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**LITERATURE SURVEY OF  
PROPERTIES OF SYNFUELS  
DERIVED FROM COAL**

Thaine W. Reynolds, Richard W. Niedzwiecki,  
and John S. Clark  
National Aeronautics and Space Administration  
Lewis Research Center

**February 1980**

Prepared for  
**U.S. DEPARTMENT OF ENERGY**  
**Energy Technology**  
**Fossil Fuel Utilization Division**

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istics were tabulated for sodium, potassium, vanadium, lead, chlorides, sulfur, and such easily dissociated nitrogens as ammonia. The fuels that were investigated include low-Btu gas, heavy and light liquid distillates, and residual liquids. Fuels processed or characterized by NASA were not included within the scope of the effort.

Natural gas and no. 2 fuel oil have been used in ground-based gas turbines for industrial and utility applications. Because of the technology base developed through commercial and military research, these fuels are presently in wide use in open-cycle gas turbines for utility peaking service. Natural gas and no. 2 fuel oil are also used in combined gas-turbine/steam-turbine cycles for intermediate duty service. However, these clean fuels are becoming scarce and expensive and may not be available for future ground-based-turbine applications. Viable future fuels for ground-based gas turbines are heavy petroleum oils in the near term and fuels derived from coal in the future. Adapting gas-turbine technology for the use of coal-derived fuels requires the development of key capabilities.

To address this need, NASA and the ERDA Office of Fossil Energy began the Critical Research and Advanced Technology Support (CRT) project with the signing of Inter-agency Agreement EF-77-A-01-2593 on June 30, 1977. Upon creation of the Department of Energy on October 1, 1977, the project was assigned to the DOE Division of Power Systems, which was renamed the Fossil Fuel Utilization Division. The CRT project will provide a gas-turbine technical data base for the DOE Integrated Coal Conversion and Utilization Systems activities, which are aimed at developing improved central-station utility power-conversion systems that use coal and coal-derived fuels.

The technical objectives of the CRT project are

- (1) To develop combustor concepts that will fire coal-derived fuels in an environmentally acceptable manner
- (2) To develop a combustion and materials data base to aid in establishing fuel specifications for advanced, fuel-flexible, stationary power-conversion systems
- (3) To develop acceptable ceramic coatings for use with coal-derived fuels
- (4) To develop a corrosion data base for combustor and turbine materials exposed to combustion products of coal-derived fuels and to correlate the data in a corrosion-life prediction model
- (5) To study the trade-offs between various gas-turbine technologies, operating conditions, and component designs

The literature survey, which is the subject of this report, is being conducted under the combustion portion of the CRT project (item 1). Additional combustion efforts include analytical modeling to determine combustor parameters that affect the conversion of fuel-bound nitrogen into oxides of nitrogen ( $\text{NO}_x$ ); flame-tube experiments to evolve fundamental concepts for minimizing the conversion of fuel-bound nitrogen into  $\text{NO}_x$ ; and evaluation of experimental combustors with coal-derived fuels at simulated gas-

turbine-combustor operating conditions. Results of these combustion efforts will be reported in forthcoming publications.

In surveying the literature, it became apparent that sufficient information on coal-derived fuels is not readily available. Thus, additional information sources were used in compiling the survey. These additional sources included monthly reports from ongoing DOE-sponsored projects and private correspondence. These sources are noted in the data tables where applicable. Since information on coal-derived fuels continues to become available, the survey will be updated to include additional data through fiscal year 1979.

### DETAILS OF LITERATURE SURVEY

Since the emphasis of this survey is on fuels from those synthetic fuels processes that are furthest along in development, data on both the processes and the fuels are continually being generated and published in progress reports by the many contractors involved. Accordingly, no survey report can contain all the latest data on the fuels of most interest. However, this report should give the general status of characterization data available to December 1977 and the physical and chemical data needed for the CRT project but currently not being obtained.

This report is arranged in the following general format:

- (1) FUEL PROPERTIES - This section includes a discussion of fuel properties of concern to the gas-turbine user and examples of the forms used to compile the data.
- (2) COAL LIQUEFACTION PROCESSES - This section describes the four major processes for converting coal into liquid fuels.
- (3) FUEL PROPERTIES DATA - This section contains physical and chemical fuel properties data, grouped by process.
- (4) DISCUSSION - This section compares the properties of various coal-derived fuels. Also fuels from the different processes are grouped by distillate category.
- (5) CONTRACT NUMBERS - This section includes a table of Federal energy contract numbers with author, company affiliation, and contract title. The contractor reports are included in the bibliography.
- (6) SOURCES OF FUEL PROPERTIES DATA - This section contains a tabulation of references 1 to 32, from which the properties data were taken.
- (7) BIBLIOGRAPHY - The bibliography lists the sources of the citations and all the published citations investigated in the literature study, by year of publication.

## FUEL PROPERTIES

Examples of the fuel analysis sheets that were used to collect physical and chemical property data for coal-derived synthetic fuels are shown in table 1 for liquid fuels and in table 2 for low-Btu gases. The lists of properties in these tables were taken from a number of sources that recommended the appropriate fuel properties for applications of advanced gas-turbine systems.

Physical property data such as pourpoint, viscosity, and distillation range are important in determining the pumping, heating, and atomizing characteristics of the fuel. Chemical properties such as elemental composition and trace-metal analyses are important in determining the combustion, emissions, and corrosion characteristics of the fuel. An excellent discussion of the importance of many properties listed in tables 1 and 2 and the use of these fuels in gas-turbine combustion systems is contained in reference 27.

Although it would be desirable to know values for all the listed properties for any given fuel, the current specifications placed upon gas-turbine fuels by users are much less comprehensive. Table 3, from reference 27, shows specifications for several types of liquid fuels for advanced gas-turbine industrial engines. The following comments on the importance of some of these specifications draw upon material contained in reference 27.

The ash and trace-metal contaminants, which are most likely to be concentrated in the higher boiling fractions during processing, can lead to turbine corrosion and deposits. Of the trace metals listed in table 1, the more critical ones appear to be vanadium, sodium, potassium, and lead.

Although no specifications are shown for the elemental compositions (C, H, N, S, O), the values of these are important in determining the combustion and emission characteristics of the fuel. Hydrogen content is a critical factor in controlling the smoke emission levels and the radiation properties of the gases in the combustor. The higher the hydrogen content of the fuel, the less tendency it has to smoke and the less tendency it has to radiate heat to the combustor walls. Fuel-bound nitrogen will contribute to the nitrogen oxide pollutant emissions, since varying amounts of fuel-bound nitrogen are converted to  $\text{NO}_x$  during the combustion process. Sulfur in fuel leads to sulfur oxides in combustion that, when combined with other trace metals, can corrode the turbine. Significant emission problems also occur with fuel-bound sulfur since it is totally converted to sulfur oxides in combustion.

The pourpoint and viscosity-temperature characteristics of the fuel are important in determining

- (1) The fuel heating that may be required to pump fuel through the system
- (2) The pump pressure requirements

(3) The fuel temperature required at the fuel nozzle for proper atomizing. (Maximum viscosities of 10 to 20 cS, depending on the fuel atomizer used, are set to obtain proper nozzle operation.)

The thermal stability of the fuel - which is the tendency to form deposits in fuel manifolds, fuel nozzles, and fuel heaters - is a most important property for the higher viscosity residual fuels. These fuels may require heating to high temperatures to meet the viscosity requirements.

Table 4, obtained from reference 27, shows some typical ranges of fuel properties applicable to current industrial gas-turbine systems.

## COAL LIQUEFACTION PROCESSES

At least four major concepts have been developed for converting coal to liquids: solvent extraction, catalytic liquefaction, pyrolysis, and indirect liquefaction. Each concept is discussed briefly here, and the status of the most important processes that use the concepts is summarized. The technology for coal liquefaction is reviewed in detail in references 33 and 34.

### Solvent Extraction

Solvent extraction is a liquefaction process in which coal is mixed with a coal-derived liquid containing relatively loosely bound hydrogen atoms. This liquid is usually called the recycle solvent. The solvent can transfer these loosely bound hydrogen atoms to the coal at temperatures to 500° C (932° F) and pressures to 275 atmospheres absolute. Heating breaks many of the physical interactions in the coal such as van der Waals forces and hydrogen bonding forces. Heating also breaks weak chemical bonds, and the solvent promotes hydrogen transfer to the broken bonds. Three processes have been developed for liquefaction of coal in the presence of a recycle solvent. In the first, the recycle solvent is hydrogenated in a separate step. In the second, hydrogen is added directly to the extraction vessel and the recycle solvent is not hydrogenated. In the third, hydrogen is added to the extraction vessel and the recycle solvent is also hydrogenated. The recycle solvent, usually an oil middle distillate of process-derived liquids, is continuously recovered and recycled to the extraction vessel. The ash in the extraction vessel often acts as a catalyst for the solvation process; its catalytic effectiveness depends on the coal properties.

Identified in these terms, the processes currently under development are

(1) Consol Synthetic Fuel (CSF)

(2) Solvent-Refined Coal (SRC)

(3) Solvent-Refined Lignite (SRL)

(4) Co-Steam

(5) Exxon Donor Solvent (EDS)

Consol Synthetic Fuel. - The CSF process (ref. 34) is under development by the Conoco Coal Development Co. (formerly Consolidation Coal Co.). Bench-scale studies were started in 1963 with support from the Office of Coal Research (OCR). A 20-ton-per-day pilot plant was built at Cresap, West Virginia, to produce gasoline from coal. This activity was halted in 1970. Fluor Engineers and Constructors, Inc., has reactivated the plant, under DOE sponsorship, to produce clean boiler fuel and distillate rather than gasoline and to test critical liquefaction process components. Shakedown operations are scheduled to be completed in fiscal year 1978 and will be followed by test run operations and testing into fiscal year 1981 (ref. 35).

The extraction reactor used in the CSF process is a stirred tank that operates at 400° C (750° F) and 10 to 30 atmospheres absolute. The hydrotreater, to hydrogenate the recycle solvent, operates at 205 atmospheres absolute. A schematic diagram of the CSF process is shown in figure 1. The process yields about 63 percent fuel oil, 25 percent char, and a high-Btu gas.

Solvent-Refined Coal. - The SRC process (ref. 34) was started in 1962 under OCR sponsorship to study the feasibility of coal de-ashing. The initial contract culminated in a 50-pound-per-hour bench-scale unit. The Electric Power Research Institute (EPRI) and Southern Company Services collaborated on a 6-ton-per-day process development unit (PDU) at Wilsonville, Alabama. Success in the PDU led to design, construction, and operation of a 50-ton-per day pilot plant at Fort Lewis, Washington. The Pittsburgh & Midway Coal Co., a subsidiary of the Gulf Oil Corp., operates the pilot plant under DOE sponsorship. A run was completed in 1977 in which 3000 tons of fuel were produced. This fuel was successfully fired in a 22.5 megawatt boiler at the Georgia Power Co. with acceptable emissions. Current plans call for continued testing at both the Fort Lewis pilot plant and the Wilsonville PDU into fiscal year 1981 (ref. 35). Gulf Mineral Resources Co. has prepared a conceptual design of a 6000-ton-per-day model of a full-scale commercial plant. Similarly, Wheelabrator-Frye, Inc., has designed a 2000-ton-per-day unit for DOE.

The original SRC process (now known as SRC-I) converts high-sulfur, high-ash coal to a nearly ash-free, low-sulfur fuel that is solid at room temperatures. A schematic diagram of the SRC-I process is shown in figure 2. Typical product compositions of SRC-I and raw coal are shown in table 5.

The Fort Lewis pilot plant was modified in 1977 to permit recycling of unconverted coal and ash. This recycling resulted in increased hydrogen addition and a product stream with a fluidity about the same as that of a no. 6 oil. A schematic diagram of this process, called SRC-II, is presented in figure 3. In this process the solidifica-



tion and solvent recovery unit is not required; the mineral residue slurry is used to produce the additional hydrogen required for the process.

The dissolver reactor in the SRC process - a vertical-tube, plug-flow reactor - operates at about 450° C (850° F) and 69 to 103 atmospheres absolute pressure. In the SRC-I process, about 1400 pounds of fuel are produced for each ton of coal (70 percent conversion efficiency by weight). Small amounts of high-Btu gas and light oil are also produced. In the SRC-II mode, the product streams include (based on weight percentage of coal): 40 to 50 percent residual oil, 6 to 12 percent fuel oil, and 2 to 5 percent naphtha. Small amounts of lighter fractions are also produced. Thermal efficiencies for both SRC-I and SRC-II are essentially the same, about 70 percent.

Solvent-Refined Lignite. - The SRL process is being developed by the University of North Dakota under contract to DOE (ref. 34). The process is based on technology derived from both the SRC and Co-Steam processes. The SRL process uses synthesis gas ( $H_2 + CO$ ) in place of the hydrogen used in the SRC process. A process diagram is shown in figure 4. A 0.5-ton-per-day PDU has been built in Grand Forks, North Dakota. Successful operation of this PDU could lead to a run with lignite in the SRC pilot plant at Fort Lewis, Washington.

Co-Steam. - The Co-Steam process is designed to convert low-ranking subbituminous coals, such as lignite, into a low-sulfur fuel oil by the noncatalytic reaction of a coal - recycle-oil slurry with carbon monoxide or synthesis gas (ref. 34). A schematic of the Co-Steam process is shown in figure 5. The stirred reactor operates at 425° C (800° F) and 275 atmospheres. The water required for the reaction is provided by the moisture contained in the low-rank coal. A 5-pound-per-hour continuous process development unit (PDU) is being built at the Grand Forks Energy Research Center, North Dakota. The PDU should be operating early in fiscal year 1979 and should continue through fiscal year 1982 (ref. 35).

Exxon Donor Solvent. - The EDS process (ref. 34) also liquifies coal in a hydrogen-donor recycle solvent. The recycle solvent is catalytically hydrogenated in a trickle-bed reactor at 260° to 450° C (500° to 850° F) and 80 to 210 atmospheres. A schematic diagram of the EDS process is shown in figure 6. Molecular hydrogen is also added to the liquefaction reactor, which operates at 425° to 480° C (800° to 900° F) and 100 to 140 atmospheres. Products are separated from heavy bottoms by flash distillation. The heavy bottoms are further processed by coking or gasification to produce additional liquids and hydrogen for the process. The process yields about 20 percent char, 54 percent oil, and about 25 percent gas. It is about 60 percent thermally efficient.

The EDS project was begun in 1966 entirely with Exxon funding. Through 1975, a 0.5-ton-per-day PDU operated successfully. With DOE and Exxon sharing the cost, a 250-ton-per-day pilot plant is being designed. Operation is scheduled to start in fiscal year 1980 (ref. 35).

## Catalytic Liquefaction

Catalytic liquefaction processes use catalysts other than the mineral matter naturally occurring in ash - ferrous compounds such as ferrous sulfate,  $\text{FeSO}_4$ ,  $\text{NiClO}_2$ ,  $\text{ZnCl}_2$ , and  $\text{SnCl}_2$  - to promote hydrogenation of the hydrogen-donor solvent. These processes have the advantage that a separate reactor to rehydrogenate the solvent is not required; catalyst deactivation and separation problems have been encountered, however.

Two main concepts are employed in catalytic liquefaction processes. In the first, the catalyst and the coal are in direct contact in the reactor, hydrogen gas is introduced, and rapid direct hydrogenation is achieved. Examples of these processes are the Bergius, University of Utah, Schroeder, and Liquid-Phase Zinc Chloride (Conoco). In the second concept, the coal and the catalyst are not in direct contact, but the suspended pelletized catalyst promotes hydrogenation of the carrier solvent, which in turn hydrogenates the coal. Examples of these concepts include H-Coal, Synthoil, Gulf-CCL, and CFFC.

Processes with catalyst and coal in direct contact. - A number of these processes have been developed. Some of the more familiar ones are described here.

**Bergius:** One of the pioneers in coal liquefaction, Bergius first converted coal into oil in 1913 (ref. 34). The process was developed commercially to produce chiefly gasoline. Fifteen plants were operated during World War II and supplied virtually all of Germany's aviation fuel requirements. Costs proved to be prohibitively high for this process, however; and thus none of those plants are now operating.

**University of Utah:** In the University of Utah process a  $\text{ZnCl}_2$  catalyst and coal are fed into a preheater and then into the reactor. The high vapor pressure of the catalyst insures direct contact with the coal at reactor conditions. Very short residence times have been achieved. About 60 percent conversion to liquids and 10 percent conversion to gases have been achieved in a 50-pound-per-hour bench-scale PDU. Catalyst recovery remains a primary technical issue (ref. 34).

**Schroeder:** The Schroeder process is similar to the University of Utah process. The catalyst is ammonium molybdate; residence times are less than 30 seconds. Product yields are about 30 percent distillable liquid, 35 percent residual liquid, 5 percent char, and 30 percent gas. Bench-scale tests of this concept were completed in 1962.

**Liquid-Phase Zinc Chloride:** The Liquid-Phase Zinc Chloride process, being developed by the Continental Oil Co., is designed to convert coal into distillates in the gasoline range by severe catalytic cracking under hydrogen pressure (ref. 34). Bench-scale tests were completed in 1977. A 1.2-ton-per-day PDU has been built by the Conoco Coal Development Co. at Library, Pennsylvania. Shakedown testing was scheduled to begin in fiscal year 1978 (ref. 35).

Processes with coal and catalyst not in direct contact. - These processes include H-Coal, Synthoil, Gulf Catalytic Coal Liquids, and Clean Fuel from Coal.

**H-Coal:** The H-Coal process (fig. 7) is being developed by Hydrocarbon Research, Inc. (HRI) from their H-Oil process, which is used to hydrotreat heavy fuel oils (ref. 2). In the H-Coal process, coal suspended in a recycle solvent is brought into contact with a particulate catalyst in an ebullating-bed reactor (fig. 8). The amount of hydrogen can be varied to produce either a low-sulfur fuel oil or a synthetic crude oil. In the ebullating-bed reactor, which operates at 450° C (850° F) and 150 to 205 atmospheres, the coal and the solvent are forced to flow through the fluidized catalytic bed; both the coal and the solvent are hydrogenated in the reactor. The relative sizes of the catalyst and coal particles are such that the catalyst stays in the reactor. Since catalyst deactivation has been rapid, however, provision is included to withdraw and add catalyst continuously.

The H-Coal process yields about four barrels of oil per ton of coal (about 74 percent conversion efficiency by weight). About 5 percent char is also produced. A self-sufficient plant would be about 64 percent thermally efficient.

Since 1964, HRI has been developing the H-Coal process in a 25-pound-per-day bench-scale unit. The OCR and an industrial consortium funded the building of a 3-ton-per-day PDU. The experimental results and economic feasibility studies were used to complete a detailed design of a 600-ton-per-day pilot plant in 1977. Catlettsburg, Kentucky, has been selected as the location. Procurement and construction is in progress; operations should begin in fiscal year 1979 (ref. 35).

**Synthoil:** The Synthoil process (ref. 34) being developed by the DOE Pittsburgh Energy Research Center (PERC) reacts coal, recycle liquid, and hydrogen in a fixed-bed catalyst with high throughflow rates (fig. 9). Life of the fixed-bed catalyst has been a problem in tests to date. Product yield and thermal efficiencies are expected to be similar to those in the H-Coal process. The Synthoil process has been developed at PERC in a 5-pound-per-day PDU. Foster-Wheeler has been awarded a contract to design and build a 10-ton-per-day pilot plant at Bruceton, Pennsylvania; operation is expected to begin in fiscal year 1979.

**Gulf Catalytic Coal Liquids:** The CCL process is a proprietary coal liquefaction development of the Gulf Oil Corp. It is similar to the Synthoil process and features a fixed-bed catalyst in a radial-flow reactor. The catalyst is claimed to have good resistance to deposition, prolonged high activity, and tolerance to metallic compounds in the coal. Bench-scale tests led to a 10-ton-per-day pilot plant at Harmersville, Pennsylvania. Design studies for a demonstration plant are being made.

**Clean Fuel from Coal:** The CFFC process is being developed by C-E Lummus. The process includes catalytic hydrodesulfurization and dissolution, an anti-solvent-promoted gravity-settling technique, distillation, and product and antisolvent recovery.

C-E Lummus has several patents on the process and has developed it to the small-pilot-plant scale.

## Pyrolysis

Pyrolysis, or carbonization, is one of the oldest techniques for obtaining liquids directly from coal. In pyrolysis, coal is heated without air or oxygen to obtain gases, liquid, and char. Pyrolytic processes typically convert about 50 percent of the coal to char, which does not presently have a ready market. Thus, these processes appear to be best suited to multiproduct plants that use char gasification to produce synthesis gas, hydrogen, or fuel gas. Pyrolytic processes include Lurgi-Ruhrgas, COED, Occidental, Toscoal, U.S. Steel Clean-Coke, and rapid hydrocarbonization.

Lurgi-Ruhrgas. - The low-pressure Lurgi-Ruhrgas pyrolytic process was developed for liquefaction of European brown coals and is the only commercialized pyrolytic process (ref. 34). A schematic diagram of the process is shown in figure 10. Pulverize coal is rapidly heated by direct contact with hot, recirculated, partially oxidized char particles. A portion of the carbonized char is withdrawn as product and the balance is rerouted to the entrained-flow reactor. Products of the process (by weight) are 50 percent char, about 18 percent liquids, and about 32 percent gases. A 1600-ton-per-day plant was built in Yugoslavia and is still operating.

COED. - The Char Oil Energy Development (COED) process (ref. 34) produces synthetic crude oil by pyrolysis of crushed coal in a series of fluidized beds. Agglomeration is prevented by operating at successively higher temperatures (fig. 11). The process has been under development by FMC Corp. since 1962. Successful operation of a 100-pound-per-hour PDU led to the design, construction, and operation of a pilot plant in Princeton, New Jersey. This plant processed 36 tons of coal per day from which it produced about 6 tons of oil, 18 tons of char, and 4 tons of gas. Design capacities were demonstrated in all parts of the pilot plant except the oil absorber tower. Pilot plant operations have been concluded and demonstrated plants have been designed.

Occidental. - The Occidental Research Corp. has been developing this pyrolytic process (ref. 34) since 1969 with its own funds. A 3.6-ton-per-day pilot plant in La Verne, California, has been operating since 1972. A 250-ton-per-day pilot plant is being designed. The process converts volatile bituminous coal to synthetic crude oil by entrained-flow, low-pressure pyrolysis (fig. 12) with very short residence times and rapid heating rates. The process stream leaves the reactor and passes through a cyclone for gas-solids separation and then to a gas-liquids collection station. The process yields about 57 percent char, 35 percent liquids, and 6 percent gas.

Toscoal. - The Toscoal process (fig. 13) is an adaptation of the oil-shale retorting technology developed by Tosco. It produces 5 to 10 weight percent liquids, 5 to 10 per-

cent gas, and the balance char. This process has been demonstrated in a 25-ton-per-day pilot plant; larger scale testing is not believed to be necessary.

U. S. Steel Clean-Coke. - The U. S. Steel Clean-Coke process (fig. 14) is a combined pyrolytic and solvent extraction process. Gases, liquids, and metallurgical grade coke are produced. Operation of a 10-inch PDU is under way and design studies have begun for a 240-ton-per-day pilot plant.

Rapid hydrocarbonization. - Occidental Research Corp. is developing the Flash Pyrolysis process (rapid heating to high temperature with short residence times) on the PDU scale. The Rocketdyne Division of Rockwell International Corp. is developing a similar process except that pyrolysis is carried out in the presence of hydrogen. Both processes are in the early development stage.

### Indirect Liquefaction

Indirect liquefaction processes first convert coal to synthesis gas ( $\text{CO} + \text{H}_2$ ) and then use the water-gas shift reaction and catalytic conversion to produce a wide range of liquids, mainly gasolines. Indirect liquefaction processes include Fischer-Tropsch, methanol synthesis, and methanol to gasoline.

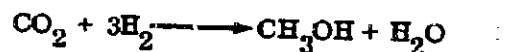
Fischer-Tropsch. - In the Fischer-Tropsch process, gasification is done in commercially available reactors (e.g., Lurgi, Winkler, Koppers-Totzek, or Wellman-Galusha). In-situ gasification may also be used. The synthesis gas is converted to liquids over an iron or cobalt catalyst. Total-process thermal efficiencies are about 40 percent. A commercial unit at SASOL in South Africa produces about 2000 barrels of gasoline per day. A new facility is under construction in South Africa that will increase production to 40 000 barrels per day of gasoline and fuel oil, about 80 percent of that country's automobile fuel needs. The process was also used by Germany during World War II.

HRL, Inc., built a 7000-barrel-per-day unit in Brownville, Texas, in which natural gas was used as the feedstock. When natural gas prices increased, however, this plant became uneconomical and was shut down. There has been renewed interest in this process in this country, however; and several development efforts are under way.

Methanol synthesis. - Methanol synthesis occurs according to either



or



Various catalysts are used to promote the reactions. Several commercial-scale plants have been built abroad, and the technology is considered off the shelf.

Methanol to gasoline. - The Mobil Oil Co., with DOE support, is developing a process for the catalytic conversion of methanol to gasoline. This process is in the PDU development stage.

## FUEL PROPERTIES DATA

The characterization data obtained from the surveyed literature have been tabulated on the fuel property forms (tables 1 and 2). The fuels are presented according to the process from which they were derived (e.g., H-Coal or Synthoil). Within any one process, characteristics have been tabulated for different boiling-range distillates, as well as for the total crude. For ease of referral to the data, the various distillate cuts have been put into three general categories: light distillates (naphtha, light oil, etc.), middle distillates (diesel fuels), and heavy distillates (heating oils and residual fuels).

All the fuel properties data surveyed are contained in this section. Tabulations are also indexed according to the sources from which the data were obtained.

Characterization data are presented in the following tables:

- (1) Data from H-Coal processes in table 3
- (2) Data from Synthoil processes in table 7
- (3) Data from SRC processes in table 8
- (4) Data from COED processes in table 9
- (5) Data from the Gulf Catalytic Coal Liquids process in table 10
- (6) Data from the Exxon Donor Solvent process in table 11
- (7) Data from the Zinc Chloride Hydrocracking process in table 12
- (8) Data from the Co-Steam Process in table 13
- (9) Data from the Flash Pyrolysis process in table 14
- (10) Data from a catalytic liquefaction process in table 15
- (11) Data from the Sea Coal process in table 16
- (12) Proposed specifications of a typical coal-derived liquid fuel in table 17
- (13) Low-Btu gas data in table 18

## DISCUSSION

### Liquid Fuels

This literature survey emphasizes those processes that are furthest along in development and are still active. This criterion could probably have restricted the search to

the liquefaction processes of H-Coal, Synthoil, Solvent-Refined Coal, and Exxon Donor Solvent. However, it was felt that including data on other processes could be useful.

It is readily apparent from casual examination of tables 6 to 18 that many of the fuel properties data of interest to this survey have not been determined for the fuels produced to date. In a few specific instances, where the fuel characterization studies were of fuels for gas-turbine engines, many more relevant property data are available. Data of this type can be found in references 5, 13, and 32.

Some of the more important property data on liquid fuels have been summarized in table 19. Plots of these data are shown in figures 15 to 17. Although different boiling ranges of the fuels are shown in table 19, all the data available for each fuel are plotted, irrespective of the type of process or the type of distillate cut.

Figure 15 shows the general trend of increasing weight percentage of hydrogen with increasing API gravity of the product, regardless of the process by which it was produced. Data for only one fuel were significantly different from the general trend.

Figure 16 shows how the weight percentage of nitrogen varied with the weight percentage of hydrogen. As hydrogenation severity is increased in the fuel production process, the fuel-bound nitrogen is decreased, as would be expected, because some fuel-bound nitrogen is converted to ammonia ( $\text{NH}_3$ ). The data for the Zinc Chloride Hydrocracking process (ref. 24), not plotted in figure 16, showed nitrogen levels significantly lower than that of any other process-derived fuel at comparable hydrogen levels. Nitrogen levels for the zinc-chloride-derived fuels were from 0.0018 to 0.0019 weight percent for hydrogen levels of 8.3 to 9.65 weight percent.

Figure 17 shows how heat of combustion varies with weight percentage of hydrogen for those few fuels for which such data were reported. Again, the trend is independent of the processing type.

### Gaseous Fuels

The low-Btu gases proposed for use in ground-based power turbine systems would be produced by air-blown gasifiers. As such, they will contain a large percentage (~50 vol %) of nitrogen, as well as some carbon dioxide ( $\text{CO}_2$ ) - neither of which contributes to the heating value of the gas mixture. The primary combustible gases from such a gasifier are hydrogen and carbon monoxide and a small amount of methane.

The heats of combustion of the most probable gases in the low-Btu mixtures are shown in the following table, which is a summary of the heat-of-combustion data in table 18. The gross volumetric heating values of hydrogen ( $\text{H}_2$ ) and carbon monoxide ( $\text{CO}$ ) are nearly identical, about 322 Btu per standard cubic foot. As a result, the heat-

Gas	Molecular weight	Heat of combustion, Btu/lb		Heat of combustion, Btu/std ft <sup>3</sup>	
		Gross	Net	Gross	Net
H <sub>2</sub>	2	60 858	51 571	322.8	272.9
CO	28	4 344	4 344	321.8	321.8
CO <sub>2</sub>	44	0	0	0	0
CH <sub>4</sub>	16	23 861	21 503	1010	910
C <sub>2</sub> H <sub>6</sub>	30	22 304	20 416	1770	1620
N <sub>2</sub>	28	0	0	0	0

ing value of a low-Btu gas mixture can be estimated closely if the volume percentage of inert gases (N<sub>2</sub> and CO<sub>2</sub>) is known. Thus

$$\text{Gross heat of combustion} = 322 - 3.22 (\text{vol \% inerts}), \text{ Btu/std ft}^3$$

A plot of this relationship is shown in figure 18. Also shown in this figure are some of the heat-of-combustion data from table 18.

Most of the references cited in table 18 give "typical" ranges of properties for these gases, rather than actual experimental data. In none of the references cited were there any data on the sulfur, alkali metals, or particulate contamination levels to be expected. These data would undoubtedly be controlled by the cleanup processes used, rather than by the gasifier type or the operating conditions.

#### CONTRACT CONDITIONS

Federal energy contract numbers relating to coal-derived synthetic fuels production and upgrading programs are listed in the following table:



Fossil energy contract FE -	Author	Company	Process and/or title
628		PAMCO (Merriam, Ka.)	Pilot plant to produce low-Btu gas from coal
1212	Jones, J. F., et al.	FMC Corp.	COED
1514	Chamberlain, R. M., et al.	W. H. Kinghouse	Advanced coal gasification system for electric power generation
1521		Foster-Wheeler	Advanced coal gasification system for electric power from coal
1527		Bituminous Coal Research	Gas generator research and development with clean fuel gas
1529		Atomics International	Molten-salt coal gasification pilot plant
1534	Peters, Bruce	Dow Chemical	Chemicals from coal (characterization and hydroprocessing studies)
1545	Patterson, R. C.	Combustion Engineering, Inc.	C-E low-Btu gasification of coal project: Phases I, II, and III
1730		IGT	Preparation of a coal conversion systems technical data book
1743	Klunjer, E. B., et al.	Conoco Coal Development Co.	Zinc Chloride Process; hydrocracking for distillate fuels
2003	Grenkovich, E. J.		Chemical characterization: handling and refining of ERC to liquid fuels
2006	Wiser, W. H.	Utah University	Applied Research and Evaluation of process concepts for gasification and liquefaction of Western coals
2010	de Rosset, et al.,	UOP, Inc.	Characterization of coal liquids
2011	Crynes, B.	Oklahoma State University	Catalysts for upgrading coal derivative liquids
2028	Katzer, J. P., et al.	Delaware University	Kinetics and mechanisms of desulfurization and denitrogenation of coal-derived liquids
2034	Berg, L., et al.	Montana State University	Catalytic hydrogenation of coal-derived liquids
2244	Knell, E. W., et al.	Occidental Research Corp.	Flash pyrolysis coal liquefaction process development
2070	Lewis, H. E., et al.	Catalytic, Inc.	ERC process operation at Wilsonville, Ala.
2286			Preparation of a coal conversion system technical data book
2292	Carlson, N.	UTC	Combined-cycle system for low-Btu gas use
2315	Sullivan, R. F.	Chevron Research	Refining and upgrading of symfuels from coal and oil shales by advanced catalytic processes
2353	Fant, B. T.	Exxon Research & Engineering	EDS coal liquefaction process development - Phase IIIa

## SOURCES OF FUEL PROPERTIES DATA

Fuel characterization data are listed, by process type, for the various distillate categories in the following table. Reference numbers in the table (1 to 32) refer to the literature where data applicable to this study were found.

The references were obtained from the extensive bibliography that follows it. Many of the citations in the bibliography repeat the data given in the references. Other citations contain no data relevant to this study. Also included in the bibliography is a list of sources.

Syncrude source	Full-range crude	Naphtha, light distillates, and light oil	Heavy naphtha, middle distillates, and wash solvent	Heavy distillates, fuel oil, and process solvent	Miscellaneous and other cuts
	Reference numbers				
H-Coal	1, 5, 6, 7, 32, (a), (b)	1, 2, 4, 6, 32, (b)	1, 2, 4, 6, 32, (a), (b)	1, 2, 6, 32, (b), (c)	3, 5, (a), (b)
Synthoil	5, 8, 9, 10, 12, 13	10	3, 10, 12	3, 10, 12	8, 11, 12
SRC	_____	5, 16, 17, 32, (a)	(e)	3, 5, 14, 16, 17, 32	14, 15, 16, 17, 32, (a)
COED	6, 18, 19, 20	_____	_____	_____	6, 13, 18, 19
Catalytic Liquid (Gulf)	21, 22	_____	_____	_____	21
Donor Solvent (Exxon)	23	_____	_____	23	_____
Zinc Chloride Hydrocracking	24	_____	_____	_____	24
Co-Steam	25	_____	_____	_____	_____
Flash Pyrolysis	26	_____	_____	_____	_____
Other liquids	13, (f)	_____	_____	_____	_____
Low-Btu gases	27 to 37 and (g)				

<sup>a</sup>Memo for record, John S. Clark of NASA Lewis Research Center, July 14, 1977.

<sup>b</sup>Meeting handout on H-Coal products for gas-turbine combined cycles, Paul H. Kydd of General Electric, Schenectady, N. Y., Jan. 9, 1975.

<sup>c</sup>Letter from G. R. Fox of General Electric Research and Development Center to Lloyd L. Sore of NASA Lewis Research Center, Feb. 18, 1977.

<sup>d</sup>Memo for record on trace element analyses of H-Coal hydroclone bottoms sample, Theodore S. Mroz of NASA Lewis Research Center, Feb. 26, 1976.

<sup>e</sup>Letter from Robert G. Sperhac of Pittsburgh & Midway Coal Mining Co. to Thaine W. Reynolds of NASA Lewis Research Center, May 16, 1975.

<sup>f</sup>Goodwin, G. G.: Amendment of Solicitation to Prospective Offerors, RFP-EF-77-R-01-2674, June 6, 1977 (Contracting Officer, ERDA).

<sup>g</sup>Riteshac, Raymond W., and Eisen, Fred: Course notes from "Synthetic Fuels from Coal," Center for Professional Advancement, July 22-24, 1974.

## REFERENCES

1. Jewitt, Carlton H.; and Wilson, George D.: Comparative Characterization and Hydrotreating of Coal, Shale and Petroleum Liquid. Am. Chem. Soc., Div. Pet. Chem., Prepr., vol. 22, no. 2, Mar. 1977, pp. 785-792.
2. Peters, Bruce C.: Chemicals from Coal: Interim Report on H-Coal. FE-1534-48, U.S. Dept. of Energy, 1977.
3. deRossett, A. J.; et al.: Characterization of Coal Liquids. FE-2010-09, Energy Research and Development Admin., 1977.
4. Holmes, S. A.; et al.: Characterization of Coal Liquids Derived from the H-Coal Process. BERC/RI-76/10, Energy Research and Development Admin., 1976.
5. Callen, Robert B.; et al.: Upgrading Coal Liquids to Gas Turbine Fuels. 1. Analytical Characterization of Coal Liquids. Ind. Eng. Chem., Prod. Res. Dev., vol. 15, no. 4, 1976, pp. 222-233.
6. Shaw, Henry; Kalfadelis, Charles D.; and Jahnig, Charles E.: Evaluation of Methods to Produce Aviation Turbine Fuels from Synthetic Crude Oils - Phase I. GRU-1PEA-75, Exxon Research and Engineering Co., 1975. (AFAPL-TR-75-10, AD-A016456.)
7. Johnson, Clarence A.; Stotler, Harold H.; and Winter, Olaf: H-Coal Prototype Program. Paper 55C - Symposium on Project Plants for Production of Clean Fuels from Coal. Nov. 11-15, 1973; 66th Annual Meeting, AIChE, Phil., Pa.
8. Schultz, Hyman; et al.: A Study of Some Trace Elements in the 1/2 Ton Per Day Synthoil Process Development Unit. Am. Chem. Soc., Div. Pet. Chem., Prepr., vol. 22, no. 2, Mar. 1977, pp. 588-592. (Also PERC/RI-77/2, 1977.)
9. Crynes, B. L.: Catalysts for Upgrading Coal-Derived Liquids. FE-2011-7, Energy Research and Development Admin., 1977.
10. Woodward, P. W.; et al.: Compositional Analyses of Synthoil from West Virginia Coal. BERC/RI-76/2, Energy Research and Development Admin., 1976.
11. Crynes, B. L.: Catalysts for Upgrading Coal-Derived Liquids. FE-2011-3, Energy Research and Development Admin., 1977.
12. Kalfadelis, Charles D.: Evaluation of Methods to Produce Aviation Turbine Fuels from Synthetic Crude Oils - Phase II, Vol. 2. GRU-2PEA-76-VOL-2, Exxon Research and Engineering Co., 1976. (AFAPL-TR-75-10, Vol. 2, AD-A036190.)