Transition
- Heat of Combustion
- Heat of Solution
- Activity Coefficient
- Fugacity Coefficient
- Heats of Reactions of Selected Reactions
- Equilibrium Constants of Selected Reactions

Vapor-Liquid Equilibria

- Critical Properties
- K-Factor
- V/L Equilibrium
- PVT and Phase Behavior

Properties of Related Processing Materials

- For Example, Catalysts, Reagents, and Treating Agents

Volume 2. Solids Storage, Preparation, and Pretreatment

- Sampling of Coal
- Projecting Data From Samples
- Coal Characteristics and Their Relationship to Utilization
- Raw-Coal Handling
- Breaking and Crushing
- Screening
- Wet Concentration of Coal
  - Coarse Coal
    - Dense-Medium Separation
    - Hydraulic Separation
  - Fine Coal
    - Dense-Medium Separation
    - Hydraulic Concentration
    - Froth Flotation
  - Dry Concentration
  - Mechanical Dewatering
  - Thermal Dewatering
  - Coal Storage and Loading
  - Refuse Removal and Disposal
  - Coal Pretreatment

Volume 3. Conversion Fundamentals

A. Gasification

- Fluid Bed
  - Steam-O_2
  - Steam-Air
  - Steam-H_2
  - Steam-H_2-CO-CO_2-N_2
- Dilute Phase
  - Entrained
    - Steam-O_2
    - Steam-Air
  - Texaco-Type
    - Steam-O_2
    - Steam-Air

Fixed Bed
- Steam-O_2
- Steam-Air

Molten Bed
- Steam-O_2

Spouting Bed

B. Liquefaction

Catalytic With H_2
- Ebullating Bed
- Fixed Bed
- Others

Catalytic Without H_2
- Ebullating Bed
- Fixed Bed
- Others

Noncatalytic
- With H_2
- Without H_2

C. Pyrolysis

Low-Temperature

High-Temperature

D. Fluid-Bed Combustion

E. High-Temperature Combustion (MHD)

Coal

Gas

Volume 4. Design Procedures (Unit Operations)

A. Fluidization

Fluid-Bed

Solid Transport

B. Fluid Flow

Single-Phase

Multiphase

C. Heat Transfer

Volume 5. Supporting Processes

- A. Gas Treating
- B. Methanation
- C. Environmental Control
  - Gas Effluents
  - Liquid Effluents
  - Solid Effluents
- D. Hydrogen Production
  - Electrothermal
  - Steam-iron
  - Other

Volume 6. Miscellaneous Products

- A. Methanol
- B. Acetylene
- C. Ammonia

Volume 7. Materials of Construction

- A. Refractories
  - Properties
  - Corrosion/Abrasion Data
- B. Ceramics
  - Properties
  - Corrosion/Abrasion Data
- C. Metals and Alloys
  - Properties
  - Corrosion/Abrasion Data
- D. Plastics
  - Properties

Volume 8. Equipment Specifications

Volume 9. Cost Data and Costing Procedures

Open File
IGT-MPR--3

INSTITUTE OF GAS TECHNOLOGY

IGT
EDUCATION - RESEARCH

3424 SOUTH STATE STREET
IIT CENTER
CHICAGO, ILLINOIS 60616
AFFILIATED WITH ILLINOIS INSTITUTE OF TECHNOLOGY