Report of Working Group on Data for Coal Gasification (1973)

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NUMERICAL DATA ADVISORY BOARD

DIVISION OF CHEMISTRY AND CHEMICAL TECHNOLOGY

NATIONAL RESEARCH COUNCIL

Report of Working Group on Data for Coal Gasification of the Panel of Private Programs

NATIONAL ACADEMY OF SCIENCES-NATIONAL ACADEMY OF ENGINEERING
NATIONAL RESEARCH COUNCIL

Washington, D. C.

NOTICE

The project which is the subject of this report was approved by the Governing Board of the National Research Council, acting in behalf of the National Academy of Sciences. Such approval reflects the Board's judgment that the project is of national importance and appropriate with respect to both the purposes and resources of the National Research Council.

The members of the committee selected to undertake this project and prepare this report were chosen for recognized scholarly competence and with due consideration for the balance of disciplines appropriate to the project. Responsibility for the detailed aspects of this report rests with that committee.

Each report issuing from a study committee of the National Research Council is reviewed by an independent group of qualified individuals according to procedures established and monitored by the Report Review Committee of the National Academy of Sciences. Distribution of the report is approved, by the President of the Academy, upon satisfactory completion of the review process.

SUMMARY and CONCLUSIONS

A working group of university, industry, and government scientists and engineers has conducted this preliminary study. They conclude that a formal effort to compile and publish a current, authoritative data compilation related to the field of coal gasification would be a useful contribution to the present state of this field. Based on the detailed outline of data in this report, they conclude that this project is feasible as well as timely.

This report presents a detailed breakdown of subjects and material that should be included in such a compilation. It includes comments on the completeness of each subject, indicates the sources and form of the data, and places subjective judgments on availability and reliability.

The Working Group was established by the Panel on Private Programs of the Numerical Data Advisory Board. The Chairman of the Working Group is Dr. Harry C. Allen, Jr., Chairman, Department of Chemistry, Clark University.

Background

The Panel on Private Programs of the Numerical Data Advisory Board has been considering the national needs for data compilation with particular reference to industry. Attention was focused on the needs of important mission-oriented fields, and clearly one of the most critical areas today is that of coal gasification. It is receiving increasing attention from many technical groups, funds have been appropriated for expanding its technical development, and it is at the center of national concern with energy needs, environmental regulations, and availability of fuel resources.

The question for the NDAB was whether to recommend a program to prepare and publish a data compilation that would serve the needs of the growing technical community concerned with research, development, design, and testing of coal gasification processes and plants. It became obvious that a preliminary study would have to be conducted in order to:

1. Determine the subjects that must be included in a meaningful data compilation on coal gasification.

2. Identify the probable sources of the required data.

3. Estimate the availability, reliability, and completeness of these data.

A working group was therefore established charged with carrying out a study that would cover the three points stated above, and on this basis evaluate the usefulness and feasibility of a program for the actual preparation and publication of the relevant data. The first meeting of this working group was on February 8, 1972.

Report of Working Group on Data for Coal Gasification

I. Composition of the Working Group

The membership of the Group was chosen so that the widest representation of backgrounds could be obtained, i. e., government, industry and academic, basic science and engineering, and major organizations active in coal gasification. The membership is:

Professor Harry C. Allen, Jr. Chairman
Department of Chemistry
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Dr. James L. Johnson
Institute for Gas Technology
3424 South State Street
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Mr. Edward J. Vidt
Westinghouse Research Center
Beulah Road
Pittsburgh, Pennsylvania 15235

In addition, Dr. Howard J. White, Jr., of the Office of Standard Reference Data, National Bureau of Standards, attended the Group's meetings of the Working Group as an observer.

Dr. H. van Olphen of the National Research Council served ably as our contact with the parent committee, arranged our meetings, and served as secretary.

II. Procedure

In order to understand the magnitude of the problem, to identify the types of data needed and to determine the availability and adequacy of data, the coal gasification process was broken down into the major steps involved in the process. Then, for each of these steps the types of data needed were listed.

This procedure provided a suitable outline which is included in the report as Appendix I. With the help of this outline, a matrix was devised in order to assess for each type of data their availability, reliability, and completeness, to determine whether the data were in a useful form, and to identify the sources of the data.

Each member of the Working Group was asked to fill out these matrices in his areas of special competence. The contributions were assembled and combined to give a master matrix that served as a basis for the final discussions and conclusions. This master matrix is included in this report as Appendix II. The Group realizes that this compilation is not complete but feels it does indicate that useful data do exist and that a compilation effort would uncover much more.

III. General Conclusions

The general conclusions of the working group are:

1. A body of relevant data does exist in many areas important to coal gasification processes.

2. For these data to be generally useful, they should be critically evaluated and compiled.

3. Both engineering data and basic physical and chemical data should be included.

4. A critically evaluated compilation of data relevant to coal gasification processes should be undertaken.

5. The compilation should culminate in a data handbook similar to A.P.I. Publications, e.g. "Technical Data Book - Petroleum Refining".

6. If a significant data compilation and evaluation effort cannot be implemented, a start should be made through the preparation of selective bibliographies.

The need for the critical evaluation arises because much of the existing data were gathered either with respect to a specific gasification process or with respect to some other coal use such as liquefaction or pipeline transportation of coal. Evaluation is needed not only to establish the validity of the data, but also to determine the extent of their applicability. Much of the existing data is a result of studies carried out in government laboratories such as those supported by the Bureau of Mines. These data are readily available in the scientific and engineering literature or in government reports that are readily available. Other data exist as the result of government supported or partially supported projects in the private sector (industry, research institutes, universities), mainly through grants and contracts funded by the Office of Coal Research. These data would be available for any compilation effort. (Appendix III) The extent to which data are available in the literature from other than these sources is not known. It is not expected to be large because until recently essentially all research done on coal and coal processing was funded by the federal government. There also exists a large body of data on coal gasification as a result of a large German effort prior to and during World War II. Many of these data have never been evaluated.

The Working Group has no ready method for including data collected in private industry from research supported by private funds. With many of the major oil companies broadening their interest to include multiple sources of energy including coal, it may be that data from the private sector can be made available through the A. P. I. Alternatively, an organization of coal producers might be formed to perform this function for coal producers, and users in general. In the past the coal industry has been content to sell coal leaving the research and development for the users.

The Working Group uncovered one project that may be a promising start for the data effort envisioned. A group at Pennsylvania State University under contract to the Office of Coal Research is making a start toward data collection on coals. Five classes of data will be considered: mining engineering, preparation, physical characterization, organic chemical analysis and petrographic analysis. One hundred fifty samples of coal from all over the United States have been collected (1/2 ton each). The data included so far has come only as a result of research programs at Penn. State. No attempt has been made to include data from the literature. Storage of these data on magnetic tape enabling selective retrieval is being worked on. Utilization data will be included as they become available. This effort could form the base for a much larger effort if a decision is made to go ahead with a compilation of data of use in coal gasification processes.

IV. Comments on specific steps in the process

During the deliberations attempts were made to delineate priorities for data collection among the sections of the outline. A by-product of this effort was the identification of several areas in which research is badly needed. The major conclusions of the discussions are summarized below:

1. Physical and chemical coal and char properties

a. Chemical Composition. A body of data exists and should be evaluated and compiled. Petrographic data is for the most part scarce and what does exist is questionable. The data are limited to 30 or 40 American coals. Considerable more research is needed on petrographic data.

b. Electrical Conductivity. Data for chars are of more interest than for coal in presently important coal gasification processes. Data on coal are of interest only to those working on underground gasification by electrical heating or for those planning to use coal as a consumable electrode in a fuel cell. Recent renewed interest in underground gasification by the AEC as well as the Bureau of Mines may increase the importance of these data on coals.

c. Thermal Properties. Both heat of combustion and thermal conductivity data are important but the availability of data is questionable especially for thermal conductivity.

d. Physical Structure. There are data available on a limited number of American coals (30-40) as well as some on British, Dutch and German coals.

The feeling is that this group of properties taken as a whole is important for correlative purposes, i. e., the determination of the usefulness of a given coal for a given gasification process.

2. Coal Preparation

There are much data available on coal preparation; however when the hardware step is reached, tests are made on the particular coal to be worked with. This is an area of lower priority.

3. Pretreatment

There are good data available which are very useful to the designer and are important to him.

4. Slurry Feed Properties

There are not much data available and what is available is scattered. Good data in this area are needed.

5. Gas-Solid Reactors

There is a sizable amount of data available, but often the coal on which it was taken is not well characterized. Traces of iron can give orders of magnitude difference in rates. A distinction should be made between coal and char. It would also be helpful to have practical process data. These depend on the sum total of the system and the reaction. Process data should be presented with an adequate description of the process (and a disclaimer in fine print).

6. Purification

Much of the information is proprietary know-how. There is little information on coal-gas systems. Particulate removal requirements depend on the end use (i. e. as turbine or as pipeline gas.) There is a body of data but its usefulness will depend on air pollution regulations. There is also a problem with H_2S for it still exists after present clean up techniques at levels too high for release to the atmosphere. No one is sure of all the compounds to be contended with and will not know until large scale plants are in operation.

7. Shift Process

Much information exists in the oil companies. At this stage one is working with cleaned-up gas so technology is available. This is a lower priority area.

8. Methanation Process

There is a large amount of data available but there remain scale-up problems particularly with respect to heat removal. The available data are generally on specific systems but nonetheless their collection in one place would be useful.

9. Environmental Effects - data available

Data should be compiled and evaluated relevant to water pollution, especially for such processes as the removal of phenols.

10. Mass and Heat Transfer

This is an area which needs data collecting.

11. Properties of Reactor and Product Cases

P. V. T. data are available for the major pure compressed gases and many binary mixtures; however, the volumetric properties of the multicomponent compressed gas mixtures have not been determined by direct experimental measurement and presently must be approximated from equation of state and mixing laws. Although such approximate calculations are adequate for most engineering purposes, they are not adequate for custody transfer of compressed gas.

Appendix 1

COAL GASIFICATION OUTLINE

I. Physical and Chemical Coal and Char Properties

a. Chemical Composition
   1. elemental (including mineral constituents)
   2. species and functional groups
   3. proximate analysis
   4. petrographic analysis

b. Electrical conductivity

c. Thermal properties
   1. thermal conductivity
   2. heat of combustion (or of formation)
   3. specific heat

d. Physical structure
   1. surface area
   2. pore distribution
   3. true and particle density
   4. adsorption properties
   5. particle shape

II. Coal Preparation

a. Drying

b. Agglomeration tendency

c. Friability

d. Particle size distribution from crushing

e. Reactivity with respect to combustion in coal piles, and dust explosions

f. Sulfur removal by mechanical treatment

III. Coal Pretreatment to Diminish Agglomerating Tendency (both reducing and oxidizing atmospheres)

a. Kinetics and chemistry as function of operating conditions and contacting system

b. Heat effects

c. Effects on subsequent gasification reactivity

d. Effects on agglomeration

e. Effects on physical and chemical coal properties (Section I.), including particle size distribution

f. Combustibility of low heating value offgas from pretreator

g. Ash fusion

IV. Slurry Feed Properties

a. Flow of slurries in pipes (viscosity, friction factors, etc.)

b. Rates and heat effects for vaporization of liquid components

c. Chemical kinetics for gas phase reaction of vaporized liquid

V. Gas-Solid Reactions

a. Coal-hydrogen, coal-carbon dioxide, coal-synthesis gas, coal-steam/air, coal-steam/oxygen, coal-steam/energy (e.g., electricity)

1. kinetics and chemistry as function of conditions and coal physical and chemical properties (Section I), including particle size
2. heat effects
3. effects on subsequent gasification reactivity
4. effects on physical and chemical coal properties (Section I)
5. effect mineral material

b. Char-hydrogen, char-carbon dioxide, char-synthesis gas, char-steam/air, char-steam/oxygen, char-steam/energy

1. kinetics and chemistry as function of conditions and char physical and chemical properties (Section I) including particle size
2. heat effects
3. effects on subsequent gasification reactivity (including combustibility for power generation)
4. effects on physical and chemical char properties (Section I)

VI. Purification (gas)

a. Particulate Removal

1. gas/solid flow properties
2. erosive properties

b. Sulfur removal

1. solution processes
2. adsorption processes
3. other

c. Oil and condensible removal

1. oil/water separation
2. vapor-liquid equilibria
3. other liquid properties

d. Carbon dioxide removal

e. Gas separation

1. molecular sieve
2. cryogenic systems
3. other

VII. Water Gas Shift Process

a. Kinetics and chemistry as function of conditions and catalyst

b. Effects of conditions on catalyst

c. Heat effects

VIII. Methanation Process

a. Kinetics and chemistry as function of conditions and catalyst

b. Effects of conditions on catalyst

c. Heat effects

IX. Environmental Effects

a. Air pollution

b. Water pollution

c. Health

X. Mass and Heat Transfer Properties of Gas/Solid Contacting Systems (fluid bed, fixed bed, moving bed, transport reactor, etc.)

XI. Properties of reactor and product gases.

a. P-V-T data

b. Other

APPENDIX II

Availability of Data Pertinent to Coal Gasification

In the course of the Working Group's deliberations, the members were asked to assess the data situation for each of the categories in Appendix I. They were asked to assess the data in three ways:

1. How available is the data?

2. How reliable i s the data?

3. How complete is the data?

The results of these assessments are compiled into Appendix II. The Working Group makes no claim that the compilation is complete but it is included to give the reader some idea about the present state of the existence of data on Coal Gasification.

In some cases the members were willing to hazard a guess as to the quality (good, fair, poor) of the data in terms of availability, reliability and completeness. The "Availability" refers to types of data; "Reliability" and "Completeness" to the individual sources. The absence of comment in these columns merely means the Working Group members could not make an assessment. Under "Source", definite references are given when they are known. In other cases the name of a scientist, cognizant of the state of data in a particular category is given.

Tabular Form for Reporting Data on Coal Gasification

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Ia - Chemical Composition 1. elemental 2. species and functional groups 4. petrographic analysis	Good	Good	Fair	H. Gluskoter (Illinois State Geological Survey) G. R. Hill (University of Utah) R. A. Friedel (USBM) and W. Spackman, P. Given (Pennsylvania State University)
Ia - Chemical Composition Ib - Electrical conductivity	Good	Adequate	Good	From customer and equipment vendors. No problem to Blaw-Knox USBM R.I. 6318, "Advances in Coal Spectroscopy," Sharkey, A.G., Shultz, J.L., Jr., Friedel, R.A. USBM R.I. 7240, "Major Ash Constituents in U.S. Coals," Abernethy, R.F., Peterson, M.J., Gibson, F.H. 1966 Book of ASTM Standards, Pt. 19, Gaseous Fuels, Coal and Coke USBM Bull. 638, "Methods of Analyzing and Testing Coal and Coke" USBM Bull. 609, "Determination of Phenols in Coal Tars and Hydroxyl Groups in Coal by Forming Trimethylsilyl Ethers,"

Tabular Form for Reporting Data on Coal Gasification

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Ia Chemical Composition				Friedman, S., et al. Chemistry of Coal Utilization, H.H. Lowry, Ed., Wiley and Sons, 1963 USBM, Pittsburgh Energy Research Center Quarterly Report, Oct.-Dec. 1971, pp. 10-51 *
Ic 2 Heat of formation (from Heat of Reaction)	Good	Good	Fair	"The Heat of Reaction of Hydrogen and Coal," Ind. Eng. Chem. Proc. Des. and Develop 7, April 1968 (244-249) Lee, A.L., Feldkirchner, H. L., Schora, F.C. and Henry, F.J.
Ic 3 Specific Heat	Good	Fair	Poor	The British Coal Utilization Research Association, Monthly Bull., XXIX, No. 2, Pt. I, 1965, "Specific Heats and Total Heat Contents of Coals and Related Materials at Elevated Temperature," Kirov, N.Y., pp. 33-60 "Enthalpy and Other Thermal Properties of Coal--A Review," Sanyal, A. Univ. of Shoffield, Fuel Soc. J., 13, 1962, pp. 55-62

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Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Ic 3 - Specific heat	Good	Poor	——	Attached nomograph #1, OCR-R & D Report #22
		Good	Fair	"Heat Capacity of Coal," American Chemical Society, Division of Fuel Chemistry Preprint 12, No. 3, 19-31 (1968) September. A.L. Lee
				"The Specific Heat of Coal," Coke Chem. U.S.S.R. 7, 9-14 (1965) Agroskin, A.A. and Goncharov, E.I.
				"Determination of the Specific Heat of Coals During Carbonization," Coke Chem. U.S.S.R. 11, 16-20 (1965) Agroskin, A.A. and Goncharov, E.I.
				Batchelor, J.D., Yavorsky, R.M. and Gorin, E., "Measurement of the Thermal Properties of Carbonaceous Materials," J. Chem. Eng. Data 4, 241-46 (1959)
				Clendenin, J.D. et al., "Thermal and Electrical Properties of Anthracite and Bituminous Coals," Trans. 7th Annual Anthracite Conference of Lehigh Univ. Bethlehem, Pa., 1949.

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Ic-3 Specific Heat	Good			Coles, G., "The Specific Heat of Coal and Its Relation to Composition," J. Soc. Chem. Ind. XLII, 435-39 (1923) Fritz, V.W. and Moser, H., "Specific Heat, Thermal Conductivity and Thermal Diffusivity of Mineral Coal, Charcoal and Coke," Feuerungstechnik 5, 97-107 (1940). Mantell, C.L., Industrial Carbon, 2nd Ed., 432. New York: D. Van Nostrand, 1947. Kazima, V.V., "Determination of the Specific Heat of Cokes," Coke Chem. U.S.S.R. 11, 26-29 (1965). Porter, H.C. and Taylor, G.B., "The Specific Heat of Coal and Its Relation to the Presence of Combined Water in the Coal Substance," Ind. Eng. Chem. 5, 289-93 (1913). Terres, V.E. et al., "The Solution of the Problem of the Origination of Fibre Coal on the Ground of Its Specific Heats," Brennstoff-Chemie 37, 366-70 (1956) June.

Tabular Form for Reporting Data on Coal Gasification

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Ic-3 Specific Heat	Good	Good	Fair	Voloshin, A.I. et al., "Determination of the Heat of Coking Under Laboratory Conditions," Coke Chem. U.S.S.R. 3, 17-20 (1962).
				Morlock, R.J., Naso, A.C., and Cameron, J.R., "Heat Requirements for Coking," Symposium on the Science and Technology of Coal, Ottawa 1967, p. 127-31.
		Good	Fair	Gomez, M., Gayle, J.B., and Taylor, A.R., Jr., "Heat Content and Specific Heat of Coals and Related Products," U.S. Bu. Mines RI 6607, 1965.
I-d Physical structure	Good	Good	Fair	Thomas (Illinois State Geological Survey)
II Coal Preparation				"Coal Preparation", J.W.Leonard, D.R. Mitchell, Editors, AIME,* 1968
IIa Drying	Good	Good	Good	
IIb Agglomeration tendency	Excellent	Excellent	?	"Chemistry of Coal Utilization" H.H. Lowry, Ed., John Wiley & Sons (1963)

*American Institute of Mining, Metallurgical, and Petroleum Engineers

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
II-c Friability	Discussions with the listed people would be the best way to complete this coal preparation information	Fair	?	D. Wolfson, A.W. Deurbrouck, U.S. Bu. Mines, Pittsburgh
II-d Particle size distribution from crushing		Fair	?	W. Abel, U.S. Bureau Mines, Morgantown, W. Va. IGT** Grinding test on coal and char performed by Allis-Chalmers Grinding Laboratory. Private Report, Oct. 25, 1965*
II-e Reactivity with respect to combustion in coal piles and dust explosions	Good	Good	Fair	Dr. VanDolah, U.S. Bu. Mines, Pittsburgh Dr. H. Lovell, Pennsylvania State University N.F.P.A. Vols. 60 and 653 U.S. Bu. Mines RI 5052, "Laboratory Explosibility Study of American Coals," Hartmann,I., Jacobson, Mr. and Williams,R.P., 1954 U.S. Bu Mines RI 6597, "Explosibility of Carbonaceous Dusts," Magy, Jr., Dorsett, A.G.,Jr., and Austin, R.C., 1965.

* Available by permission
** Institute for Gas Technology

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
II-f Sulfur removal by mechanical treatment				USBM R.I. 7174, "Preparation Characterisitcs of Coal, etc.," Zeilinger, J.E., and Deurbrouck, A.W., 1968, contains bibliography.
III Coal Pretreatment				
III-a Kinetics and chemistry as function of operating conditions	Fair	Poor	——	Chemistry of Coal Utilization, H.H. Lowry, Ed., John Wiley & Sons (1963) p. 997
III-b Heat effects	Good	Fair	Fair	"The Heat of Reaction of Hydrogen and Coal," Ind. Eng. Chem. Proc. Des. and Develop. 7. April 1968 (244-249). Lee, A.L., Feldkirchner, H.L., Schora, F.C. and Henry, J.J.
III-c Effects on subsequent gasification reactivity	Good	Fair	Fair	"Reactivity of Coals in High-Pressure Gasification with Hydrogen and Steam," Ind. Eng. Chem. Proc. Des. and Develop. 2, April 1963 (153-62). Feldkirchner, H.L. and Linden, H.R. "Fluid-Bed Pretreatment of Bituminous Coals and Lignite-Direct Hydrogenation of Chars to Pipeline Gas." K.C. Channabasappa and H.R. Linden. Industrial and Engineering Chemistry 50, 637-44 (1958) April.

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
III-d Effects on agglomeration	Good	Good	Fair	ibid. "Coal Pretreatment in Fluidized Bed," V.C. Kavlick and B.S. Lee, Advances in Chemistry Series No. 68, 8-17, Wash. D.C. ACS, 1967. Various publications by IGT and FML under OCR sponsorship USBM, Pittsburgh Energy Research Center, Quarterly Report, Oct.-Dec. 1970, pp. 66-70; Quarterly Report, Jan.-March 1971, pp. 62-67; Quarterly Report, April-June 1971, pp. 80-85; Quarterly Report, July-Sept. 1971, pp. 94-103; Quarterly Report, Oct.-Dec. 1971, pp. 112-119* USBM, Pittsburgh Energy Research Center, Quarterly Report, Jan.-March 1971, pp. 43-59; Quarterly Report, July-Sept. 1971, p. 136. * "Coal Pretreatment in Fluidized Bed." V.C. Kavlick and B.S. Lee, Advances in Chemistry Series No. 68, 8-17, Wash. D.C. ACS, 1967. Channabasappa and Kavlick Papers

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Process Operation

Type of Critical Data	Availability			
III e Effects on physical and chemical coal properties	Good	Good	Fair	IGT Bulletin No. 39 (To be published in 1972)
III-g Ash Fusion	Fair	Good	Fair	Chemistry of Coal Utilization, H.H.Lowry, Ed., John Wiley & Sons (1963), p.827
IV Slurry Feed Properties				
IV-a Flow of slurries in pipes	Good	Good	Good	"Slurry Piping Systems: Trends," Chemical Engineering June 28, 1971, p. 74-90, Aude, T.C., Cowper, N.T., Thompson, T.L. and Wasp, E.J. Thomas, D.G., Transport Characteristics of Suspension: VII - A Note on the Viscosity of Newtonian Suspensions of Uniform Spherical Particles. J. Colloid Science, 20, No. 3, pp. 267-277 (1965). Wasp, E.J., et al. Deposition Velocities, Transition Velocities and Spatial Distribution of Solids in Slurry Pipelines. First International Conf. on the Hydraulic Transport of Solids in Pipe. Coventry, England (Sept. 1970).*

*Limited availability

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
IV-a Flow of slurries in pipes				Hanks, R.W., Pratt, D.R. On The Flow of Bingham Plastic Slurries in Pipes and Between Parallel Plates, Soc. of Petrol. Engrs. J., pp. 342-345 (Dec. 1967). Job, A.L., Transport of Solids in Pipelines, With Special Reference to Mineral Ores, Concentrates, and Unconsolidated Deposits (A Literature Survey), Dept. of Energy, Mines and Resources of Canada, Information Circular 230 (Oct. 1969). "The Transportation of Solids in Steel Pipelines," Colorado School of Mines Research Foundation (1963). The Longest, Largest Coal Slurry Pipeline Ever Built, Coal Mining and Processing, Feb. 1971, pp. 8-11. Wasp, E.J., Thompson, T.L., Aude, T.C. Slurry Pipeline Economics and Application, presented at First International Conf. on the Hydraulic Transport of Solids in Pipes, Coventry, England (Sept. 1970).

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
IV-a Flow of slurries in pipes	——	——	——	None Available
V Gas-Solid Reactions				Chemistry of Coal Utilization, H.H. Lowry, Ed., Wiley & Sons, 1963, pp. 892-1014
V-a-1 Kinetics & chemistry as function of conditions & coal physical & chemical properties	Good	Good	Fair	"Gasification of Brown Coal with Hydrogen in a Continuous Fluidized-Bed Reactor," J. Inst. Fuel 33, 422-35 (1960) Sept., T.J. Birch, et al. "The Mechanism of Hydrogeneration of Coal to Methane," Aust. J. Chem. 20, 1561-70 (1967) Aug., J.D. Blackwood, et al. "Reactivity of Coals in High Pressure Gasification with Hydrogen and Steam," I&EC Process Des. Develop. 2, 153-62 (1963) April, H.L. Feldkirchner, et al. R.W. Hiteshue (Various USBM Publications) "The Rapid High-Temperature Hydrogenation of Coal Chars," J. Inst. Fuel, 38, 13-23 (1965) Jan; PT 2, ibid, 378-91 (1965) Sept. F. Mosely, et al.

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
V-a-1 Kinetics & chemistry as function of conditions and coal physical & chemical properties				"Continuous Pressure Gasification of Pulverized Coal in Suspension". C.G. von Fredersdorff, and E.J. Pyrcioch. American Gas Association Proceedings - 1952, 685-701. "Reaction of Carbon with Carbon Dioxide and with Steam" IGT Research Bulletin No. 19, Chicago, 1955 "Gasification of Pulverized Coal in Suspension." C.G. von Fredersdorff, E.J. Pyrcioch and E.S. Pettyjohn. Inst. of Gas Tech. Research Bulletin No. 7, Chicago, 1957. "The Direct Methanation of Coal," Paper Presented at 158th National Meeting of the ACS, Division of Fuel Chemistry, New York, Sept. 7-12, 1969. R.L. Zahradnick, et al.

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
V-a-1 Kinetics & chemistry as function of conditions and coal physical and chemical properties	Fair	Good	Fair	H.F. Feldmann (Various U.S.B.M. Publications)
-4 Effects on physical and chemical coal properties	Fair	Good	Fair	
V-a-1 Kinetics & chemistry as function of conditions	Fair	Good	Fair	IGT Bulletin No. 39, 1972
-3 Effects on subsequent gasification reactivity	Fair	Good	Fair	
-4 Effects on physical and chemical char properties	Fair	Good	Fair	

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
V-b Char-hydrogen, -carbon dioxide, -synthesis gas, -steam/air, -steam/oxygen, -steam/energy	By permission	Good	Fair	Various IGT Reports to A.G.A. and OCR.
V-b-1 Kinetics & chemistry as function ofconditions and chair physical & chemical properties including particle size.	Good	Good	Fair	"Phase II, Bench Scale Research on CSG Process-Laboratory Physico-Chemical Studies", Office of Coal Research, U.S. Dept. of Interior, R&D Report No. 16, Interium Report No. 3, Book 2, OCR Contract No. 14-01 0001-415. Washington,D.C.: U.S. Government Printing Office, 1970, E.P. Curran et al. "Kinetics of Carbon Gasification by Steam: Effect of High Temperature Pretreatment on Reactivity of Low Temperature Char to Steam and Carbon Dioxide," Ind. Eng. Chem. 44, 1051-57 (1952) May. E. G. Goring, et al. "Kinetics of Carbon Gasification by Steam: Mechanism of Interaction of Low Temperature Char and Steam-Hydrogen Mixtures at 1600°F," Ind.Eng.Chem 45, 2386-91 (1953) Nov. R.W. Hiteshue (Various USBM Publications)

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
V-b-1 Char-hydrogen,-carbon dioxide, -synthesis gas, -steam/air, -steam/oxygen, -steam/energy				"Carbon-Steam Reaction Kinetics From Pilot Plant Data," Ind. Eng. Chem. 50, 1289-96 (1958) Sept. W.E. May, et al. "Steam-Oxygen Gasification of Fine Sizes of Coal in Fluidized Bed at Elevated Pressure," Trans. Inst. Chem. Eng. 39, 3-27 (1961) A.M. Squires. "Kinetics of Carbon Gasification: Interaction of Hydrogen With Low Temperature Char at 1500° to 1700°F," Ind. Eng. Chem. 47, 820-25 (1955) April, C.W. Zielke, et al. "Kinetics of Carbon Gasification: An Emperical Correlation for Predicting Differential Rates of Carbon Gasification and Methane Formation Can Be Used For Interpreting Pilot Runs and Extrapolating Pilot Designs to Commercial Scale," Ind. Eng. Chem. 49, C.W. Zielke, et al.

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
V-b-1 kinetics and chemistry as function ofconditons & char physical & chemical properties.	Good	Good	Fair	J.D. Blackwood (Australia-Various Publications)
V-b-3 effects on subsequent gasification reactivity (inc. combustibility for power generation)	Good	Good	Fair	IGT Bulletin No. 39 , 1972
V-a-2 heat effects	Poor	Poor	——	"Chemistry of Coal Utilization", H.H. Lowry, Ed., John Wiley & Sons (1963), p. 895
V-b-2 heat effects	Poor	Poor	——	
b-3 effects on subsequent gasification reactivity	Poor	Poor	——	

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Behavior of raw coal in hydrogen atomsphere	Reasonable	Good		Hiteshue, R.W. AGA, Synthetic Pipeline Gas Symposium, 1966
Kinetics of hydrogasification of Disco char - Dilute-Phase and Fluid-Bed Reactors	Good	Good	Wide range of conditions	Wen and Huebler, I&EC Process Design & Dev., v. 4, No. 2, 1965
Kinetics of hydrogasification of carbonized coals-entrained reactor system	Good	Good	Goes to very high pressure	Moseley and Paterson, J. Inst. of Fuel, Sept. 1965
Mechanism of hydrogasifying raw coal in synthesis gas in an entrained reactor	Good	Good	Variety of feeds	Zahradnik & Glenn -Fuel Div. Preprints, 158 Nat. ACS Meeting
Differential reactor data with raw coal-hydrogen rapid heatup rates	Good	Good	Covers one type of coal but over a wide range of temperature & pressure	Hiteshue, Friedman, and Madden, USBM RI 6376
Yield data for IGT two-stage process feeding pretreated coal and steam-hydrogen mixtures. Continuous fluid-bed reactor-some dilute-phase tests	Good	Good	Restricted to conditions that are commercially desirable	Lee, Pyrcioch & Schora, ACS Fuel Division Preprints

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Yield data for dilute-phase hydrogasification of raw coal kinetics continuous dilute-phase reactor	Good	Good	Limited to raw bituminous coal	Feldmann, Simons, Mima, and Hiteshue, ACS Fuel Division Preprints
Kinetics for converting coal char to methane by hydrogenation-fixed and fluid beds	Good	Good	Limited to one coal char & some certifically prepared carbons	Blackwood and McCarthy, Aust. J. Chem.,1966, v. 19
Kinetics of converting coal chars to methane by hydrogenation differential reactor	Good	Good	Limited to Disco char	Zielke & Gorin, I&EC, v. 47, No. 4
Fixed-bed reactor hydrogasifying cokes and coal	Limited	Good	Lower pressure	Dent, International Conf. on Coal Gasification, Liege, 1954
Means of avoiding agglomeration in fluid-bed hydrogasification of coal	Good	Good	Pressures to 500 psig, temp. to 700° C	Kawa et al., USBM
Yield data for the direct hydrogasification of Disco char in a continuous fluid-bed reactor	Good	Good	Limited to Disco char	Pyrcioch and Lindne, I&EC, v. 52, No. 7, July 1960
Heat of Reaction of Coal and Coal Char With Hydrogen (2)	Good	Too few data to determine	More data needed	Lee, A.L. et al I&EC Process, Design and Development, v. 7, No. 2, April 1968

Tabular Form for Reporting Data on Coal Gasification

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Thermal Conductivity and Specific Heat of Coal & Ccke	Good	Good	800°F upper temp. limit	Batchelor, Yavorsky and Gorin J. Chem. & Eng. Data, v. 4, No. 3, July 1959
Specific Heat of Coal of Varying Volatile Meter	Good	Good	Very	A.L. Lee, ACS Fuel Chem. Preprints, v. 12, No. 3, 1968
Fluidization Properties of Porous Chars	Good	Good	Considers chars formed by dilute-phase hydro gasification	Feldman, H.F., Kiang, K., & Yavorsky, ACS Fuel Chem. Preprints, Wash. D.C.
VI Purification (gas)				
VI-a-1 gas/solid flow properties	Poor	——	——	Chemical Engineering Handbook, 4th Ed., R.H. Perry, McGraw Hill Book Co. (1963)
VI-a Particulate removal -b Sulfur removal				USBM, Pittsburgh Energy Research Center, Quarterly Report Oct.-Dec. 1970, pp.71-75; Quarterly Report Jan.-March 1971, pp. 68-75; Quarterly Report April-June 1971, pp.86-87*
VI-c By-product water purification				USBM, Pittsburgh Energy Research Center, Quarterly Report July-Sept. 1971, pp.107-113; Quarterly Report, April-June 1971, pp.113-115; Quarterly Report, Oct.-Dec. 1971, pp. 123-125*

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
VI (tar) Thermodynamic and physical properties of polynuclear aromatic heterocyclic, phenolic, etc., compounds in tar separated from gasifier gas	Rather scarce but some available	Some is excellent but most of poor quality	Very incomplete	Scattered in scientific literature
VI-b,d,e Removal of H_2S, SO_2, COS, CO_2, CO, NO_x, Thiophene, etc.	Equilibrium absorption isotherms of these gases on various solid and liquid absorbents as a function of pressure are scattered throughout chemical literature	Moderate		Chemistry of Coal Utilization, H.H. Lowry, Ed., Wiley & Sons, 1963, pp. 1014-1022
Removal of Sulfur Oxides from Flue Gases by Various Absorbents				USBM, Pittsburgh Energy Research Center, Quarterly Report, Oct.-Dec. 1970, pp. 182-192; Quarterly Report, Jan.-March 1971, pp. 168-180; Quarterly Report, April-June 1971, pp. 217-232 *

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
Simultaneous Removal of Sulfur and Nitrogen Oxides from Flue Gases				USBM, Pittsburgh Energy Research Center, Quarterly Report, July-Sept. 1971, pp. 164-172; Quarterly Report, Oct.-Dec. 1971, pp. 183-198 *
Catalytic Decomposition of NO_x				USBM, Pittsburgh Energy Research Center, Quarterly Report, Oct.-Dec. 1970, pp. 179-181; Quarterly Report, Jan.-March 1971, pp. 164-167; Quarterly Report, April-June 1971, pp. 208-216 *
VII Water Gas Shift Process	Good	Adequate	Good	From process Licensors Commercial
VII-c Heat effects Equilibrium constants, equilibrium compositions, Enthalpies for gaseous mixtures $CO + H_2O \rightleftarrows H_2 + CO_2$	Good	Fair	Fair	Chemistry of Coal Utilization, H.H. Lowry, Ed., John Wiley & Sons, 1963 API Project 44 Tables on "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds" JANAF Thermochemical Tables NBS Circular 564 (1955), Tables of Thermal Properties of Gases Thermodynamic Functions of Gases, Vols. I, II, and II, F. Din, Ed. Butterworths, 1962

*Available
By permission,
Director of Bureau of Mines

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
VII-b Effects of conditions on catalyst	Poor	Poor	——	From Bureau of Mines and IGT publications
VIII Methanation Process	Good	Good	Fair	ACS-"Methanation for Coal Hydrogasification," A.L. Lee, H.L. Feldkirchner, D.G. Tajbl. Sept. 1970. Chem. Eng. Prog. 44, 553-66 (1948) W.W. Akers, R.R. White, "Kinetics of Methane Synthesis." IGT Res. Bull. 31, H.A. Dirksen, H.R. Linden, "Pipeline Gas From Coal By Methanation of Syn Gas" AIChE J. 2, 59-62 (1956) S. Weller USBM RI 5046, 1954. Gas Res. Board GRD 51 London, 1949 USBM RI 6126. 1962 USBM RI 6609. 1965 USBM RI 5137. 1955

Tabular Form for Reporting Data on Coal Gasification

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
VIII-a Kinetics & chemistry as function of conditions & catalyst -b Effects of conditions on catalyst				USBM, Pittsburgh Energy Research Center, Tech. Progress Report - 24, "A Process to Make High-BTU Gas from Coal," April 1970 Chemistry of Coal Utilization, H.H. Lowry, Ed., John Wiley & Sons, 1962
VIII-a Kinetics & chemistry as function of conditions & catalyst -b Effects of conditions on catalyst -c Heat effects				USBM, Pittsburgh Energy Research Center, Quarterly Report, Oct.-Dec. 1970, pp. 77-86; Quarterly Report, Jan.-March 1971, pp. 114-119; Quarterly Report, Oct.-Dec. 1971, pp. 130-140*
VIII-c Heat effects Equilibrium constants equilibrium compositions Enthalpies for gaseous mixtures of $3H_2 + CO = CH_4 + H_2O$			Tables of thermo functions, H,S,G,C_p,Z,K for various mixtures of H_2, CO, CH_4, H_2O, N_2 298 → 1000 K 0 → 100 atm	Chemistry of Coal Utilization, H.H. Lowry, Ed., John Wiley & Sons, 1963 API Project 44 Tables on "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds." JANAF Thermochemical Tables NBS Circular 564 (1955), Tables of Thermal Properties of Gases

Process Operation

Type of Critical Data	General Availability	Reliability of available data	Completeness of available data	Sample Sources of Data
				Thermodynamic Functions of Gases, Vols. I and II, F. Din, Ed., Butterworths, 1962
IX Environmental Effects				
IX-c carcinogenicity of effluents, particularly polynuclear aromatic and heterocyclic hydrocarbons. Relation to physical and thermodynamic properties				Survey of Compounds Which Have Been Tested for Carcinogenic Activity, U.S. Department of Health, Education, and Welfare, 1969
				From equipment vendors
XI-a P-V-T Properties H, S, G, Z for H_2, CH_4, C_2H_6, N_2 Mixtures	Good	Adequate	Good	Chemistry of Coal Utilization, H.H. Lowry, Ed., John Wiley & Sons, 1963
				API Project 44 Tables on "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds"
				JANAF Thermochemical Tables
				NBS Circular 564 (1955), Tables of Thermal Properties of Gases
				Thermodynamic Functions of Gases, Vols. I and II, F. Din, Ed., Butterworths, 1962