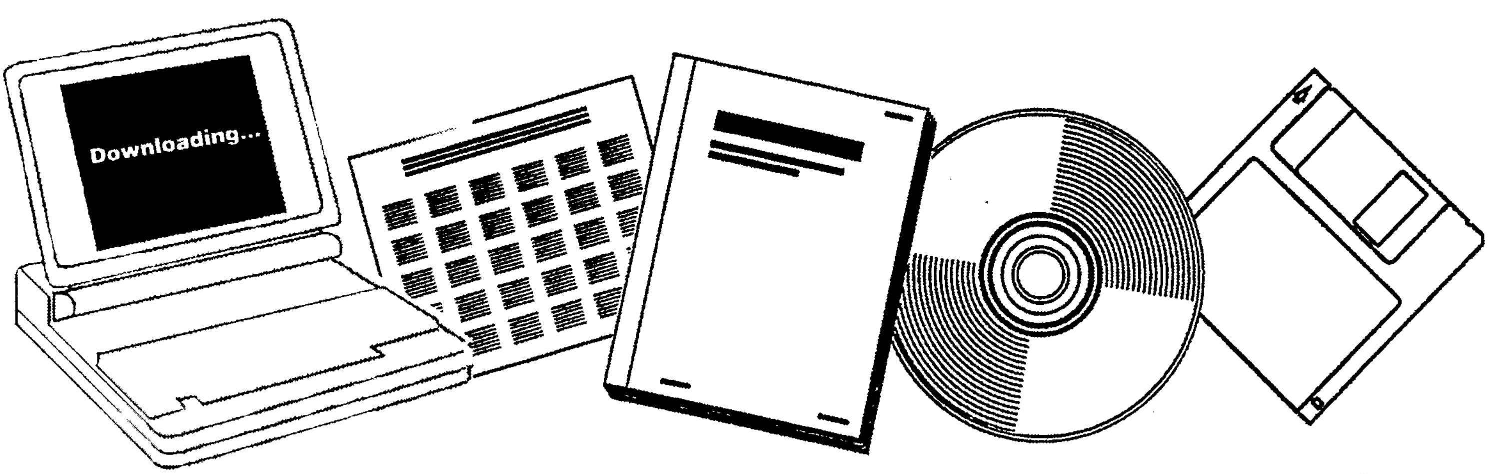
OPTIMIZATION OF COAL GASIFICATION PROCESSES. MONTHLY PROGRESS REPORT FOR PERIOD JANUARY--DECEMBER 1972

WEST VIRGINIA UNIV., MORGANTOWN

JAN 1972



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OPTIMIZATION OF COAL GASIFICATION PROCESSES

Monthly Progress Reports for the
Period January - December 1972

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OPTIMIZATION OF COAL CONVERSION PROCESSES
PROGRESS REPORT NO. 53
JANUARY 1972

to

Office of Coal Research
Contract No. 14-01-0001-497

During the last two months, two coal gasification processes proposed by the U. S. Bureau of Mines, known as the "Synthane Process" and the "Hydrane Process", have been studied and mathematically optimized. Their respective thermal and carbon efficiencies and their costs have been compared to the other processes described in our Interim Report, written on September 15, 1971. This study is almost completed and we are now drafting a supplemental report giving the results of these evaluations, the report to be completed within two weeks.

The modified computer program to use ambient air instead of high pressure oxygen to produce fuel gas in now operational. The program yields the calorific values of the produced gas, the air requirements and the exit gas compositions for various steam-coal ratios and carbon conversions. The initial calculations were made for a gasification reaction at 80 psig and 1700°F. Since these units usually operate above 2000°F, these calculations will be repeated for a range of higher reaction temperatures.

The efforts to use the new mathematical technique, "Complex Method of Optimization", to more efficiently coordinate the various process sub-systems into an optimized overall process is still continuing. The calculation method has proved to be successful; however, difficulties in certain process subsystem simulations have prevented the obtaining of useful results. These problems are expected to be solved soon.

Process descriptions and operating data are being assembled for the various coal liquefaction processes now being actively developed for potential commercialization. The previous OCR reports concerning these processes have been requested and a literature search is underway to gain background knowledge in this reaction area. The first objective will be the survey of the various process flow schemes to determine which subsystems we have already evaluated during the gasification study.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES
PROGRESS REPORT NO. 54
FEBRUARY 1972

to

Office of Coal Research
Contract No. 14-01-0001-497

In the last few months, studies were made of the "Hydrane Process" and the "Synthane Process", two coal gasification systems developed by the U. S. Bureau of Mines. A supplemental report will soon be issued describing the optimization of these processes and comparing their carbon useage and thermal efficiencies with other coal gasification processes described in our Interium Report, September 15, 1971. To reduce the production of unwanted char, the overall process was reevaluated assuming higher carbon conversions, up to 85%. The results of this study will be included in the supplementary report available soon.

The new mathematical technique "Complex Method of Optimization" was used to coordinate the various subsystems of the "Hydrane Process" into an optimized overall process. The thermal efficiency, defined as;

$$\%\ \text{Efficiency} = \frac{Q_G}{Q_C + E_p - E_R}$$

where; Q_G = Heat Content of Product Gas Leaving Plant
Q_c = Heat Content of Coal Used for Gasification
E_p = Energy Required for Process
E_R = Energy Recovered From the Process

This optimized value for the thermal efficiency ranges from 72 to 76%, varying with changes in the flow scheme.

The costs of the sulfur recovery plants were not considered in the original process plant cost studies and are now being sized and the estimated installed costs added to the already reported plant investments. The processes to convert the gaseous H_2S to elemental sulfur represent a significant portion of the overall plant capital investment. A sensitivity study is being undertaken to determine the effect of varying the various bare equipment costs portions on the final cost of the manufactured fuel gas.

The study of the production of low-BTU fuel gas using low pressures and ambrient air instead of high pressure oxygen has now completed the reaction-modeling of the gasification chamber and our interests are now concerned with the positioning of various steam and gas turbines in the exit gas lines to utilize the sensible heat available from this process.

The review of various coal liquifaction processes have led us to choose two processes; "Project COED" (F.M.C. Corporation) and the "Solvent-Refined Coal" (Pittsburgh & Midway Coal Company): as our initial candidates for optimization in this process area. The "Project COED" contains a number of process steps very similar to steps in the coal-gasification studies we have already undertaken in our optimization project. The "S.R.C." Project is chosen because its process steps are rather simple and the ashless-low sulfur product can be used as a raw material for other coal-to-gas or coal-to-oil processes that we have already studied or intend to study in the future.

C.Y. Wen

C.Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 55

MARCH 1972

to

Office of Coal Research

Contract No. 14-01-0001-497

The writing of the supplementary report to our September 15, 1972, Interium Report is partially completed. This supplement will consolidate and up-date the findings given in the previous detailed publication and is intended as a summary of our optimization investigations and will also include studies of some coal-to-gas processes not described in the previous volume.

In our previous studies, Consolidation Coal's "CO_2 Acceptor Process" was evaluated using lignite as the raw material. A material balance has now been completed on this process using bituminous coal, and the results of this study will be included in the supplemental report. Initial results indicate that the carbon utilization efficiency for bituminous coal lies between the Bituminous Coal's "BI-GAS Process" and the U. S. Bureau of Mines' "Synthane Process."

Sensitivity studies evaluating the effect of various individual cost factors on the overall gas cost indicates a 2.1 to 3.6 cent difference per million Btu will be reflected in the final productions cost by a 10% change in the bare capital equipment cost. An increase of 2 to 4 cents per million Btu is the effect of a 10% decrease in the stream factor (using

95% on-stream time as the mean). The sensitivity of cost changes in the direct materials (catalyst and other chemicals, excluding coal) were found to be insignificant. The major overall cost effect is, of course, the purchase price of raw coal.

Studies on a process to produce low-Btu gas from partial air-gasification at realtively low operating pressures are now concerned with recognizing the optimum process thermal efficiencies for various arrangements of steam and gas turbines in the effluent product gas stream.

The studies of the coal-to-liquid fuel processes are still concerned with collecting the current research and development data from the various investigators and to gaining a good basic understanding of the proposed processes and their alternatives. The formulation of a general material balance computation program has been started and integration of coal gasification processes with coal liquefaction processes will be attempted.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 56

APRIL 1972

to

Office of Coal Research

Contract No. 14-01-0001-497

The first draft of the supplementary report to our September 15, 1971, Interim Report is nearly complete. This report, consolidating and updating the findings of the detailed Interim Report, is expected to be issued in the next few weeks.

In the proposed fuel-gas generation systems, the required steam and electrical power can be generated using different kinds of fuel, such as raw coal, char produced from the gasification reaction and mixtures of the two fuels-raw coal and char. The char is the partially reacted solid by-product produced in the hydrogasifier. The computations of the thermal efficiency of hte "Hydrane Process" (U. S. Bureau of Mines) were studied using the three sources of fuel for steam and electricity. The results of this optimization study indicated that the highest thermal efficiencies can be realized by using mixtures of raw coal and char.

The study of the production of low BTU fuel gas using air and in a low pressure reactor continues, with emphasis on the placement of the steam and gas turbines to realize the optimum efficiency from the overall system.

A process performance study has been made of the "Project COED" (F.M.C. Corporation) process. A number of interrelationships of its several subsystems have been recognized and understood. In the next few months, this process and the "S.R.C. Process" will be studied in greater detail.

C. Y. Wen

C. Y. Wen, Director

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 57

MAY-JUNE 1972

to

Office of Coal Research

Contract No. 14-01-0001-497

Our efforts in the last two months have been mainly directed at preparing and releasing several papers and reports describing our studies of the coal gasification processes.

(a) "Efficiency of Coal Gasification Processes", Paper No. XX In it the thermal efficiencies of eight alternative processes to produce high Btu pipeline gas from coal are computed and compared.

(b) "Optimization of Alternate Coal Gasification Processes for Pipeline Gas Production". This supplementary report summarizes the study results contained in the comprehensive O.C.R. Interim Report; "Optimization of Coal Gasification Processes", R & D Report No. 66, Interim Report No. 1, 1972; recently published on this project. In the Appendix of the new report are process descriptions and optimization study results for three alternative processes studied after the Interim Report was submitted for publication. These recently studied processes are similar to, but not identical with, the U. S. Bureau of Mine's "Hydrane" and "Synthane" Processes and Consolidation Coal's "CO_2 Acceptor Process" using bituminous coal.

(c) "Comparison of Alternate Coal Gasification Processes for Pipeline Gas Production", Paper submitted for presentation before the 65th Annual Meeting, American Institute of Chemical Engineers, New York, New York, November 26-30, 1972. This paper is basically the same as the above report, Item (b), except the Appendix has been deleted.

The initial emphasis in the study of low Btu fuel gas production has been concentrated on the arrangement of various gas and steam turbine units in the gas stream following the combustion chamber to recognize the maximum overall efficiency of the energy recovery system. Our interests are now centered on the low-Btu gas generator system, investigating several reactor arrangements, such as a coal pyrolysis unit whose product char is gasified in a separate synthesis gas generator (fed with steam and air) to provide the inert fluidizing and heat-supplying gases for the pyrolyzer. Our efforts will be concentrated in this study area for the next several months to optimize and compare the thermal efficiencies of the many methods by which this low-Btu gas can be produced from the coal.

The study of the coal liquefaction processes remain concentrated on the various reaction systems of the "COED Process" (F.M.C. Corporation) and the "S.R.C. Process" (Pittsburgh & Midway Coal Mining Company). Areas of immediate concern for mathematical modeling are the coal dissolvation and coal pyrolysis systems.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 58

JULY 1972

to

Office of Coal Research

Contract No. 14-01-0001-497

Coal Gasification to Low-Btu Gas

The efforts in this study are now concentrated on the coal pyrolysis and gasification steps to maximize the thermal and carbon efficiencies.

Two gas production schemes are being studied initially. In one, Case I, all the gas is produced in an air-fed, low-pressure (100 psig) gasifier consuming raw coal. In the second scheme, Case II, the raw coal is fed to a devolatilizer which is fluidized by synthesis gas. This synthesis gas is generated in an air-fed, low pressure gasifier which is fueled by the devolatization char.

Preliminary results indicate that the devolatilizer-gasifier system, Case II, has a slightly higher thermal efficiency (by 4%) than does the single chamber gasifier, Case I. Also the product gas from the Case II system has a higher caloric value which may beneficially affect the combustion chamber efficiency and/or equipment cost in the power generation section of the overall process.

Next, the gas generation section will be coupled with the gas combustion and electrical power generation sections to optimize the overall low-Btu gas production and power generation process.

Conversion of Coal to Liquid Fuels

After a preliminary investigation of some typical coal-to-liquid conversion processes now under development (COED, H-Coal, SRC, University of Utah Process, etc.), we are now in the process of dividing the various process schemes into subsystems so that each subsystem can be examined in detail, modeled and finally optimized. Complexing the study structure will be the fact that many different products can be produced. The quantity distribution of these products can be arbitrary, within certain limits set by the mass balance relationships, and will be likely justified mostly by the assumed economic criteria and product demand. This analysis to define the subsystems will be finished by September 1st.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 59

AUGUST 1972

to

Office of Coal Research

Contract No. 14-01-0001-497

Coal Gasification to Low-Btu Gas

The efforts in this study continue to be concerned with maximizing the thermal and carbon efficiencies of the coal pyrolysis and/or gasification stages of the process.

Among a number of alternate schemes considered, conceptual flowscheme of the overall process to generate electrical power via coal-derived low-Btu synthesis gas is illustrated in the attached Figure 1. Raw coal is fed into either a pyrolyzer or into a gasifier or into both. In the combination gasifier-pyrolysis system illustrated in Figure 1, the pyrolysis char and supplementary raw coal (if needed) is gasified with air and steam to form a synthesis gas composed of N_2, CO, CO_2 and H_2. This synthesis gas is fed to the pyrolyzer to act as a carrier to remove the volatiles evolved from the raw coal feed. The gasifier operates at 1800-2300°F and the pyrolyzer operates at 1400-1500°F. Heat is removed (steam being generated) before the gas enters the char separators. The char is fed into the gasifier and the solid-free fuel gas then enters the purification units where the CO_2 and sulfur compounds are removed to acceptable fuel gas concentrations. The clean low-Btu gas is then burned in the comubstion chamber with excess air. The heat generated in the chamber and the hot effluent gas are used in cycles involving the most optimum combination of steam and gas turbines to generate the electrical power.

At the present time we are evaluating the gasification-pyrolysis steps, comparing a fuel-gas generating system involving both gasifier and pyrolyzer (as illustrated) with a system utilizing an air and steam-fed synthesis gas generator alone. Preliminary computations, without mathematical optimization, indicate that these two systems have very close thermal and carbon efficiency values. One choice of operating conditions may favor one system while another operating condition choice may swing the system favoritism in reverse. Upon coupling the gas generation subsystems with the rest of the gas combustion-electrical power generation subsystems, we will employ mathematical optimization on both gas generating alternates using either the lowest capital equipment cost or the lowest gas manufacturing price as the objective function of the optimization. Included in the overall process economics will be the gas purification and the sulfur recovery costs.

Conversion of Coal To Liquid

The preliminary results of the study to divide the various coal-to-liquid process schemes into subsystems has indicated that the unit processes of low-temperature coal pyrolysis, coal dissolvation into organic solvents with or without hydrogenolysis and heavy oil hydrogenation, among others, are definite subsystems which must be investigated in detail. Our initial efforts will be directed at the low-temperature coal pyrolysis, investigating not only the recent research in this step in the "COED Process" and in the "Project Seacoke", but also analyzing and utilizing the research results produced over the last fifty years. This detailed analysis of research data to be used to formulate the various reaction models are now underway.

C. Y. Wen

C. Y. Wen, Project Director

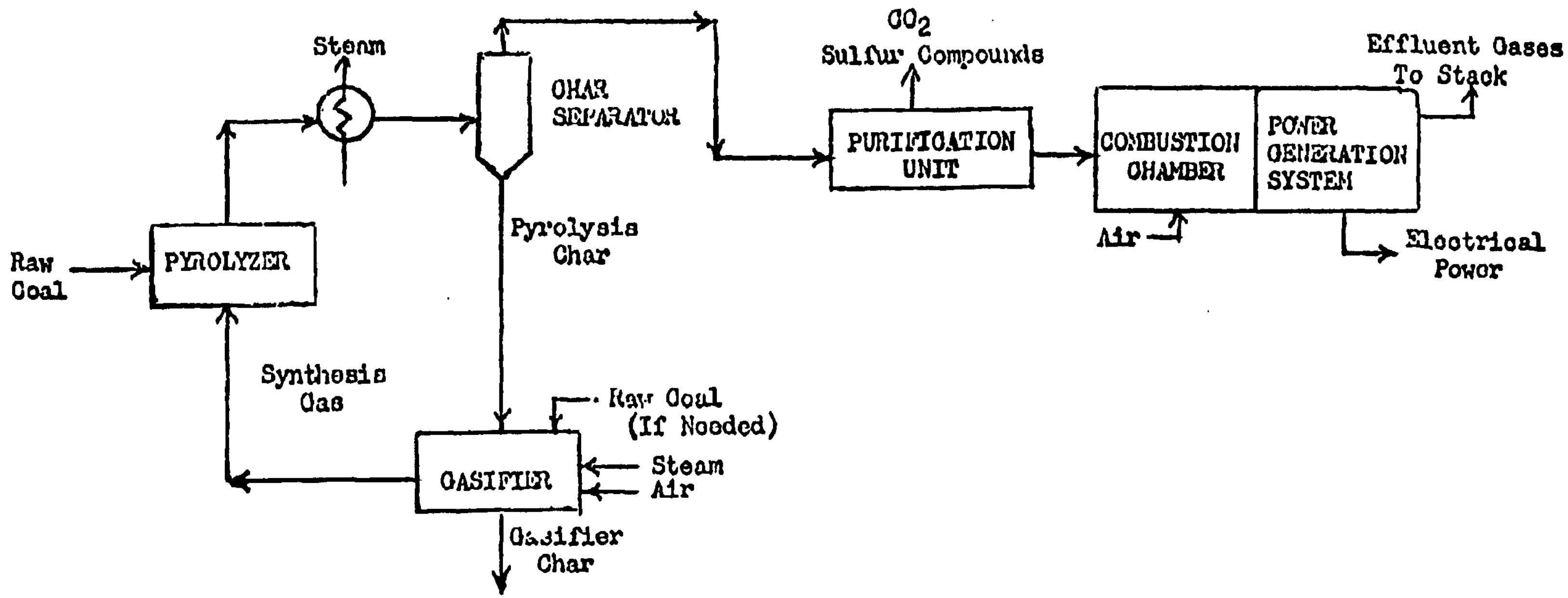

FIGURE 1: A CONCEPTUAL FLOWSCHEME FOR ELECTRICAL POWER GENERATION VIA LOW-BTU, COAL-DERIVED GAS PRODUCTION

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 60

SEPTEMBER 1972

to

Office of Coal Research
Contract No. 14-01-0001-497

Conversion of Coal to Low-Btu Gas

Current efforts in this study continue to be concerned with deriving a conceptual flowscheme for the production of low-Btu gas by coal gasification, and in evaluating some of the alternative choices in the process path.

The generalized conceptual flowscheme was illustrated and described in our last month's report (Progress Report No. 59, August, 1972, O.C.R. Contract No. 14-01-0001-497). Some of the alternative subsystems being examined are:

(a) Coal Pyrolyzing Reactor: Will its presence in coordination with an air- and steam-fed Gasifier (for the pyrolysis char) mean higher carbon and/or thermal efficiencies than the efficiencies obtained when raw coal is directly gasified in a single high-temperature reactor?

(b) Coal Pyrolysis (if needed) and Gasifier Reactors: What are the most advantageous design and operating conditions?

(c) Gas Purification Subsystem: What purification techniques will yield the highest overall plant efficiencies? The sulfur compounds must be removed, but the presence of carbon dioxide in the gas entering the combustion chamber may or may not be advantageous to the efficiency of the overall process. In our studies of the high-Btu gas-from-coal processes ("Optimization of Coal Gasification Processes", R & D Report No. 66, Interim Report No. 1, Office of Coal Research, 1972, we limited our considerations in the gas purification subsystems to only a few well-known alternative scrubbing techniques. This study will be broadened.

(d) Combustion Chamber and Power Generation Subsystem: What is the optimum among the power cycle arrangements? In this area we will have to rely on the published expertise of the power industry; however, we can evaluate several of their recommended alternatives with regard to the rest of our gas production flowscheme.

The statements above list some of the various questions we are seeking to answer in our study. We have made considerable progress in resolving Question (a). It seems that the pyrolyzer does indeed aid in increasing the overall thermal efficiency of the gas production subsystem. However, the question is unresolved as to whether this efficiency increase will justify the additional costs of the separate pyrolyzing reactor. Questions (b) and (d) have been incorporated into a generalized calculation procedure in preparation for mathematical optimization. We are now initiating the new study into the various low-Btu gas purification processes.

Conversion of Coal to Liquids

A study leading to the preparation of a mathematical model simulating the low-temperature pyrolysis of coal has been initiated. Relationships involving the material and heat balances are being derived. In addition, the available reports of the "COED Process" and the "Project Seacoke" are being searched to extract experimental information which can be used in deriving and computing the "quasi-equilibrium" and kinetic relationships involving the aqueous, oil and gaseous products in the relatively low-temperature (600°-1200°F) reaction regime.

C. Y. Wen

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 61

OCTOBER 1972

to

Office of Coal Research

Contract No. 14-01-0001-497

Conversion of Coal to Low-Btu Gas

The efforts continue in developing process systems to produce low-Btu gas by air-fed coal pyrolysis and/or gasification reactions.

During October the model of the CO_2 Acceptor Process (Consolidation Coal Company) was studied to determine if the sulfur removal can be more efficiently accomplished by the adsorption-reaction of the sulfur compounds with dolomite during the coal gasification, than if the sulfur were removed as H_2S in the reactor effluent stream and then the fuel gas cleaned in a separate, later purification subsystem. This study is still continuing with the results expected soon.

The kinetic model of coal pyrolysis in the high temperature range (above 1000°F) is also under investigation for use later in designing the reactor subsystem.

Conversion of Coal to Liquids

Efforts are underway to develop a kinetic model for later use in predicting the production rates, versus temperature, of the several products from coal pyrolysis. In this first simplified version of the model, these potential products are subdivided into four divisions; (a) aqueous products (b) liquid hydrocarbons, (c) gaseous hydrocarbons, and (d) char. Reported experimental data from early work in the "Project

COED" (F.M.C. Corporation) are being utilized, as well as data reported in literature by other research investigators: Tests for the reliability of the model for various reactor systems are planned as soon as the model has been prepared.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES

PROGRESS REPORT NO. 62

NOVEMBER 1972

to

Office of Coal Research

Contract No. 14-01-0001-497

Conversion of Coal to Low-Btu Gas

This study continues to concentrate its effort on the development of a kinetic model for the pyrolysis of the coal, particularly at the higher temperatures above 1000°F. Although we are experiencing some difficulties in deriving the form of the model, some general reaction trends seem apparent. In order to maximize the production of non-condensible caloric compounds (the gaseous fuels; CO, H_2, CH_4, C_2H_6, etc.), one should (a) approach a high temperature, flash reaction for the evolution of the volatile product effluent from the solid coal particle, and then (b) hold this evolved volatile matter in the high temperature range for a prolonged time period, after it has left the solid, in order to "crack" as much of the higher-molecular weight molecules into the non-condensible synthetic fuel compounds. Work in deriving and utilizing this pyrolysis kinetic model will be continued.

Conversion of Coal into Liquids

Efforts continue in developing a kinetic model to use in predicting the production rates of the several products; non-condensible compounds, condensible hydrocarbons, aqueous compounes and residue char;

from the pyrolysis reaction of coal, particularly in the lower temperature range (below 1000°F) where each compound class has a significant evolution rate. The reaction system is quite complex which has hindered the theoretical derivation of the kinetic model. Certain simplifying assumptions are now being proposed and tested against the experimental data available in literature.

C. Y. Wen, Project Director

OPTIMIZATION OF COAL CONVERSION PROCESSES
PROGRESS REPORT NO. 63
DECEMBER 1972

to

The U. S. Office of Coal Research
Contract No. 14-01-0001-497

Conversion of Coal to Low-Btu Gas

Efforts in this study continue in the developing and refining of models to predict the production of low-Btu gas via the high-temperature pyrolysis (above 1000°F) of coal and the later gasification of the char to produce the fluidizing gases for the coal pyrolyzer. A paper entitled "Production of Low Btu Gas Involving Coal Pyrolysis and Gasification" has been written and submitted to O.C.R. for permission to present at the Dallas, Texas, ACS Meeting in April 1973. In this paper, some experimental coal pyrolysis data, obtained earlier at West Virginia University, are presented and analyzed. From this data analysis, some general reaction trends, which the pyrolysis model must simulate, were derived and discussed.

The emphasis of this study will now concentrate on the refinement of the coal pyrolysis model and then shift to the use of the model to design, optimize and economically evaluate the entire (coal)-to-(low Btu gas)-to-(electric power) conversion system.

Conversion of Coal into Liquids

The goal of this study has been shifted slightly to involve the optimization of a coordinated multi-product coal conversion system similar to the conceptual flowscheme of the COED Process (FMC Corporation). The emphasis of this study will be mainly directed at the optimized utilization of the large amount of char being generated in the present process design. Some char utilization alternatives to be examined are (a) conversion to high-Btu gas, (b) conversion to low-Btu gas for electrical power generation, and (c) production of hydrogen.

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C. Y. Wen, Project Director

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