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AN ANALYSIS OF COAL HYDROGASIFICATION PROCESSES

FINAL REPORT

By Dr. Michael Epstein
Dr. Tan-Ping Chen
Dr. Mohamed A. Ghaly

BECHTEL CORPORATION
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ABSTRACT

Bechtel Corporation has conducted a program for the Department of Energy (DOE) to investigate the operability potential and scaleup feasibility of the Cities Service, Rocketdyne, Pittsburgh Energy Research Center (PERC), and Brookhaven National Laboratory coal hydrogasification processes. As part of the program objective, a reactor model study has been performed for each of the processes, and a conceptual, full-scale hydrogasification reactor design has been generated. The entrained-downflow reactor systems operate at temperatures up to 2,000°F and pressures up to 3,000 psi. Reactor product is primarily methane, with smaller amounts of ethane, BTX, light oils, and carbon-oxides.

Bechtel has collected and analyzed bituminous, subbituminous, and lignite coal hydrogasification and hydropyrolysis data from Rocketdyne, Cities Service, PERC, and Brookhaven National Laboratory. The data have been entered into a computerized data base for ease of evaluation and tabulation. Semi-empirical correlations for predicting overall carbon conversion efficiency and carbon selectivity to gaseous products have been fitted to the data. The results show that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar values of overall carbon conversion and carbon selectivity to gaseous products for subbituminous coal under comparable operating conditions; therefore, the test data at Rocketdyne and Cities Service should be scalable to a PDU or commercial-size reactor, within the region investigated. The results also show that overall carbon conversion (or reactivity) for bituminous coal is greater than the reactivity for subbituminous or lignite coals at reduced residence time and/or pressure.

A conceptual design of a full-scale hydrogasification reactor has been generated, on the basis of the subbituminous coal data gathered in the Cities Service and Rocketdyne reactors, together with the predictive reactor performance models fitted to the data. The hydrogasification stage has a configuration similar to the Rocketdyne reactor assembly, which incorporates an entrained-downflow reactor chamber and high-efficiency injector nozzles which produce coal heatup rates in excess of 100,000°F/sec. For the design conditions of 50 percent overall carbon conversion and 100 percent carbon selectivity to gas, predicted operating variable levels for reactor gas temperature, pressure, and residence time were 1,875°F, 1,500 psig, and 1,100 milliseconds, respectively.

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Section 1

INTRODUCTION AND BACKGROUND

In rapid-rate coal hydropyrolysis, pulverized coal particles are contacted with hot, high-pressure hydrogen for a short period of time. Typical conditions include temperatures of 1,000°F to 2,000°F, hydrogen partial pressures of 500 to 3,000 psi, and particle residence times of 0.05 to 10 seconds. Reaction products are primarily methane, with smaller amounts of ethane, benzene and its derivatives, light oils, and carbon-oxides. Agglomeration of caking coals is avoided by rapidly heating the coal particles at rates in excess of 10,000°F/sec to reaction temperature.

Rapid rate hydropyrolysis of coal involves a number of complex chemical and transport phenomena which are not well understood. These phenomena include devolatilization of the solid coal, hydrogenation of reactive volatile matter, hydrogenation of char, diffusion of volatile matter from the coal particles, and intrusion of hydrogen to stabilize the reactive volatiles or react with the active char. Excellent reviews of the subject have been presented by Anthony and Howard,[1] Pyrcioch et al.,[2] and Russel, et al.[3]

For the past several years, a number of studies have been conducted on the rapid-rate hydropyrolysis of various rank coals. These studies have included laboratory-scale experiments at CUNY;[4] bench-scale experiments at PERC,[5] Cities Service,[6] and Brookhaven;[7] and small pilot-scale experiments at Rocketdyne.[8] Some of these studies have emphasized the production of both gas and liquid products (hydropyrolysis or hydrogenation); others have emphasized the production of only gas (hydrogasification).

PERC involvement in the direct hydrogasification of coal to produce high-Btu gas dates back to the late 1950's and has led to the design of several laboratory reactors over a period of 10 years. In 1966, PERC began the development of a free-fall, dilute-phase (FDP) tubular reactor designed to feed coal at up to 25 lb/hr. Since 1966, the PERC FDP reactor has generated a substantial quantity of data on the hydrogasification of various rank coals.

Since 1976, Rocketdyne has been performing experimental studies sponsored by the DOE for the hydrogasification and hydropyrolysis (partial liquefaction) of bituminous and subbituminous coals in two entrained-downflow tubular reactors of 1/4- and 1-ton/hr coal capacity. Coal particles and hot hydrogen gas are mixed inside a specially designed injector element, which can produce coal heatup rates in excess of 500,000°F/sec.

Since 1975, Cities Service has been performing experimental studies on hydrogasification of a subbituminous coal and hydropyrolysis (rapid hydrogenation) of a lignite coal. The hydrogasification program has been funded by the DOE, and the hydropyrolysis program has been funded by Cities Service. The bench-scale system incorporates entrained-downflow tubular and helical reactors designed to feed coal at up to 5 lb/hr. Preheated hydrogen and coal are mixed inside a high-velocity coaxial injector nozzle to produce coal heating rates in excess of 100,000°F/sec. An injected stream of cryogenically cooled hydrogen at the reactor outlet quenches the reaction.

Since 1975, Brookhaven National Laboratory has been performing an experimental study on rapid hydrogenation (flash hydropyrolysis) of a lignite coal. Although major emphasis in this study has been to maximize liquid hydrocarbon yield, an appreciable yield of hydrocarbon gases (mainly methane and ethane) has been obtained. The bench-scale system incorporates an entrained-downflow tubular reactor, designed to feed coal at up to 2 lb/hr.

Bechtel Corporation has conducted a program for the DOE to investigate the operability potential and scaleup feasibility of the Cities Service, Rocketdyne, PERC, and Brookhaven National Laboratory coal hydrogasification processes relating to DOE plans for a hydrogasification process development unit (PDU). As part of the program objective, a reactor model study has been performed for each of the processes, and a conceptual, full-scale hydrogasification reactor design has been generated. Work on this program was initiated in February 1977 and was concluded in April 1978. This report presents the results of the Bechtel program.

Section 2

SUMMARY AND CONCLUSIONS

Bechtel Corporation has conducted a program for the Department of Energy (DOE) to investigate the operability potential and scaleup feasibility of the Cities Service, Rocketdyne, Pittsburgh Energy Research Center (PERC), and Brookhaven National Laboratory rapid-rate coal hydrogasification processes. As part of the program objective, a reactor model study has been performed for each of the processes, and a conceptual, full-scale hydrogasification reactor design has been developed.

2.1 DATA COLLECTION AND DATA CORRELATION

Bechtel has collected and analyzed rapid-rate hydrogasification data from (1) 60 Rocketdyne tests using bituminous and subbituminous coals, (2) 67 Cities Service tests using lignite and subbituminous coals, (3) 42 PERC tests using bituminous and lignite coals, and (4) 48 Brookhaven tests using lignite coal. The data have been entered into a computerized data base for ease of evaluation and tabulation.

The Rocketdyne tests were conducted in two entrained-downflow reactor systems of 1/4- and 1-ton/hr coal capacity. The Cities Service and Brookhaven bench-scale tests were conducted in entrained-downflow reactors of 5 and 2 lb/hr coal capacity, respectively. PERC performed its testing in a free-fall, dilute-phase reactor with a coal capacity of 25 lb/hr.

The reactor systems were operated at reactor outlet gas temperatures of 900°F to 1,960°F, pressures of 500 to 3,000 psi, and particle residence times of 60 to 12,000 milliseconds. Overall carbon conversion varied from 13 to 71 percent; carbon selectivity to gas varied from 25 to 100 percent. Reactor products were primarily methane, with smaller amounts of ethane, BTX, light oils, and carbon-oxides.

Semiempirical correlations for predicting overall carbon conversion efficiency and carbon selectivity to gaseous products have been fitted to the bituminous, subbituminous, and lignite data using a computerized multiple-regression statistical analysis. The correlations and the results predicted from the correlations should be considered as preliminary, since the collected data are still being revised and updated by Rocketdyne, Cities Service, PERC, and Brookhaven.

2.2 REACTOR SCALABILITY AND OPERABILITY

The developed subbituminous coal correlations show that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar values of overall carbon conversion and carbon selectivity to gaseous products under comparable operating conditions. Therefore, the results of testing at Rocketdyne and Cities Service should be scalable to a PDU or commercial-size reactor, within the region investigated. Information with respect to the effect of hydrogen-to-coal ratio on reactor performance, however, could not be obtained from the collected data.

Reactor operability during the Rocketdyne 1/4- and 1-ton/hr testing and the Cities Service bench-scale testing has been good. The Rocketdyne tests, however, have been of relatively short duration (less than 10 minutes). Longer duration tests are required to demonstrate the operability of the Rocketdyne reactor system.

2.3 MECHANISM OF CARBON CONVERSION TO PRODUCTS

For bituminous coal, predicted overall carbon conversion increases with increasing gas temperature and predicted selectivity to gas increases with increasing temperature and residence time. The fact that predicted overall carbon conversion (or reactivity) is not a statistically significant function of residence time suggests that nearly all of the carbon conversion for bituminous coal occurs through devolatilization within a relatively short period of time in the reactor; i.e., there is little direct methanation of char. The fact that selectivity to gas is a significant function of residence time suggests that the initial higher (liquid) hydrocarbon products of devolatilization are cracked down to lower hydrocarbon products as gas residence time increases.

For subbituminous coal, predicted overall carbon conversion increases with increasing coal particle residence time and gas temperature. At high particle residence times, conversion increases with increasing hydrogen partial pressure; at low particle residence times, conversion decreases with increasing hydrogen partial pressure. This increase in overall carbon conversion with residence time suggests that conversion of carbon to products occurs throughout the length of the reactor. The reversal effects of pressure on carbon conversion suggests a two-step mechanism for hydrogasification: pyrolysis-controlled devolatilization at short residence time, and pressure-controlled hydrogenation of char at longer residence time.

For subbituminous coal, predicted selectivity to methane increases with increasing temperature and particle residence time. At high temperatures, methane selectivity increases with hydrogen partial pressure; at low temperatures, methane selectivity decreases with increasing hydrogen partial pressure. This increase in carbon selectivity to methane with increasing residence time suggests that for subbituminous coal, the initial higher hydrocarbon products of devolatilization and, perhaps, products of direct char hydrogenation are cracked down to methane as residence time increases.

The Cities Service lignite test program was conducted under both entrained-flow (high gas velocity) and free-fall (low gas velocity) reactor operating conditions. For entrained-flow operation, particle residence time is approximately equal to gas residence time; for free-fall operation, particle residence time is less than gas residence time. A statistical analysis of the Cities Service lignite data showed that overall carbon conversion was a significant function of particle, rather than gas, residence time.

For lignite coal, predicted overall carbon conversion increases with increasing gas temperature, particle residence time, and hydrogen partial pressure. The fact that overall conversion increases with residence time suggests that, as with subbituminous coal, conversion of carbon to products occurs throughout the length of the reactor.

For the Rocketdyne, Cities Service, and Brookhaven data, it was not possible to determine separately the effects of both hydrogen partial pressure and reactor pressure on carbon conversion. This is because the hydrogen partial pressure was nearly equal to reactor pressure for a majority of the tests; i.e., hydrogen partial pressure and reactor pressure are confounded. Additional data are required, with methane or inert gas addition to the reactor gas, to determine the separate effects of hydrogen partial pressure and total pressure on conversion.

A thermodynamic equilibrium computer model predicts that for the operating range used in the reactor systems, methane is the major hydrocarbon product present at equilibrium. Higher hydrocarbon products, such as ethane, ethylene, or benzene, are present only in trace amounts. Therefore, reactor systems that produce significant quantities of ethane or BTX are operating in a kinetically controlled regime, far removed from equilibrium.

The Rocketdyne, Cities Service, and Brookhaven data were generated within a regime that is controlled by the kinetics of carbon conversion to products. This is due primarily to the relatively large hydrogen-to-coal ratios (0.2 to 2.0 lb/lb) used in the testing. For these hydrogen-to-coal ratios, the predicted carbon conversion at equilibrium is 100 percent for all tests; i.e., at infinite residence time, all of the carbon in the coal would be converted to methane. It was not possible, therefore, to determine the effect of hydrogen-to-coal ratio on carbon conversion from the collected data. Additional data are required at lower hydrogen-to-coal ratios (0.05 to 0.3 lb/lb) to determine this effect.

The carbon conversion in the PERC reactor is controlled by the thermodynamic equilibrium between the carbon in the coal (or char) and the reaction products. This is due in large part to the relatively high gas residence times (75 to 220 seconds) and low hydrogen-to-coal ratios (0.03 to 0.12 lb/lb) used in the testing. At these low hydrogen-to-coal ratios, the predicted carbon conversion at equilibrium (at infinite residence time) for the PERC tests was between 40 and 65 percent with lignite coal and between 15 and 35 percent with bituminous coals. As expected, methane was the major hydrocarbon product.

2.4 COMPARISON BETWEEN COALS

Predicted overall carbon conversion (or reactivity) for bituminous coal is greater than the reactivity of subbituminous and lignite coals at reduced residence time and/or pressure. In addition, the reactivity of lignite coal is greater than that of subbituminous coal at increased temperature and increased pressure.

Subbituminous coal gives higher predicted gas selectivity than bituminous or lignite coals at low residence time and high temperature. At larger residence times, bituminous coal gives the highest predicted selectivity to gas.

2.5 OPERATING VARIABLE LEVELS FOR FULL-SCALE REACTOR DESIGN

Operating variable levels for a full-scale hydrogasification reactor have been selected and are based on the subbituminous coal data gathered in the Rocketdyne and Cities Service reactors and the reactor performance models fitted to the data. The conceptual full-scale hydrogasification stage has a configuration similar to the Rocketdyne reactor assembly, which incorporates an entrained-downflow tubular reactor chamber. Coal particles and hot hydrogen are mixed inside high-efficiency injector elements, producing coal heatup rates in excess of 500,000°F/sec.

An economic study has shown that the cost of SNG produced from the reactor facility decreases as carbon conversion in the hydrogasification stage increases. An overall carbon conversion of 50 percent was selected as the reactor design basis, since that value is close to the maximum conversion obtained to date in the Cities Service and Rocketdyne subbituminous coal testing and is above the char balance point. (At the char balance point, the quantity of unreacted char from the hydrogasification stage is just sufficient to produce the required process hydrogen in the hydrogen production stage.) A coal feed rate of 108 tons/hr was selected on the basis of a recommendation by Rocketdyne for a maximum coal capacity for a single injector element of 3 tons/hr and a maximum number of 36 injector elements per head.

A carbon selectivity to gas of 100 percent was selected as the reactor design basis by the DOE. A reactor design pressure of 1,500 psig was chosen because at pressures less than 1,500 psig, the predicted maximum reaction temperature required for 100 percent carbon selectivity to gas is greater than 1,900°F. (Temperatures greater than 1,900°F are considered excessive and are outside the range of the Cities Service and Rocketdyne subbituminous coal testing.) A hydrogen-to-coal ratio of 0.4 lb/lb was chosen since this value is within the lower range investigated by Rocketdyne.

From the fitted models, at a reactor pressure of 1,500 psig and at conditions of 50 percent overall carbon conversion and 100 percent carbon selectivity to gas, the predicted reactor exit gas temperature is 1,875°F and the predicted particle residence time is 1,100 milliseconds. The predicted carbon selectivity to methane and carbon monoxide are 86 and 13 percent, respectively.

2.6 CONCEPTUAL DESIGN FOR FULL-SCALE REACTOR

The hydrogasification reactor vessel consists of two sections. The upper section of the vessel contains a shell and tube heat exchanger, and the lower section includes a hydrogasifier and a cyclone separator. The hydrogasification reactor would have a length roughly between 10 and 30 feet, depending on the gas velocity.

In the hydrogasification section, hot hydrogen at 1,740°F is contacted with coal feed at 77°F in a total of 36 injector nozzles; each nozzle handles a maximum of 3 tons of coal per hour. The nozzles are arranged in single rank in a circle. Coal enters each through a central tube, and hot hydrogen enters through annular nozzles around the coal tubes.

Char and product gas flow downward in an entrained-flow manner through the annuli formed by the inner wall of the reactor vessel shell and the outer shell of a central pipe (or duct) through which the product gas leaves the hydrogasifier. The coal char solids and the gas stream are separated in a cyclone which sends the product gas stream back up through the central pipe or duct and sends the char downward through a cyclone dipleg. The char next collects in a surge volume section and is held there as a feed material for hydrogen production. The cyclone is constructed so that it can be moved vertically and hence could be used to control the residence time of char and gas inside the reactor. A gas or water quench system is also installed near the bottom of the central pipe to provide an extra or standby facility for quickly controlling the reaction, if necessary.

Product gas from the hydrogasifier cyclone flows upwards through the tube side of a shell and tube heat exchanger, where it is cooled from about 1,875°F to about 1,100°F by heat exchange with cold feed hydrogen flowing downward through the exchanger shell side. The hydrogen stream is assumed to enter at 100°F and is heated to about 1,000°F. The hydrogen effluent from the exchanger is further heated to about 1,740°F by combustion with oxygen, which is injected into the hydrogen stream near the exchanger outlet.

Section 3

OBJECTIVES AND SCOPE

The program, "An Analysis of Coal Hydrogasification Processes," was performed for the Department of Energy (DOE) by Bechtel Corporation under DOE Contract No. EF-77-A-01-2565. Work on this program was initiated on February 1, 1977 and was concluded on April 30, 1978.

The major objective of the program was "to conduct an analytical study which will investigate the operability potential and scaleup feasibility of the Cities Service, Rocketdyne, and Pittsburgh Energy Research Center (PERC) coal hydrogasification processes, relative to DOE plans for a hydrogasification process development unit (PDU)." To accomplish the objective, four sequential program tasks were established.

The primary objective of Task I was to conduct a survey of information in the public domain relating to the above three hydrogasification processes. This survey was supplemented with visits to the process contractors for discussion, expansion, and updating.

The primary objective of Task II was to perform a detailed analysis of the data, as required to evaluate the information for a pilot plant application. Consideration was given to reactor heat and mass balances, reaction kinetics, actual or predicted data on the product gas yield and composition, and all other relevant factors. In addition, conceptual designs, where available, were analyzed for potential operational problems and scaling.

Task III had two primary objectives: (1) to perform a reactor model study, where available data permit, for each of the three processes; and (2) to generate a conceptual, full-scale, reactor design in consultation with DOE. The reactor model study attempted to predict, where possible, overall carbon conversion, carbon selectivity to gas, and carbon selectivity to methane for the three processes. In conjunction with the modeling study, a sensitivity analysis was performed to determine the influence of the degree of uncertainty of the basic information used in the prediction of reactor performance.

The primary objectives of Task IV were to: (1) identify critical data gaps and point out specific data that are missing and are required for reliable pilot plant design; (2) recommend experiments to acquire the necessary data, and estimate the number of experiments and manhours needed to obtain these data; and (3) assess the impact on the process design phase, in case the necessary data cannot be experimentally determined.

Section 4

DATA COLLECTION AND ANALYSIS

Bechtel has collected and analyzed bituminous, subbituminous, and lignite coal hydrogasification and hydropyrolysis data from Rocketdyne, Cities Service, PERC, and Brookhaven National Laboratory. The data have been entered into a computerized data base for ease of evaluation and tabulation. A computer listing of all of the data contained in the data base is presented in Appendix A. Properties of the coals used in the testing are given in Appendix B.

Owing to the period of performance for this program, no data received after February 1978 were entered into the data base for evaluation. Moreover, the data and analyses presented in this section should be considered as preliminary, since a portion of the data is still being revised and updated by Rocketdyne, Cities Service, PERC, and Brookhaven.

The subject matter discussed in this section fulfills the contractual requirements for Tasks I and II.

4.1 ROCKETDYNE DATA COLLECTION AND ANALYSIS

Rocketdyne is performing experimental studies on hydrogasification and hydropyrolysis (partial liquefaction) of bituminous and subbituminous coals in two entrained-downflow tubular reactor systems of 1/4- and 1-ton/hr coal capacity. The units are designed to feed coal at design temperatures as high as 2,000°F and pressures as high as 1,500 psi.

Coal particles and hot (1,500°F to 3,000°F) hydrogen gas are mixed inside a high-efficiency injector element, which produces coal heatup rates in excess of 500,000°F/sec. The hydrogen gas is heated first in a fired heat exchanger, then by partial combustion through oxygen addition in a preburner. A water spray quenches the reaction. More detailed descriptions of the reactor systems have been given by Gray[8] and by Oberg.[9]

Computer listings of selected Rocketdyne partial liquefaction and hydrogasification data from January 1977 through January 1978 are presented in Tables 4-1 and 4-2, respectively. A computer listing of all of the Rocketdyne data contained in the data base is found in Appendix A. Properties of the bituminous and subbituminous coals tested are given in Appendix B.

Rocketdyne has calculated overall carbon conversions from the feed coal and main char assay data. The quantity of char was calculated, however, by forcing an ash balance between the coal and char. Conversion to gas was obtained from gas flow rate and gas composition measurements. (Recently, conversion to gas has been calculated by forcing a carbon balance between the coal, char, and reaction products. This will be discussed further in Subsections 4.1.2 and 4.1.3.) Conversion to liquid products was derived from information concerning light oils collected in the product condenser, condensible hydrocarbons (BTX and higher hydrocarbons) in the gas samples, and benzene extractables in the chars.

Bechtel has calculated conversion and selectivity to reaction products from the measured gas and liquid compositions, where available, and the measured total conversions to gas and liquid. Not enough information was available to calculate carbon conversion and selectivity to hydrocarbon and carbon-oxide gases for the partial liquefaction tests (Table 4-1), or to light oil and BTX for the hydrogasification tests (Table 4-2).

4.1.1 Partial Liquefaction Program — Bituminous Coal

The Rocketdyne bituminous coal partial liquefaction test program is being conducted under DOE Contract EX-76-C-01-2044. The reported data (Runs 5

Table 4-1

ROCKETDYNE PARTIAL LIQUEFACTION DATA
FOR BITUMINOUS COALS

RUN DESIG-NATION	DATE	COAL* TYPE	REACTOR	OVERALL FRACTION CARBON CONVERTED	CARBON SELEC-TIVITY TO GAS	CARBON SELEC-TIVITY TO METHANE	CARBON SELEC-TIVITY TO ETHANE	CARBON SELEC-TIVITY TO BTX	OUTLET GAS TEMP (DEG F)	REACTOR PRESSURE (PSIG)	HYDROGEN PARTIAL PRESSURE (PSIG)	GAS VEL-OCITY (FT/SEC)	GAS RESI-DENCE TIME (MSEC)	HYDROGEN TO COAL RATIO (LB/LB)	MEAN PARTICLE SIZE (MICRONS)
5	1/31/77	BTM-1	1 TPH	.382					1290.	1000.	940.	32.30	155.	.250	56.
6	2/ 3/77	BTM-1	1 TPH	.542	0.397			.089	1700.	1000.	930.	39.70	126.	.478	56.
7	2/ 7/77	BTM-1	1 TPH	.615	0.483			.013	1950.	1000.	920.	42.00	119.	.775	56.
8	2/17/77	BTM-1	1 TPH	.596	0.485			.089	1690.	1000.	920.	18.20	274.	.365	56.
9	2/22/77	BTM-1	1 TPH	.645	0.760			.002	1880.	1500.	1390.	12.20	410.	.365	56.
10	3/ 1/77	BTM-1	1 TPH	.609	0.782			.056	1570.	1500.	1400.	10.20	490.	.314	56.
11	3/ 4/77	BTM-1	1 TPH	.627	0.968			.027	1650.	1500.	1420.	7.90	634.	.334	56.
12	3/ 9/77	BTM-1	1 TPH	.576	0.672			.123	1680.	1000.	940.	11.80	424.	.333	56.
13	3/23/77	BTM-1	1 TPH	.560	0.334			.055	1720.	1000.	930.	79.40	63.	.292	56.
14	3/25/77	BTM-1	1 TPH	.597	0.472			.097	1770.	1500.	1400.	51.00	98.	.397	56.
15	3/29/77	BTM-1	1 TPH	.560	0.359			.066	1660.	700.	650.	111.00	45.	.403	56.
16	4/ 4/77	BTM-1	1 TPH	.573	0.412			.058	1690.	1000.	930.	72.50	69.	.443	56.
17		BTM-1	1 TPH	.592	0.434			.083	1740.	1010.	940.	78.10	64.	.507	56.
18		BTM-1	1 TPH	.519	0.343			.071	1630.	1000.	930.	74.60	67.	.409	56.
19		BTM-1	1 TPH	.562	0.256			.034	1590.	520.	480.	147.00	34.	.429	56.
20		BTM-2	1 TPH	.540	0.341			.085	1600.	1000.	930.	63.30	79.	.293	52.
21		BTM-2	1 TPH	.590	0.403			.132	1690.	1000.	930.	78.10	64.	.458	52.
22		BTM-2	1 TPH	.570	0.389			.047	1630.	500.	470.	87.70	57.	.370	52.
23		BTM-2	1 TPH	.600	0.355			.120	1640.	1000.	930.	79.40	63.	.469	36.
24		BTM-2	1 TPH	.638	0.434			.172	1770.	1000.	930.	82.00	61.	.528	36.
25		BTM-2	1 TPH	.630	0.365			.154	1920.	1000.	930.	41.30	121.	.656	36.
26	9/ 9/77	BTM-2	1 TPH	.615	0.382			.122	1720.	1000.	940.	39.10	128.	.485	36.
27	9/14/77	BTM-2	1 TPH	.571	0.366			.095	1610.	1000.	950.	37.30	134.	.472	36.
28	9/16/77	BTM-2	1 TPH	.587	0.433			.123	1770.	1000.	940.	39.70	126.	.491	52.
29	9/21/77	BTM-2	1 TPH	.576	0.477			.151	1720.	1500.	1400.	23.60	212.	.418	52.
30	9/23/77	BTM-2	1 TPH	.546	0.441			.097	1630.	1000.	940.	36.80	136.	.435	52.
31	9/27/77	BTM-2	1 TPH	.628	0.712			.135	1940.	1500.	1400.	23.90	209.	.505	52.
32	9/29/77	BTM-2	1 TPH	.622	0.441			.138	1840.	1000.	930.	39.40	127.	.452	52.
34	10/ 4/77	BTM-2	1 TPH	.479	0.378			.071	1530.	1000.	940.	75.80	66.	.414	52.
37	10/31/77	BTM-2	1 TPH	.482	0.427			.083	1570.	1000.	940.	19.60	255.	.304	52.
38	11/ 8/77	BTM-2	1 TPH	.462	0.329				1410.	1000.	950.	18.50	271.	.313	52.
39	11/ 9/77	BTM-2	1 TPH	.513	0.468			.105	1660.	1000.	940.	20.20	247.	.296	52.
40	11/10/77	BTM-2	1 TPH	.481	0.486			.098	1590.	1000.	950.	22.20	225.	.279	52.
41	11/11/77	BTM-2	1 TPH	.432	0.382			.049	1430.	1000.	950.	20.90	239.	.243	52.
42	11/14/77	BTM-2	1 TPH	.518	0.502			.139	1690.	1000.	950.	23.60	212.	.249	52.

*BTM-1 is Kentucky #9/14 bituminous HvCb coal from the Colonial Mine of the Pittsburgh and Midway Mining Co.

BTM-2 is Kentucky #9 bituminous HvAb coal from the Hamilton No. 2 Mine of the Island Creek Coal Co.

Table 4-2

ROCKETDYNE HYDROGASIFICATION DATA
FOR BITUMINOUS AND SUBBITUMINOUS COALS

RUN DESIG-NATION	DATE	COAL* TYPE	REACTOR	OVERALL FRACTION CARBON CONVERTED	CARBON SELEC-TIVITY TO GAS	CARBON SELEC-TIVITY TO METHANE	CARBON SELEC-TIVITY TO ETHANE	CARBON SELEC-TIVITY TO BTX	OUTLET GAS TEMP (DEG F)	REACTOR PRESSURE (PSIG)	HYDROGEN PARTIAL PRESSURE (PSIG)	GAS VEL-OCITY (FT/SEC)	GAS RESI-DENCE TIME (MSEC)	HYDROGEN TO COAL RATIO (LB/LB)	MEAN PARTICLE SIZE (MICRONS)
011- 7	9/21/77	BTM-1	1/4 TPH	.473	0.421	.317	.044		1670.	1000.	950.	24.40	615.	.356	
011- 8	9/29/77	BTM-1	1/4 TPH	.535	0.583	.492	.009		1810.	1010.	950.	31.60	475.	.421	
011- 9	10/ 4/77	BTM-1	1/4 TPH	.588	0.724	.655	.002		1960.	1500.	1420.	21.60	695.	.499	
011-10	10/ 7/77	BTM-1	1/4 TPH	.588	0.707	.643	.0		1910.	1490.	1410.	21.70	690.	.506	
300- 2	1/ 6/78	BTM-3	1/4 TPH	.707	0.973	.885	.0		1980.	1500.	1310.	10.20	1465.	.643	
300- 3	1/ 9/78	BTM-3	1/4 TPH	.500	0.872	.648	.092		1600.	990.	870.	13.60	1100.	.342	
300- 4	1/11/78	BTM-3	1/4 TPH	.595	0.827	.687	.062		1860.	1000.	870.	14.90	1010.	.509	
300- 5	1/16/78	BTM-3	1/4 TPH	.480	0.775	.477	.194		1470.	990.	900.	12.80	1170.	.548	
300- 6	1/17/78	BTM-2	1/4 TPH	.627	0.903	.831	.003		1820.	1490.	1280.	10.00	1500.	.469	
300-11	2/10/78	BTM-2	1/4 TPH	.644	0.961	.882	.002		1910.	1500.	1320.	15.90	945.	.519	
300-12	2/16/78	BTM-2	1/4 TPH	.650	0.992	.915	.0		1910.	1500.	1320.	4.39	3415.	.489	
011- 2	8/30/77	SUBBTM	1/4 TPH	.289	0.495	.246	.118		1470.	1020.	960.	25.00	600.	.592	
011- 4	9/ 9/77	SUBBTM	1/4 TPH	.361	0.837	.640	.006		1900.	990.	930.	28.00	535.	.512	
011- 5	9/15/77	SUBBTM	1/4 TPH	.364	0.629	.451	.036		1730.	1000.	940.	26.10	575.	.401	
011-11	10/14/77	SUBBTM	1/4 TPH	.436	0.991	.819	.002		1840.	1500.	1410.	22.10	680.	.569	
011-12	10/18/77	SUBBTM	1/4 TPH	.392	0.714	.423	.140		1590.	1500.	1430.	18.60	805.	.559	
011-13	10/21/77	SUBBTM	1/4 TPH	.321	0.692	.330	.206		1470.	1500.	1440.	19.10	785.	.535	
011-14	10/28/77	SUBBTM	1/4 TPH	.278					1560.	1010.	790.	28.47	527.	.418	
011-15	11/ 2/77	SUBBTM	1/4 TPH	.298					1710.	1130.	840.	22.69	661.	.331	
011-16	11/21/77	SUBBTM	1/4 TPH	.470	1.000	.872	.0		1760.	1480.	1390.	10.60	1420.	.550	
011-17	11/28/77	SUBBTM	1/4 TPH	.407	0.860	.627	.081		1530.	1500.	1430.	8.70	1725.	.576	
011-22	12/14/77	SUBBTM	1/4 TPH	.354	0.867	.675	.003		1760.	1000.	880.	13.60	1105.	.392	
011-23	12/19/77	SUBBTM	1/4 TPH	.292	0.849	.384	.243		1420.	990.	900.	12.90	1165.	.364	
011-24	12/21/77	SUBBTM	1/4 TPH	.382	0.911	.725	.0		1800.	1000.	890.	15.40	975.	.705	
300- 1	1/ 4/78	SUBBTM	1/4 TPH	.459	0.935	.780	.0		1830.	1500.	1310.	10.60	1420.	.675	

*BTM-1 is Kentucky #9/14 bituminous HvCb coal from the Colonial Mine of the Pittsburgh and Midway Mining Co.

BTM-2 is Kentucky #9 bituminous HvAb coal from the Hamilton No. 2 Mine of the Island Creek Coal Co.

BTM-3 is Illinois #6 bituminous HvCb coal.

SUBBTM is Montana Rosebud subbituminous coal.

through 42 in Table 4-1)[9,10] were generated in the 1-ton/hr reactor facility. The coals tested were a Kentucky bituminous #9/14 HvCb and a Kentucky bituminous #9 HvAb.

The partial liquefaction tests were conducted at reactor outlet gas temperatures of 1,290°F to 1,950°F, particle (or gas) residence times of 61 to 634 milliseconds, and reactor pressures of 520 to 1,500 psig. Overall carbon conversion varied from 38 to 65 percent; carbon selectivity to gas varied from 25 to 97 percent. The maximum carbon conversion of 65 percent (Run 9) was obtained at a reactor exit gas temperature of 1,880 °F and a residence time of 212 milliseconds. The maximum selectivity to gas of 97 percent (Run 11) was obtained at an exit gas temperature of 1,650°F and a residence time of 634 milliseconds.

A summary of carbon and hydrogen mass balances for Runs 5 through 24 has been given by Oberg.[9] The quantity of char for each run was calculated by requiring an ash balance between the coal and char. For Runs 5 through 16, the carbon and hydrogen in the liquid components were obtained by difference; for Runs 17 through 24, the actual measured liquid compositions were used in the mass balances. The carbon and hydrogen material balances for Runs 17 through 24 ranged from 88 to 101 percent and 93 to 115 percent, respectively. It is assumed that most of the error in the carbon balances is due to errors in gas and liquid sampling and analysis. No ash balances were reported by Rocketdyne.

4.1.2 Hydrogasification Program — Bituminous Coal

The Rocketdyne bituminous coal hydrogasification program is being conducted under DOE Contract EX-77-C-01-2518. The reported data (Runs 011-7 through 300-12 in Table 4-2)[11,12,13] were generated in the 1/4-ton/hr reactor system. The bituminous coals tested were a Kentucky #9/14 HvCb, a Kentucky #9 HvAb, and an Illinois #6 HvCb. Properties of the coals are given in Appendix B.

The bituminous coal tests were conducted at reactor outlet gas temperatures of 1,600°F to 1,980°F, particle (or gas) residence times of 475 to 3,415 milliseconds, and reactor pressures of 991 to 1,500 psig. Overall carbon conversion varied from 47 to 71 percent; carbon selectivity to gas varied from 42 to 99 percent. The maximum carbon conversion of 71 percent (Run 300-2) was obtained at a reactor gas temperature of 1,980°F and a residence time of 1,465 milliseconds. The maximum selectivity to gas of 99 percent (Run 300-12) was obtained at an exit gas temperature of 1,910°F and a residence time of 3,415 milliseconds.

Probable uncertainties in the values for carbon conversion for bituminous Runs 011-7, 8, 9, and 10 have been mentioned by Rocketdyne;[14] these uncertainties stem mainly from the relatively short durations (approximately 3 minutes) of the tests, which, owing to operational problems, had all been terminated prematurely. For these tests, marked variations occurred among the product gas samples taken at various time intervals, and an average of these samples was used to calculate the conversions.

Poor overall carbon balances, ranging from 80 to 85 percent, were reported by Rocketdyne for bituminous Runs 011-7, 8, 9, and 10.[11] "Unaccounted-for" carbon conversion in the gas and/or liquid, therefore, ranged from 15 to 20 percent. (It is assumed that the carbon in the char, which is calculated by forcing an ash balance, is correct.)

From August to November 1977, Rocketdyne determined the conversion to gas for each test from the average gas composition and flow rate. It was assumed that any "unaccounted-for" carbon conversion represented entrained liquids in the product gas.[11] As mentioned previously, carbon balances during that period were poor. In January 1978, Rocketdyne revised its procedure for determining gas and liquid product conversion by assuming that all "unaccounted-for" carbon was distributed in the product gas, rather than relying on the metered gas flow rate.[12] This revised procedure is consistent with the calculation used by Cities Service to determine gas and liquid carbon conversions (see Subsection 4.2).

To date, Rocketdyne has presented gas and liquid product conversion data based on the revised procedure only for bituminous Runs 300-2 through 300-12.[12,15] Corrected values for the preceding 011-series tests (Runs 011-7 through 011-10) will be reported by Rocketdyne in the near future.

4.1.3 Hydrogasification Program — Subbituminous Coal

The Rocketdyne Montana Rosebud subbituminous coal hydrogasification program is also being conducted under DOE Contract EX-77-C-01-2518, in the 1/4-ton/hr reactor facility. The reported tests (Runs 011-2 through 300-1 in Table 4-2)[11,12] were conducted at reactor outlet gas temperatures of 1,420°F to 1,900°F, particle (or gas) residence times of 527 to 1,725 milliseconds, and reactor pressures of 987 to 1,500 psig.

Overall carbon conversion for the tests ranged from 28 to 47 percent; carbon selectivity to gas ranged from 50 to 100 percent. The maximum carbon conversion of 47 percent and carbon selectivity to gas of 100 percent were obtained in Run 011-16 at a reactor temperature of 1,756°F and a particle residence time of 1,420 milliseconds.

Methane was mixed with the hydrogen gas stream fed to the reactor in subbituminous coal Runs 011-14 and 011-15 to simulate the recycle of raw product gases. Since the measured reactant flow rates and product gas analyses for the two runs were inconsistent with C, H, and O material balances,[11] the results obtained from these two tests are uncertain. Significant fluctuations in reactor flows, particularly in Run 011-14, remain essentially unexplained.

Probable uncertainties in the values for carbon conversion for subbituminous Runs 011-2, 4, and 5 have been mentioned by Rocketdyne.[11] As with the bituminous tests discussed in Subsection 4.1.2, these uncertainties stem mainly from the relatively short durations (approximately 3 minutes) of the tests, which, owing to operational problems, had all been terminated prematurely.

Relatively poor overall carbon balance of about 90, 108, 112, and 114 percent have been reported by Rocketdyne[11,12] for subbituminous Runs 011-5, 22, 24, and 300-1, respectively. No values were reported for Runs 011-14 and 15. The remaining eight subbituminous tests had relatively good carbon material balances ranging from 95 to 105 percent, i.e., "unaccounted-for" gas and/or liquid carbon conversion from 5 to -5 percent. No ash balances have been reported for the subbituminous tests.

As mentioned in Subsection 4.1.2, Rocketdyne revised its procedure for determining gas and liquid product conversion in January 1978. This was done by forcing a carbon balance between the coal, char, and gaseous products.[12] Subbituminous coal data using this revised procedure have been received only for Runs 011-22, 23, 24, and 300-01.[12] Corrected values for the preceding 011-series tests (011-2 through 17) will be reported by Rocketdyne in the near future. It should be noted, however, that the corrections for the earlier 011-series tests will all be less than about 5 percent gas conversion, except for Run 011-5, which will have a correction of about 10 percent conversion to gas.

4.2 CITIES SERVICE DATA COLLECTION AND ANALYSIS

Cities Service has performed experimental studies on hydrogasification of a subbituminous coal and hydropyrolysis (rapid hydrogenation) of a lignite coal. The bench-scale system incorporates an entrained-downflow tubular reactor that is designed to feed coal at up to 5 lb/hr at design temperatures up to 1,700°F and pressures up to 3,000 psi.

Preheated hydrogen and coal are mixed inside a high-velocity coaxial injector nozzle to produce coal heating rates in excess of 100,000°F/sec. The mixture then passes through the reactor tube, which is electrically heated through the walls to maintain adiabatic operation. An injected stream of cryogenically cooled hydrogen at the reactor outlet quenches the reaction. A more detailed description of the reactor system has been given by Combs and Greene.[6]

Computer listings of selected Cities Service hydropyrolysis and hydrogasification data from 1975 through December 1977 are presented in Tables 4-3 and 4-4, respectively. A computer listing of all of the Cities Service data contained in the data base is presented in Appendix A. Properties of the coals tested are given in Appendix B.

Cities Service has calculated overall carbon conversion for each test from the measured quantities of carbon in the coal and char. For these tests, the char production rate was measured directly; i.e., a forced ash balance was not required. Conversion to gas and liquids was determined by assuming that all "unaccounted-for" carbon was distributed in the product gas. Conversion to liquid products was obtained from measurements of light oils collected in the product condenser and heavier hydrocarbons analyzed in the gas samples.

4.2.1 Hydrogenation Program — Lignite Coal

Cities Service has conducted company-funded, bench-scale, rapid-hydrogenation tests with a North Dakota lignite coal. These tests have focused on the production of high-value aromatic liquids and methane. Results from some of the tests (Runs 1 through 25 in Table 4-3) have been reported by Rocketdyne[16] as part of DOE Contract EX-77-C-01-2518. Properties of the lignite coal are given in Appendix B.

The lignite tests used five different reactors, which were chosen to accommodate the desired residence times and feed flow rates. Four of the reactors were entrained-flow (EF) reactors; three of these were helical tubes with diameter-length combinations of 1/2 inch by 20 feet, 1/4 inch by 60 feet, and 3/8 inch by 63 feet; the fourth was a 1-inch-diameter vertical tube 4 feet in length. The fifth reactor was a free-fall (FF), vertical, 1-inch-diameter tube with quench probes at various lengths.

The lignite tests were conducted at reactor outlet gas temperatures of 1,000°F to 1,660°F, particle residence times of 70 to 6,290 milliseconds, gas residence times of 70 to 24,900 milliseconds, and reactor pressures of 300 to 2,000 psig. Overall carbon conversion ranged from 20 to 49 percent; selectivity to gas ranged from 60 to 83 percent. Results from Run 8 have not been included, since Cities Service has reported[17] that possible temperature excursions may have occurred.

Gas, liquid, and char analyses for each of the 25 Cities Service lignite tests have not been made available. Cities Service has reported,[18] however, a poor carbon balance of 60 to 70 percent for Runs 1 to 6 and a greatly improved carbon balance of 92 to 97 percent for Runs 7 to 25.

4.2.2 Hydrogasification Program — Subbituminous Coal

Cities Service has conducted bench-scale hydrogasification tests with Montana Rosebud subbituminous coal as part of the Rocketdyne DOE Contract EX-77-C-01-2518. The tests employed a number of helical and vertical entrained-flow (EF) reactors designed to accommodate the desired residence times and feed flow rates.

Table 4-3

CITIES SERVICE HYDROGENATION DATA
FOR LIGNITE COAL

RUN DESIGNATION	DATE	COAL TYPE	REACTOR	OVERALL FRACTION CARBON CONVERTED	CARBON SELECTIVITY TO GAS	CARBON SELECTIVITY TO METHANE	CARBON SELECTIVITY TO ETHANE	CARBON SELECTIVITY TO BTX	OUTLET GAS TEMP (DEG F)	REACTOR PRESSURE (PSIG)	HYDROGEN PARTIAL PRESSURE (PSIG)	GAS VELOCITY (FT/SEC)	GAS RESIDENCE TIME (MSEC)	HYDROGEN TO COAL RATIO (LB/LB)	MEAN PARTICLE SIZE (MICRONS)
1	1975-6	LIGNITE	FF*	.472	0.650			.286	1580.	1500.	1500.	0.49	6300.	1.400	175.
2	1975-6	LIGNITE	FF	.434					1500.	1500.	1500.	0.46	6600.	1.300	250.
3	1975-6	LIGNITE	FF	.366	0.645	.243	.197	.276	1480.	1500.	1500.	0.50	3000.	1.300	200.
4	1975-6	LIGNITE	FF	.377	0.602	.276	.196	.263	1430.	1500.	1500.	0.45	6800.	1.600	470.
5	1975-6	LIGNITE	FF	.323	0.666	.300	.183	.232	1500.	750.	750.	0.90	1700.	1.200	200.
6	1975-6	LIGNITE	FF	.435	0.703	.345	.214	.195	1510.	1500.	1500.	0.40	7700.	0.900	190.
7	1975-6	LIGNITE	FF	.369	0.732	.382	.157	.206	1620.	580.	580.	1.70	1800.	1.400	190.
8	1975-6	LIGNITE	FF	.816	0.825	.635	.089	.162	1480.	2960.	2960.	0.20	14700.	1.000	190.
9	1975-6	LIGNITE	EF	.429	0.758	.361	.226	.203	1530.	1000.	1000.	7.70	2400.	2.000	190.
10	1975-6	LIGNITE	FF	.374	0.768	.382	.160	.152	1460.	1500.	1500.	0.30	10400.	0.480	190.
11	1975-6	LIGNITE	FF	.430	0.815	.498	.109	.102	1540.	1500.	1500.	0.12	24700.	0.180	56.
12	1975-6	LIGNITE	FF	.492	0.834	.482	.110	.205	1490.	2000.	2000.	0.28	10800.	0.900	190.
13	1975-6	LIGNITE	FF	.326	0.684	.273	.156	.126	1510.	1000.	1000.	0.74	1300.	1.200	190.
14	1975-6	LIGNITE	EF	.383	0.710	.337	.154	.188	1570.	1000.	1000.	77.50	800.	1.200	190.
15	1975-6	LIGNITE	EF	.479	0.791	.532	.109	.207	1620.	1500.	1500.	24.00	2500.	1.000	190.
16	1975-6	LIGNITE	EF	.310	0.803	.423	.123	.177	1620.	500.	500.	58.30	1000.	1.300	150.
17	1975-6	LIGNITE	EF	.442	0.743	.380	.156	.208	1530.	1000.	1000.	6.70	3000.	1.500	150.
18	1975-6	LIGNITE	EF	.443	0.670	.255	.153	.108	1320.	1500.	1500.	23.50	2500.	1.600	150.
19	1975-6	LIGNITE	EF	.327	0.719	.156	.128	.092	1480.	1000.	1000.	46.60	90.	2.300	109.
20	1975-6	LIGNITE	FF	.197	0.726	.096	.076	.046	1000.	1000.	1000.	0.17	24900.	0.170	109.
21	1975-6	LIGNITE	EF	.331	0.662	.202	.142	.069	1550.	1000.	1000.	48.90	70.	1.200	109.
22	1975-6	LIGNITE	EF	.343	0.819	.449	.082	.157	1620.	300.	300.	44.60	1300.	1.500	109.
23	1975-6	LIGNITE	EF	.341	0.716	.264	.152	.138	1660.	1000.	1000.	58.00	70.	2.400	161.
24	1975-6	LIGNITE	EF	.321	0.745	.305	.171	.181	1600.	1000.	1000.	13.80	290.	1.900	161.
25	1975-6	LIGNITE	EF	.369	0.721	.279	.157	.125	1590.	1000.	1000.	57.30	70.	5.100	63.

*FF refers to a free-fall reactor; EF refers to an entrained-flow reactor.

Table 4-4

CITIES SERVICE HYDROGASIFICATION DATA
FOR SUBBITUMINOUS COAL

RUN DESIG- NATION	DATE	COAL TYPE	REACTOR	OVERALL FRACTION CARBON CONVERTED	CARBON SELEC- TIVITY TO GAS	CARBON SELEC- TIVITY TO METHANE	CARBON SELEC- TIVITY TO ETHANE	CARBON SELEC- TIVITY TO BTX	OUTLET GAS TEMP (DEG F)	REACTOR PRESSURE (PSIG)	HYDROGEN PARTIAL PRESSURE (PSIG)	GAS VEL- OCITY (FT/SEC)	GAS RESI- DENCE TIME (MSEC)	HYDROGEN TO COAL RATIO (LB/LB)	MEAN PARTICLE SIZE (MICRONS)
MR- 4	6/13/77	SUBBTM	EF	.390					1520.	500.	500.	20.90	1530.	1.400	45.
MR- 1	6/16/77	SUBBTM	EF	.319	0.837	.266	.216	.107	1520.	500.	500.	9.00	433.	0.760	45.
MR-10	6/22/77	SUBBTM	EF	.214	0.593	.182	.150	.093	1500.	1500.	1500.	9.40	423.	0.830	45.
MR-13	6/27/77	SUBBTM	EF	.397	0.710	.370	.209	.134	1530.	1500.	1500.	16.60	1090.	0.800	45.
MR-14	6/29/77	SUBBTM	EF	.431	0.814	.513	.146	.121	1630.	1500.	1500.	17.00	1060.	0.740	45.
MR-28	7/ 6/77	SUBBTM	EF	.275	0.724	.247	.204	.065	1530.	1000.	1000.	12.80	307.	0.790	45.
MR-29	7/ 8/77	SUBBTM	EF	.344	0.773	.340	.235	.125	1630.	1000.	1000.	12.80	307.	0.990	45.
MR-30	7/12/77	SUBBTM	EF	.324	0.772	.401	.204	.173	1710.	1000.	1000.	12.30	321.	0.850	45.
MR-11	7/15/77	SUBBTM	EF	.255	0.718	.298	.224	.114	1610.	1500.	1500.	13.00	303.	0.780	56.
MR-12	7/19/77	SUBBTM	EF	.321	0.726	.330	.231	.156	1660.	1500.	1500.	12.60	312.	0.750	56.
MR-25	7/21/77	SUBBTM	EF	.359	0.710	.331	.234	.178	1520.	1000.	1000.	16.60	1090.	0.980	56.
MR-26	7/25/77	SUBBTM	EF	.382	0.780	.458	.170	.217	1620.	1000.	1000.	16.50	1090.	0.880	56.
MR-27	7/27/77	SUBBTM	EF	.402	0.794	.585	.057	.206	1700.	1000.	1000.	16.40	1100.	0.930	56.
MR-15	7/29/77	SUBBTM	EF	.453	0.775	.541	.102	.216	1660.	1500.	1500.	16.40	1100.	0.870	56.
MR- 2	8/ 3/77	SUBBTM	EF	.339	0.770	.327	.224	.156	1610.	500.	500.	29.40	318.	0.890	56.
MR- 3	8/ 5/77	SUBBTM	EF	.330	0.797	.352	.109	.148	1710.	500.	500.	29.50	317.	0.970	56.
MR-16	8/ 8/77	SUBBTM	EF	.379	0.715	.256	.172	.127	1520.	1500.	1500.	14.30	653.	0.910	56.
MR-17	8/10/77	SUBBTM	EF	.430	0.765	.319	.153	.165	1600.	1500.	1500.	14.30	654.	1.240	56.
MR-18	8/12/77	SUBBTM	EF	.430	0.751	.316	.128	.191	1640.	1500.	1500.	14.20	656.	0.930	56.
MR-37	8/16/77	SUBBTM	EF	.334	0.784	.338	.168	.180	1540.	750.	750.	25.20	2300.	1.080	56.
MR-38	8/18/77	SUBBTM	EF	.414	0.754	.488	.065	.244	1650.	770.	770.	20.10	2860.	0.970	56.
MR-39	8/22/77	SUBBTM	EF	.455	0.809	.475	.009	.185	1730.	750.	750.	20.70	2770.	0.980	56.
MR- 5	8/24/77	SUBBTM	EF	.418					1630.	500.	500.	63.50	910.	1.230	56.
MR-20	9/15/77	SUBBTM	EF	.460	0.741	.352	.230	.220	1520.	1600.	1600.	18.10	3190.	0.910	56.
MR-21	9/20/77	SUBBTM	EF	.507	0.740	.438	.134	.252	1590.	1600.	1600.	17.80	3250.	0.940	56.
MR-22	9/22/77	SUBBTM	EF	.548	0.754	.471	.100	.243	1610.	1600.	1600.	17.60	3160.	0.920	56.
MR- 9	10/12/77	SUBBTM	EF	.456	0.686	.346	.206	.211	1520.	1600.	1600.	27.10	2130.	1.070	56.
MR-47	10/14/77	SUBBTM	EF	.478	0.713	.381	.186	.222	1570.	1600.	1600.	25.20	2268.	1.140	56.
MR-19	10/18/77	SUBBTM	EF	.516	0.715	.411	.149	.254	1610.	1600.	1600.	24.90	2310.	1.000	56.
MR-35	10/20/77	SUBBTM	EF	.412	0.709	.359	.189	.209	1550.	1000.	1000.	17.60	2780.	0.990	56.
MR-36	10/24/77	SUBBTM	EF	.473	0.702	.446	.074	.249	1640.	1000.	1000.	15.90	3508.	0.850	56.
MR-40	10/26/77	SUBBTM	EF	.506	0.759	.534	.024	.237	1690.	1000.	1000.	16.60	3365.	0.950	56.
MR-32	10/28/77	SUBBTM	EF	.456	0.706	.309	.217	.215	1540.	1000.	1000.	24.40	2320.	0.860	56.
MR-33	11/ 8/77	SUBBTM	EF	.465	0.671	.387	.084	.308	1650.	1000.	1000.	24.50	2320.	0.940	56.
MR-34	11/ 9/77	SUBBTM	EF	.462	0.658	.442	.028	.331	1690.	1000.	1000.	23.70	2400.	0.930	56.
MR-23	11/11/77	SUBBTM	EF	.426	0.681	.324	.192	.291	1540.	1000.	1000.	11.50	1540.	0.880	56.
MR-24	11/14/77	SUBBTM	EF	.409	0.741	.423	.093	.200	1650.	1000.	1000.	12.70	1400.	0.910	56.
MR-31	11/16/77	SUBBTM	EF	.447	0.747	.463	.022	.197	1720.	1000.	1000.	12.20	1450.	0.940	56.
MR- 6	11/18/77	SUBBTM	EF	.432	0.697	.319	.220	.162	1510.	1600.	1600.	12.30	1450.	0.850	56.
MR- 8	11/21/77	SUBBTM	EF	.465	0.710	.366	.187	.196	1600.	1600.	1600.	12.10	1460.	0.770	56.
MR- 7	11/22/77	SUBBTM	EF	.410	0.712	.359	.212	.207	1560.	1600.	1600.	12.10	1470.	0.810	56.
MR-48	12/14/77	SUBBTM	EF	.392	0.796	.482	.005	.179	1750.	500.	500.	16.40	3486.	0.890	56.

The reported subbituminous tests (Runs MR-4 through MR-48 in Table 4-4)[11,12] were conducted at reactor outlet gas temperatures of 1,500°F to 1,750°F, particle (or gas) residence times of 303 to 3,510 milliseconds, and reactor pressures of 500 to 1,600 psig. Overall carbon conversion ranged from 26 to 55 percent; carbon selectivity to gas ranged from 59 to 84 percent. The maximum carbon conversion of 55 percent was obtained in Run MR-22 at a gas temperature of 1,610°F, a residence time of 3,160 milliseconds, and a pressure of 1,600 psig.

Cities Service has reported[12] ash balances (and char balances, presumably) for the tests ranging from 85 to 112 percent. This indicates possible maximum errors of about ±13 percent in the measured overall carbon conversions. Cities Service has also reported[12] actual carbon balances ranging from 83 to 111 percent. As mentioned previously, Cities Service has assumed that all "unaccounted-for" carbon is distributed in the product gas.

Greene[12] has presented a series of plots for the Cities Service subbituminous data. These plots revealed that at larger residence times carbon conversion increases with increasing pressure, and at smaller residence times carbon conversion decreases with increasing pressure. The plots also showed that temperature and pressure interacted in the same manner as residence time and pressure.

With regard to the reversal effect of pressure on carbon conversion, Greene has postulated the following:[12]

> "The observations regarding the reversal effect of pressure on carbon conversion suggests a two-step mechanism of hydrogasification: pyrolysis-controlled devolatilization and pressure-controlled hydrogenation. During the initial pyrolysis stage, hydrocarbons are evolved from thermal cracking of bonds in the coal structure. The hydrogen fed to the reactor along with the coal has essentially no effect on the chemical reactions occurring in this stage of hydrogasification. In fact, increased hydrogen pressure retards the evolution of volatiles by inhibiting the diffusion of these products from the coal pores into the bulk gas phase. Thus, increasing the total pressure

of the gas increases the reaction time required for the pyrolysis products to escape from the particle. During this time, the hydrogen partial pressure within the pores of the coal particle is much lower than that of the bulk gas phase. Once the pyrolysis products have diffused into the bulk gas stream, hydrogen can counter-diffuse into the particle. At this point, the second stage of hydrogasification, namely, hydrogenation (or char methanation) predominates."

4.3 PERC DATA COLLECTION AND ANALYSIS

PERC involvement in the direct hydrogasification of coal to produce high-Btu gas dates back to the late 1950's and has led to the design of several laboratory reactors over a period of about 10 years. The design of these reactors was crucial to solving the major problem of direct processing of agglomerating raw coals to produce methane.

Since 1966, PERC has been performing an experimental study on the hydrogasification of various rank coals in a free-fall, dilute-phase, tubular reactor, 3.26 inches in diameter and 5 feet in length. The unit is designed to feed coal at up to 25 lb/hr at design temperatures as high as 1,800°F and pressures as high as 3,000 psi. Preheated hydrogen mixes with the coal, and the mixture falls through the electrically heated reactor tube.

A computer listing of selected data from PERC hydrogasification tests conducted since 1974 in the free-fall, dilute-phase reactor is presented in Table 4-5. A computer listing of all of the PERC data contained in the data base is given in Appendix A. The coals used during the testing were a high-volatile A bituminous (HvAb), a high-volatile C bituminous (HvCb), and a North Dakota lignite. Analyses of the coals are found in Appendix B.

The series of bituminous coal tests conducted during 1974 (Runs IHR-178 through IHR-163 in Table 4-5)[5] were of relatively short duration. Since 1974, PERC has conducted a number of longer duration tests (Runs 120 through 135B in Table 4-5)[19] with both bituminous and lignite coals, and has made progress toward reaching the goal of operating the free-fall reactor for extended periods. So far, the longest continuous reported operation has been 45 hours in Run 134.

Two sets of calculated overall carbon conversions are listed in Table 4-5: the first set was computed by Bechtel and was based on coal and product gas analyses; the second set was computed by PERC and was based on coal and char analyses. The two sets of calculations should give close results for runs with good carbon balance closures. Obviously, the calculated conversions based on gas and char do not agree well for a majority of the IHR runs, or for Runs 131 to 135A.

In Table 4-5, carbon selectivities to gaseous products were calculated by Bechtel from reported product gas analyses;[5,19] gas velocity was computed using the average of the reported inlet and outlet gas flow rates and the reactor cross-sectional area; and gas residence time was computed using the reactor heated length and the gas velocity. The mean hydrogen partial pressure was calculated from the logarithmic mean of the measured inlet and outlet hydrogen concentrations in the gas stream. Insufficient data were available to calculate carbon conversions and selectivities to liquid products.

No particle residence time data have been reported for the long-duration tests, since they appear to depend on the degree of backmixing and aerodynamic drag on the coal particles, which are still subjects of ongoing study and experiment at PERC. A range of 1 to 2 seconds was reported for the particle residence time for the earlier IHR runs.[5] It should be noted that PERC has reported only reactor wall temperatures (and not gas temperatures) for the tests.

The PERC tests have been conducted at reactor wall temperatures of 1,200°F to 1,650°F, gas residence times of 54 to 220 seconds, reactor pressures of 500 to 2,000 psig, and hydrogen-to-coal ratios of 0.03 to 0.14 lb/lb. For the long-duration tests, overall carbon conversion (based on the average of char and gas analysis) ranged from about 39 to 54 percent, whereas selectivity to gas ranged from 83 to 100 percent. As will be shown in Subsection 5.3, at the relatively low hydrogen-to-coal ratios and relatively high gas residence times employed in the PERC tests, the overall carbon conversion is controlled by the thermodynamic equilibrium between the carbon in the coal and the reaction products (primarily methane and carbon oxides).

Table 4-5

PITTSBURGH ENERGY RESEARCH CENTER
HYDROGASIFICATION DATA

RUN DESIG-NATION	DATE	COAL* TYPE	OVERALL FRACTION CARBON CONVERTED BASED ON GAS ANALYSIS	OVERALL FRACTION CARBON CONVERTED BASED ON CHAR ANALYSIS	CARBON SELEC-TIVITY TO GAS	CARBON SELEC-TIVITY TO METHANE	CARBON SELEC-TIVITY TO ETHANE	REACTOR WALL TEMP (DEG F)	REACTOR PRESSURE (PSIG)	MEAN HYDROGEN PARTIAL PRESSURE (PSIG)	GAS VEL-OCITY (FT/SEC)	GAS RESI-DENCE TIME (SEC)	HYDROGEN TO COAL RATIO (LB/LB)
IHR-178	1974	BTM-1	.135	.281	0.473	0.420	0.025	1470.	1000.	853.	.0401	124.7	.0718
IHR-167	1974	BTM-1	.141	.250	0.556	0.488	0.040	1470.	1000.	368.	.0420	119.1	.0298
IHR-156	1974	BTM-1	.168	.250	0.660	0.556	0.020	1560.	1000.	340.	.0447	111.9	.0320
IHR-176	1974	BTM-1	.173	.240	0.700	0.617	0.008	1560.	1000.	339.	.0448	111.5	.0319
IHR-190	1974	BTM-1	.182	.220	0.809	0.723	0.009	1560.	1000.	347.	.0475	105.2	.0333
IHR-183	1974	BTM-1	.189	.362	0.517	0.470	0.0	1560.	1000.	454.	.0412	121.3	.1051
IHR-177	1974	BTM-1	.240	.308	0.773	0.724	0.006	1560.	1000.	737.	.0416	120.1	.0701
IHR-166	1974	BTM-1	.162	.256	0.625	0.563	0.004	1560.	1200.	411.	.0368	135.8	.0321
IHR-165	1974	BTM-1	.180	.242	0.744	0.682	0.004	1560.	1500.	516.	.0300	166.5	.0335
IHR-157	1974	BTM-1	.208	.300	0.737	0.663	0.003	1560.	2000.	627.	.0232	215.3	.0329
IHR-172	1974	BTM-1	.185	.280	0.650	0.629	0.004	1560.	2000.	665.	.0228	219.0	.0355
IHR-186	1974	BTM-1	.221	.334	0.671	0.614	0.0	1650.	500.	361.	.0415	120.6	.0547
IHR-173	1974	BTM-1	.164	.314	0.516	0.478	0.006	1650.	1000.	371.	.0442	67.9	.0330
IHR-147	1974	BTM-1	.189	.250	0.736	0.628	0.016	1650.	1000.	388.	.0463	108.0	.0372
IHR-146	1974	BTM-1	.182	.256	0.691	0.621	0.012	1650.	1000.	348.	.0459	109.0	.0338
IHR-182	1974	BTM-1	.144	.260	0.550	0.488	0.008	1650.	1000.	393.	.0934	53.6	.0374
IHR-181	1974	BTM-1	.269	.332	0.804	0.729	0.0	1650.	1000.	680.	.0458	109.2	.0695
IHR-151	1974	BTM-1	.160	.242	0.802	0.744	0.012	1650.	1100.	369.	.0422	118.4	.0342
IHR-153	1974	BTM-1	.269	.233	0.773	0.708	0.004	1650.	1100.	783.	.0380	131.7	.0727
IHR-149	1974	BTM-1	.192	.250	0.852	0.816	0.004	1650.	1200.	436.	.0399	125.4	.0366
IHR-160	1974	BTM-1	.196	.242	0.802	0.744	0.012	1650.	1500.	509.	.0310	161.5	.0374
IHR-158	1974	BTM-1	.214	.250	0.852	0.816	0.004	1650.	2000.	640.	.0240	208.7	.0352
IHR-154	1974	BTM-1	.200	.240	0.700	0.617	0.008	1650.	2000.	671.	.0241	207.3	.0368
IHR-192	1974	BTM-2	.081	.191	0.398	0.298	0.063	1200.	1000.	561.	.0437	114.5	.0501
IHR-191	1974	BTM-2	.137	.251	0.514	0.343	0.116	1340.	1000.	494.	.0435	115.0	.0411
IHR-161	1974	BTM-2	.237	.298	0.755	0.708	0.0	1650.	1000.	397.	.0482	103.8	.0432
IHR-164	1974	BTM-2	.262	.278	0.888	0.813	0.0	1650.	1200.	409.	.0431	116.0	.0373
IHR-162	1974	BTM-2	.233	.278	0.781	0.723	0.0	1650.	1500.	488.	.0322	155.3	.0326
IHR-163	1974	BTM-2	.248	.263	0.924	0.833	0.008	1650.	2000.	670.	.0248	201.9	.0343
120	1976	LIGNITE	.379	.409	0.961	0.597	0.024	1650.	1000.	679.	.0595	84.1	.0578
122	1976	BTM-2	.321	.337	0.955	0.834	0.033	1650.	1000.	736.	.0525	95.2	.0800
124A	1976	BTM-2	.256	.316	0.810	0.671	0.041	1650.	1000.	669.	.0404	123.6	.0490
124B	1976	BTM-2	.240	.272	0.890	0.768	0.011	1650.	1000.	601.	.0338	147.7	.0420
128A	6/76	BTM-2	.337	.360	0.933	0.825	0.0	1650.	1000.	705.	.0402	124.5	.0727
128B	6/76	BTM-2	.321	.298	1.067	0.943	0.0	1650.	1000.	655.	.0345	145.0	.0640
130	12/ 7/76	LIGNITE	.430	.434	0.827	0.532	0.0	1650.	1000.	738.	.0533	93.9	.0670
131	12/ 7/76	LIGNITE	.663	.332	1.669	1.151	0.0	1650.	1000.	752.	.0660	75.7	.1422
132	1/11/77	LIGNITE	.493	.317	1.297	0.842	0.0	1650.	1000.	714.	.0515	97.1	.0863
133	3/77	LIGNITE	.546	.330	1.182	0.948	0.0	1650.	1000.	755.	.0565	88.5	.0850
134	3/77	LIGNITE	.509	.442	0.826	0.652	0.0	1650.	1000.	748.	.0570	87.7	.0823
135A	4/77	LIGNITE	.650	.440	1.232	0.730	0.0	1650.	1000.	708.	.0752	119.7	.0899
135B	4/77	LIGNITE	.481	.507	0.791	0.454	0.0	1650.	1000.	664.	.0481	187.1	.0560

*BTM-1 is Pittsburgh Seam HvAb coal.

BTM-2 is Illinois No. 6 HvCb coal.

LIGNITE is North Dakota lignite coal from the Baukol-Noonan Mine.

Detailed material balances (overall, carbon, hydrogen, and ash) have been reported by PERC[5] for the early IHR series bituminous tests. For these runs, reported carbon, hydrogen, and ash balances ranged from 89 to 99 percent, 86 to 107 percent, and 92 to 113 percent, respectively.

Detailed material balances have also been reported[19] for a number of the more recent long-duration tests. On the basis of coal as received, the overall mass balances for Runs 120 to 128B ranged from 92 to 98 percent, the carbon balances from 94 to 102 percent, and the hydrogen balances from 86 to 100 percent. Material balances have not yet been reported for Runs 130 to 135B because of an unexpectedly low ash recovery.

4.4 BROOKHAVEN DATA COLLECTION AND ANALYSIS

Brookhaven National Laboratory has been performing an experimental study on rapid gas-phase hydrogenation (flash hydropyrolysis) of a lignite coal. Although major emphasis in this study has been to maximize liquid hydrocarbon yield, an appreciable yield of hydrocarbon gases (mainly methane and ethane) has been obtained. The bench-scale system incorporates an entrained-downflow tubular reactor, 1 inch inside diameter by 8 feet long, with a 3-foot cooling section below.

The unit is designed to feed coal at up to 2 lb/hr at design temperatures to 1,500°F and pressures to 4,000 psi. The coal used to date is a North Dakota lignite with an average particle size less than 150 microns. Preheated hydrogen mixes with the coal, and the mixture then falls through the reactor tube, which is electrically heated through the walls. A more detailed description of the reactor system has been given by Fallon.[7]

During the reporting period, all of the published[7,20,21] Brookhaven lignite data were entered into the computerized data base. A computer listing of selected data is presented in Table 4-6. A computer listing of all of the Brookhaven data contained in the data base is presented in Appendix A.

The Brookhaven tests were conducted at reactor pressures of 1,000 to 3,000 psig, reactor wall temperatures of 890°F to 1,500°F, particle residence times of approximately 2 to 12 seconds, gas residence times of approximately 11 to 56 seconds, and hydrogen-to-coal ratios of approximately 0.5 to 6 lb/lb. Gas residence time was calculated by Bechtel using the inlet reactor conditions and the reactor length. Particle residence times for the earlier 18 tests (Runs 5 through 18C) were not available from Brookhaven. It should be noted that Brookhaven has reported only reactor wall temperature (and not gas temperature) for the tests.

The Brookhaven results given in Table 4-6 show overall carbon conversions ranging from 13 to 89 percent and carbon selectivity to gas ranging from

Table 4-6

BROOKHAVEN HYDROPYROLYSIS DATA FOR LIGNITE COAL

RUN DESIGNATION	DATE	COAL TYPE	OVERALL FRACTION CARBON CONVERTED	CARBON SELECTIVITY TO GAS	CARBON SELECTIVITY TO METHANE	CARBON SELECTIVITY TO ETHANE	REACTOR WALL TEMP (DEG F)	HYDROGEN PARTIAL PRESSURE (PSIG)	HYDROGEN TO COAL RATIO (LB/LB)	GAS VELOCITY (FT/SEC)	GAS RESIDENCE TIME (SEC)	PARTICLE RESIDENCE TIME (SEC)
5	1976	LIG	.365	.737	.334	.164	1290.	1500.	3.38	.226	35.3	
7	1976	LIG	.301	.781	.312	.146	1290.	1500.	1.39	.239	33.4	
8	1976	LIG	.398	.721	.339	.0	1290.	1500.	5.80	.462	17.3	
9	1976	LIG	.215	.879	.265	.148	1200.	1500.	2.20	.439	18.2	
10	1976	LIG	.459	.649	.259	.137	1290.	2000.	1.48	.177	45.2	
11	1976	LIG	.171	.760	.158	.094	1110.	1500.	3.62	.415	19.3	
12	1976	LIG	.129	.977	.155	.085	890.	1500.	4.85	.309	25.9	
13A	1976	LIG	.330	.867	.258	.139	1200.	1500.	5.63	.408	19.6	
13B	1976	LIG	.234	.855	.299	.167	1200.	1500.	0.90	.378	21.2	
14	1976	LIG	.566	.716	.387	.143	1430.	1500.	2.33	.481	16.6	
15	1976	LIG	.586	.759	.449	.089	1500.	1500.	2.80	.500	16.0	
16A	1976	LIG	.444	.722	.399	.131	1430.	1500.	0.98	.447	17.9	
16B	1976	LIG	.396	.714	.394	.134	1430.	1500.	1.40	.447	17.9	
16C	1976	LIG	.580	.705	.409	.133	1430.	1500.	1.53	.447	17.9	
17	1976	LIG	.692	.711	.397	.133	1410.	1500.	0.95	.426	18.8	
18A	1976	LIG	.860	.693	.367	.165	1370.	2100.	1.28	.286	28.0	
18B	1976	LIG	.822	.695	.354	.167	1370.	2100.	0.98	.286	28.0	
18C	1976	LIG	.888	.703	.359	.164	1370.	2100.	0.94	.286	28.0	
21	11/ 5/76	LIG	.428	.717	.348	.178	1340.	2000.	1.24	.213	37.5	8.6
22	1/13/77	LIG	.475	.680	.356	.168	1380.	2000.	1.32	.272	29.5	11.4
23	1/25/77	LIG	.448	.596	.368	.109	1450.	2000.	1.46	.240	33.4	12.2
24	1/27/77	LIG	.595	.655	.469	.094	1480.	2000.	3.62	.278	28.7	11.5
25	1/28/77	LIG	.381	.714	.336	.171	1340.	2000.	2.24	.270	29.6	11.1
26	1/31/77	LIG	.360	.647	.275	.150	1290.	2000.	2.20	.263	30.4	11.3
27	2/ 2/77	LIG	.388	.696	.317	.165	1360.	2000.	1.86	.273	29.3	11.2
28	2/ 3/77	LIG	.438	.710	.388	.148	1420.	2000.	2.29	.282	28.3	11.2
29	2/ 3/77	LIG	.358	.771	.377	.156	1420.	1500.	1.92	.342	23.4	10.5
46	4/26/77	LIG	.511	.818	.538	.115	1430.	2000.	0.42	.284	28.2	9.9
47	4/27/77	LIG	.467	.722	.358	.212	1450.	2000.	1.13	.273	29.3	8.3
48	5/ 6/77	LIG	.325	.800	.422	.178	1430.	1500.	0.66	.396	20.2	6.5

Table 4-6 (Cont'd)

RUN DESIG-NATION	DATE	COAL TYPE	OVERALL FRACTION CARBON CONVERTED	CARBON SELEC-TIVITY TO GAS	CARBON SELEC-TIVITY TO METHANE	CARBON SELEC-TIVITY TO ETHANE	REACTOR WALL TEMP (DEG F)	HYDROGEN PARTIAL PRESSURE (PSIG)	HYDROGEN TO COAL RATIO (LB/LB)	GAS VELOCITY (FT/SEC)	GAS RESIDENCE TIME (SEC)	PARTICLE RESIDENCE TIME (SEC)
49	5/ 9/77	LIG	.637	.804	.557	.104	1440.	1500.	0.97	.345	23.2	6.8
50A	5/12/77	LIG	.407	.779	.474	.135	1470.	1500.	0.91	.380	21.1	6.8
50B	5/12/77	LIG	.591	.934	.766	.076	1470.	2500.	1.04	.224	35.8	8.8
51A	5/13/77	LIG	.503	.847	.630	.093	1470.	2000.	1.08	.264	30.3	8.1
51B	5/13/77	LIG	.634	.964	.801	.091	1470.	3000.	1.26	.171	46.9	9.5
52	5/16/77	LIG	.587	.818	.555	.164	1380.	3000.	0.89	.181	44.2	9.5
53	5/17/77	LIG	.482	.869	.643	.180	1430.	3000.	1.32	.176	45.5	9.5
55	6/ 7/77	LIG	.611	.975	.881	.074	1470.	3000.	0.51	.160	50.0	9.5
56	6/15/77	LIG	.384	.792	.477	.190	1380.	3000.	0.89	.143	56.1	10.0
57	6/16/77	LIG	.492	.758	.429	.207	1370.	3000.	1.23	.150	53.5	9.9
58	6/20/77	LIG	.497	.831	.551	.111	1380.	2000.	0.53	.201	39.8	8.7
59	6/21/77	LIG	.478	.799	.502	.142	1380.	1500.	0.61	.295	27.1	7.4
60A	6/23/77	LIG	.627	.986	.871	.030	1470.	2500.	0.63	.179	44.6	9.2
60B	6/23/77	LIG	.601	.938	.837	.035	1470.	2500.	0.63	.179	11.1	2.3
61A	6/27/77	LIG	.518	.809	.519	.158	1380.	2500.	0.62	.165	48.5	9.6
61B	6/27/77	LIG	.454	.722	.445	.156	1380.	2500.	0.62	.165	12.1	2.4
62	6/28/77	LIG	.663	.807	.572	.139	1380.	3000.	0.58	.134	59.6	2.5
63	6/29/77	LIG	.353	.824	.405	.167	1380.	1000.	0.60	.438	18.3	6.4

60 to 99 percent. Several tests conducted under comparable conditions of temperature, pressure, residence time, and hydrogen-to-coal ratio have resulted in some discrepancies. For example, two product samples drawn in Run 16 (16B and 16C) gave substantially different carbon conversions: one was 40 percent; the other was 58 percent. Also, comparable Runs 48 and 49 and comparable Runs 52 and 56 gave significantly different conversions for approximately the same operating conditions. In addition, several anomalously high values of carbon conversion have been reported for Runs 17, 18A, 18B, and 18C. Some of the discrepancies may be due to (1) analytical errors, (2) reactor transient behavior that gives rise to large differences between measured wall temperature and gas/particle temperature, or (3) fluctuations in coal feed.

Actual mass balances for carbon, hydrogen, oxygen, nitrogen, and sulfur have been presented by Brookhaven[20,21] for all the lignite tests listed in Table 4-6. Almost all tests show good balance closures.

Section 5

REACTOR MODELING

This section gives the semiempirical correlations developed for predicting overall carbon conversion and carbon conversion to gaseous products for the Rocketdyne, Cities Service, PERC, and Brookhaven reactors using bituminous, subbituminous, and lignite coals. The proposed correlations have been fitted to the data using a computerized multiple-regression statistical analysis. A computer listing of all the data contained in the data base is presented in Appendix A. Properties of the coals used are found in Appendix B.

The correlations presented in this section should be considered as preliminary, since a portion of the collected data are still being revised and updated by Rocketdyne, Cities Service, PERC, and Brookhaven.

The subject matter discussed in this section fulfills the contractual requirements under Task III to perform reactor model studies.

5.1 NOMENCLATURE

The following nomenclature will be used in this section:

d_p = Mean particle diameter

E = Activation energy

H/C = Hydrogen-to-coal ratio

k_0 = Forward reaction rate frequency factor

k_1 = Forward reaction rate constant

k_2 = Reverse reaction rate constant

K = Equilibrium constant

P = Total pressure

P_{H_2} = Hydrogen partial pressure

R = Gas constant

t_R = Particle or gas residence time

t_{RG} = Gas residence time

t_{RP} = Particle residence time

T = Reaction temperature

T_G = Maximum gas temperature (or reactor gas outlet temperature)

u_G = Superficial gas velocity

X = Weight fraction overall carbon conversion

X_A = Weight fraction carbon conversion of species A

X_{CO} = Weight fraction carbon conversion to CO

X_{CO_2} = Weight fraction carbon conversion to CO_2

X_G = Weight fraction carbon conversion to gas

X_M = Weight fraction carbon conversion to methane

X^* = Weight fraction overall carbon conversion at equilibrium

X_A^* = Weight fraction carbon conversion of species A at equilibrium

X_G^* = Weight fraction carbon conversion to gas at equilibrium

X_M^* = Weight fraction carbon conversion to methane at equilibrium

$\alpha_1, \alpha_2, \ldots \alpha_9$ = Fitted coefficients

Φ_G = Weight fraction carbon selectivity to gas

Φ_{CO} = Weight fraction carbon selectivity to CO

Φ_{CO_2} = Weight fraction carbon selectivity to CO_2

Φ_M = Weight fraction carbon selectivity to methane

$\psi, \psi_G, \ldots$ = Fitted functions of independent (operating) variables

5.2 DEVELOPMENT OF A REACTOR MODEL FOR PREDICTION OF CARBON CONVERSION

Rapid hydropyrolysis of coal is an extremely complex process, which involves a number of reversible heterogeneous and homogeneous reactions.[1,2] Coal (or carbon) conversion kinetics during rapid devolatilization and subsequent hydrogenation are not well understood, and a majority of the models developed to correlate carbon conversion data have been more or less empirical. The principal correlative tool in most studies has been a simple first-order kinetic model for the irreversible reaction $C + 2H_2 \longrightarrow CH_4$. An integration of this simple model, assuming the Arrhenius form for the reaction rate coefficient, gives:

$$X = 1 - \exp\left[-k_o \exp(-E/RT) P_{H_2} t_R\right] \tag{1}$$

The above model, however, has not satisfactorily correlated data from different sources, where rate of heating, hydrogen-to-coal ratio, coal particle size, and coal type have differed markedly.[1]

Bechtel has proposed the following model for correlating overall carbon conversion to the operating variables:

$$X = X^* \left[1 - \exp(-\psi)\right] \tag{2}$$

with

$$\psi = \alpha_1 (t_{RG})^{\alpha_2} (t_{RP})^{\alpha_3} \exp(\alpha_4 P) \exp(\alpha_5 P_{H_2}) \exp(\alpha_6 H/C) (d_p)^{\alpha_7} \exp(-\alpha_8/T_G) (X^*)^{\alpha_9} \tag{3}$$

The coefficients, α_1 through α_9, have been fitted to the data using a computerized multiple-regression statistical analysis. Note that maximum reactor gas temperature, T_G, has been chosen as the correlating temperature variable for this study.

The proposed model, which consists of an equilibrium component, X^*, and a kinetic component, $[1-\exp(-\psi)]$, satisfies a number of boundary constraints. For example, as residence time or temperature approaches zero, conversion approaches zero, and as residence time approaches infinity, conversion approaches the equilibrium conversion limit, X^*.

The form of Equation 2 has been influenced by the similar form of an integrated, first-order kinetic model for the reversible homogeneous reaction $A \rightleftarrows B$, where one mole of reactant produces one mole of product. The analytical expression for conversion of A to B for this reaction is:

$$X_A = X_A^* \left\{ 1-\exp\left[-(k_1+k_2)t_R\right]\right\} \tag{4}$$

with

$$X_A^* = k_1/(k_1 + k_2) = K/(1 + K) \tag{5}$$

Assuming the Arrhenius form for the forward reaction rate coefficient, and combining Equations 4 and 5 gives:

$$X_A = X_A^* \left\{ 1-\exp\left[-(k_o/X_A^*)\exp(-E/RT)t_R\right]\right\} \tag{6}$$

The proposed model has also been used to correlate the available data for carbon conversion to gas and methane. The models for X_G and X_M, therefore, are written as:

$$X_G = X_G^* \left[1-\exp(-\psi_G)\right] \tag{7}$$

$$X_M = X_M^* \left[1-\exp(-\psi_M)\right] \tag{8}$$

where the fitted functions ψ_G and ψ_M have the same form as ψ in Equation 3.

As will be shown in the following subsection, the values for X^*, X_G^*, and X_M^* are close to unity for all of the Rocketdyne, Cities Service, and Brookhaven tests. Because of this, the effect of X^* on the kinetic component of Equation 2 could not be obtained; i.e., the value of the fitted coefficient α_9 in Equation 3 could not be determined from the data.

The reaction mechanism for conversion of carbon to CO and CO_2 during coal hydropyrolysis is not well understood. The Rocketdyne and Cities Service data have shown, however, that within the region investigated, X_{CO} is a monotonically increasing function of temperature and residence time and X_{CO_2} is a monotonically decreasing function of temperature and residence time. Thus, the following model is proposed for correlating the CO and CO_2 conversion data:

$$X_{CO} = 1-\exp(-\psi_{CO}) \tag{9}$$

$$X_{CO_2} = 1-\exp(-\psi_{CO_2}) \tag{10}$$

where the fitted functions ψ_{CO} and ψ_{CO_2} have the same form as ψ in Equation 3.

Carbon selectivities to gas, methane, CO, and CO_2 are obtained from the predicted values of conversion to products and the predicted overall carbon conversion. That is, $\Phi_{Product} = X_{Product}/X$

5.3 PREDICTION OF EQUILIBRIUM CARBON CONVERSION AT REACTOR OPERATING CONDITIONS

Owing to the complexity of coal hydropyrolysis, a thermodynamic equilibrium computer model, PEP[22] (Propellant Evaluation Program), has been used to predict the thermodynamic equilibria for the test data. PEP considers a reaction system of carbon (β-graphite), hydrogen, oxygen, and hydrocarbon gases within a temperature and pressure range normally encountered in coal hydropyrolysis.

At a given temperature, pressure, and relative weights of initial reactants, PEP predicts the concentration of species that appear in significant amounts at equilibrium. For the operating range used in the reactor systems, the results from PEP indicate that methane is the major hydrocarbon product present at equilibrium. Higher hydrocarbon products, such as ethane, ethylene, or benzene, are present only in trace amounts. PEP also predicts that significant quantities of CO and CO_2 can be present in the gas phase at equilibrium. Note that for these conditions the equilibrium overall carbon conversion, X^*, and the equilibrium conversion to gas, X_G^*, are equal.

Figures 5-1 and 5-2 predict the fraction overall carbon conversion at equilibrium for the bituminous and subbituminous coals tested by Rocketdyne and Cities Service. The equilibrium conversions are shown as a function of reaction temperature and hydrogen-to-coal ratio, for a reactor pressure of 1,500 psig. Since there are fewer product gas moles than reactant gas moles during hydropyrolysis, X^* (or X_G^*) increases with increasing pressure.

As expected, X^* decreases with increasing temperature and with decreasing hydrogen-to-coal ratio. Also, subbituminous coal gives larger values of X^* than bituminous coal at comparable hydrogen-to-coal ratios. This observation is attributed to the following:

- The carbon content of the subbituminous coal is less than the carbon content of the bituminous coal. Therefore, more hydrogen is available for conversion of the subbituminous coal at the same level of hydrogen-to-coal ratio

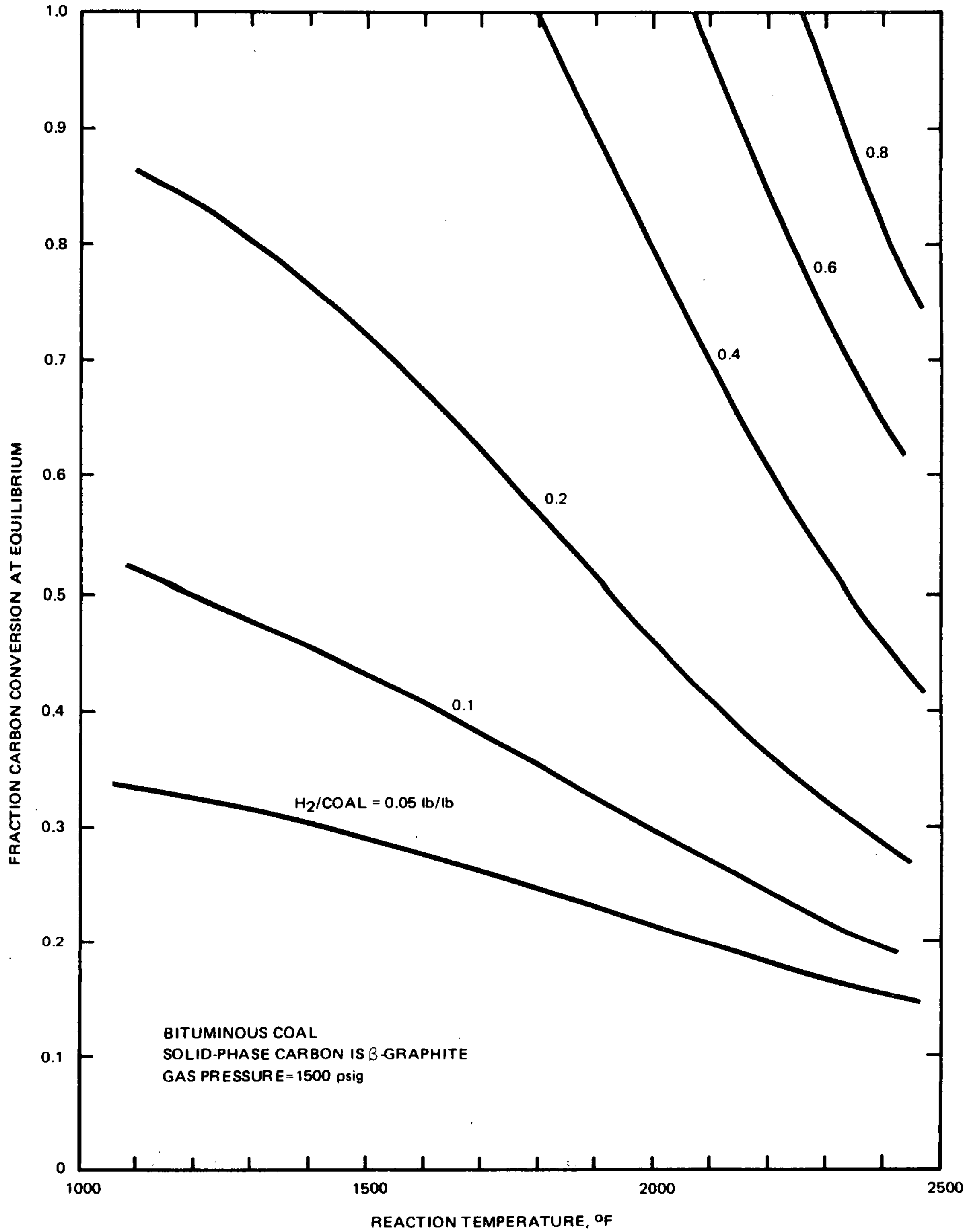

Figure 5-1. Predicted Fraction Carbon Conversion at Equilibrium for Bituminous Coal

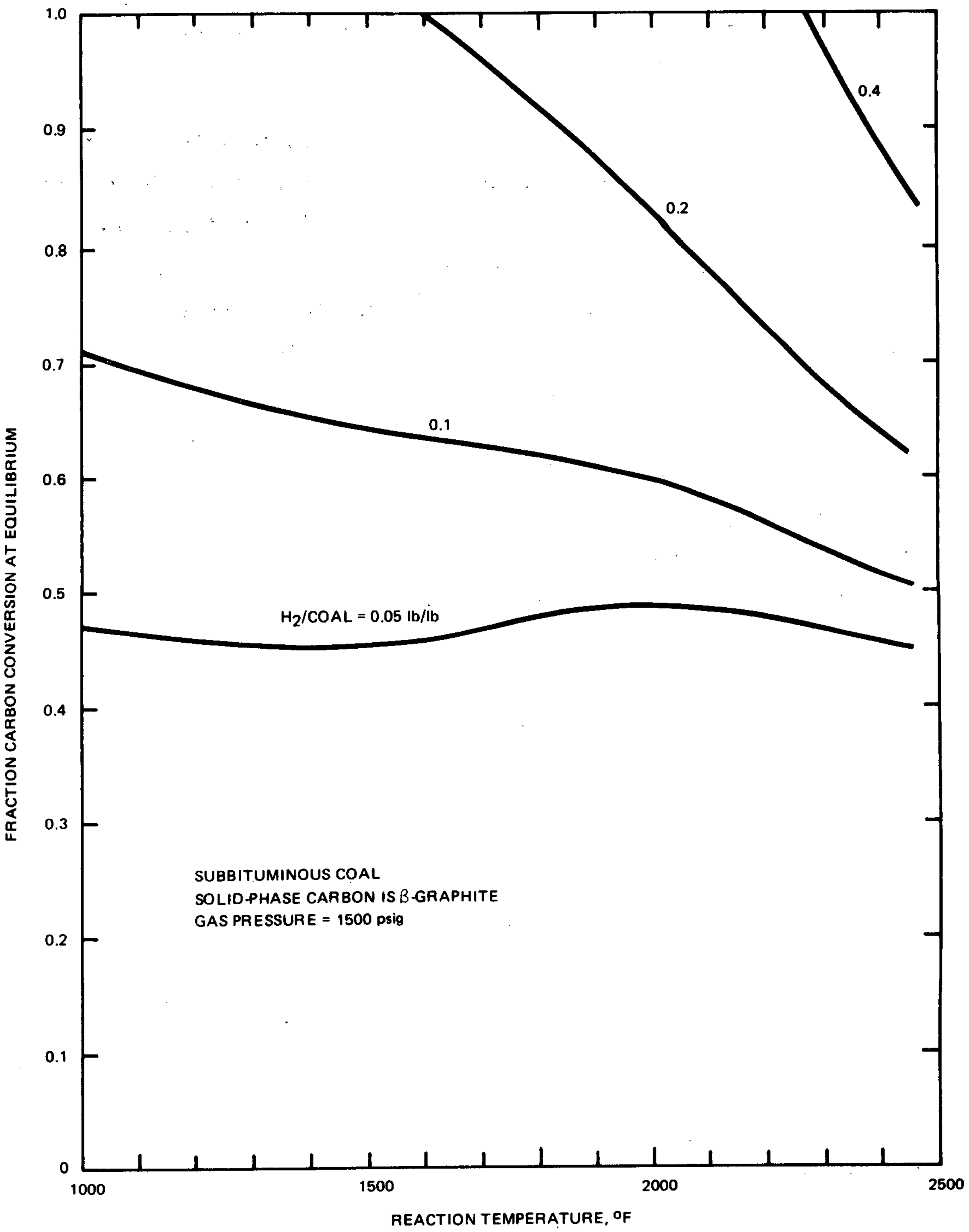

Figure 5-2. Predicted Fraction Carbon Conversion at Equilibrium for Subbituminous Coal

- The oxygen content of the subbituminous coal is greater than the oxygen content of the bituminous coal, resulting in larger conversions of carbon to CO and CO_2 for the subbituminous coal

Figure 5-3 predicts the equilibrium carbon conversion to methane for the subbituminous coal tested by Rocketdyne and Cities Service. (Conversion to methane has not been fitted to the proposed model for bituminous or lignite coal.) The equilibrium conversions are shown as a function of temperature and hydrogen-to-coal ratio, for a reactor pressure of 1,500 psig. Again, as expected, X_M^* decreases with increasing temperature and with decreasing hydrogen-to-coal ratio.

PEP predicts an equilibrium overall fraction carbon conversion and conversion to gas of unity (100 percent conversion) for all of the Rocketdyne, Cities Service, and Brookhaven tests. This is due primarily to the high levels of hydrogen-to-coal ratio, which varies from about 0.2 to 2.0 lb/lb (see Tables 4-1 through 4-6 and Figures 5-1 and 5-2). PEP also predicts that the equilibrium fraction of carbon converted to methane is nearly unity for a majority of the Rocketdyne and Cities Service subbituminous tests (see Tables 4-2 and 4-4 and Figure 5-3). For these conditions, Equations 2, 3, 7, and 8 simplify, with $X^* = X_G^* = X_M^* = 1$.

The predicted equilibrium overall fraction carbon conversions for the PERC tests are, however, all less than unity, because the PERC reactor has operated at extremely low hydrogen-to-coal ratios, varying from 0.03 to 0.12 lb/lb (see Table 4-5). Predicted values of X^* for the PERC tests are shown in Table 5-1.

As mentioned previously, PEP assumes that the carbon present is β-graphite. Other studies[23,24,25] have indicated that the carbon present at equilibrium may be amorphous carbon, which has a higher reactivity than β-graphite. Therefore, the predictions of X^* given in this section should be considered as approximate, and possibly on the low side.

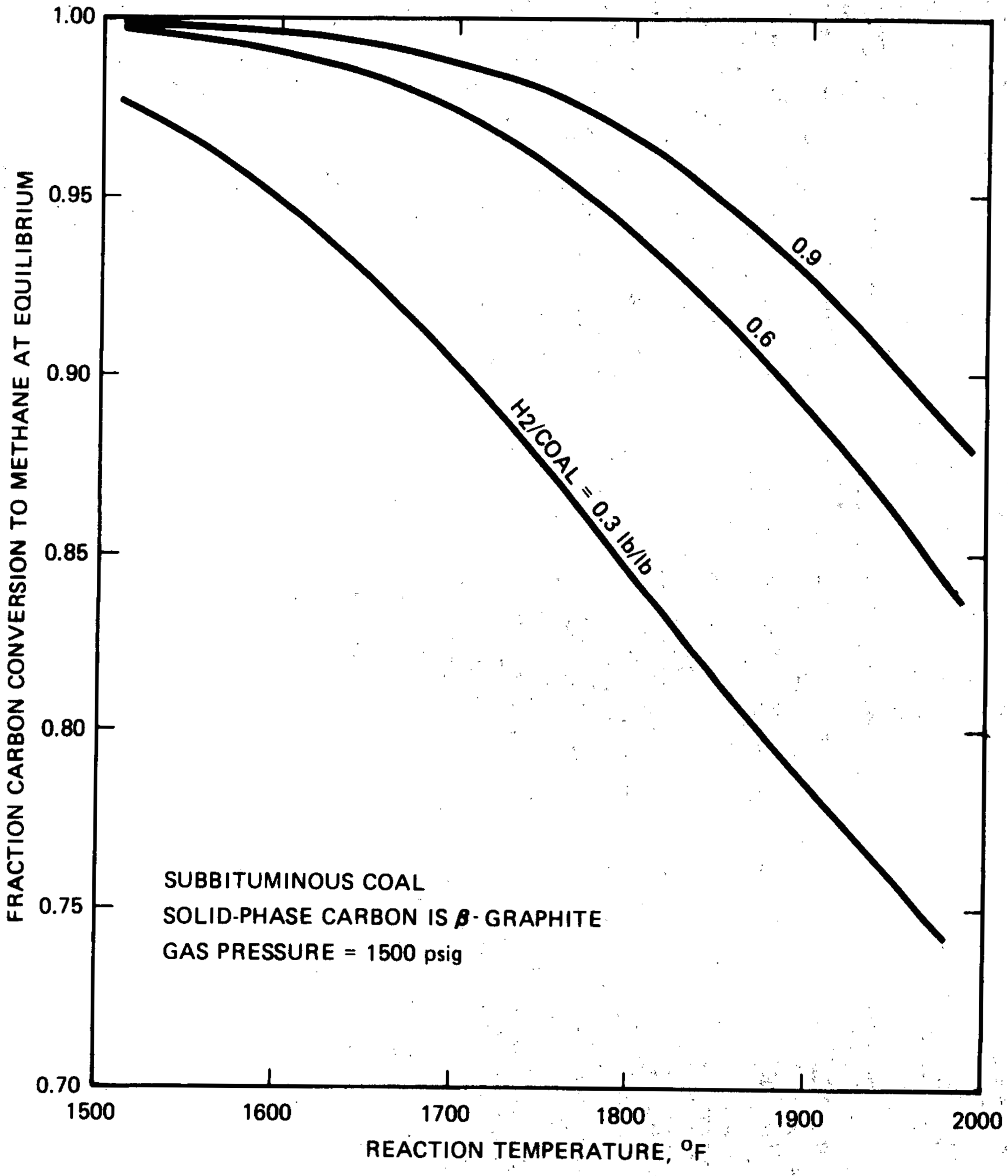

Figure 5-3. Predicted Fraction Carbon Conversion to Methane at Equilibrium for Subbituminous Coal

Table 5-1

PREDICTED VALUES OF CARBON CONVERSION AT EQUILIBRIUM FOR THE PERC TESTS

Run Designation	Coal Type	Reactor Wall Temp., °F	Reactor Pressure, psig	Hydrogen-to-Coal Ratio, lb/lb	Measured Average Fraction Carbon Converted	Overall Fraction Carbon Converted at Equilibrium
IHR-178	HvAb	1,470	1,000	0.0718	0.208	0.331
IHR-167	HvAb	1,470	1,000	0.0298	0.196	0.192
IHR-156	HvAb	1,560	1,000	0.0320	0.209	0.180
IHR-176	HvAb	1,560	1,000	0.0319	0.207	0.180
IHR-190	HvAb	1,560	1,000	0.0333	0.201	0.184
IHR-183	HvAb	1,560	1,000	0.1051	0.276	0.340
IHR-177	HvAb	1,560	1,000	0.0701	0.274	0.298
IHR-166	HvAb	1,560	1,200	0.0321	0.209	0.188
IHR-165	HvAb	1,560	1,500	0.0335	0.211	0.200
IHR-157	HvAb	1,560	2,000	0.0329	0.254	0.206
IHR-172	HvAb	1,560	2,000	0.0355	0.233	0.214
IHR-186	HvAb	1,650	500	0.0547	0.278	0.206
IHR-173	HvAb	1,650	1,000	0.0330	0.239	0.173
IHR-147	HvAb	1,650	1,000	0.0372	0.220	0.181
IHR-146	HvAb	1,650	1,000	0.0338	0.219	0.171
IHR-182	HvAb	1,650	1,000	0.0374	0.202	0.182
IHR-181	HvAb	1,650	1,000	0.0695	0.300	0.271
IHR-151	HvAb	1,650	1,100	0.0342	0.201	0.174
IHR-153	HvAb	1,650	1,100	0.0727	0.251	0.286
IHR-149	HvAb	1,650	1,200	0.0366	0.221	0.185
IHR-160	HvAb	1,650	1,500	0.0374	0.219	0.193
IHR-158	HvAb	1,650	2,000	0.0352	0.232	0.200
IHR-154	HvAb	1,650	2,000	0.0368	0.220	0.204
IHR-192	HvCb	1,200	1,000	0.0501	0.136	0.308
IHR-191	HvCb	1,340	1,000	0.0411	0.194	0.258
IHR-161	HvCb	1,650	1,000	0.0432	0.268	0.214
IHR-164	HvCb	1,650	1,200	0.0373	0.270	0.205
IHR-162	HvCb	1,650	1,500	0.0326	0.256	0.203
IHR-163	HvCb	1,650	2,000	0.0343	0.256	0.217
120	Lignite	1,650	1,000	0.0578	0.394	0.416
122	HvCb	1,650	1,000	0.0800	0.329	0.318
124A	HvCb	1,650	1,000	0.0490	0.286	0.248
124B	HvCb	1,650	1,000	0.0420	0.256	0.229
128A	HvCb	1,650	1,000	0.0727	0.349	0.300
128B	HvCb	1,650	1,000	0.0640	0.310	0.278
130	Lignite	1,650	1,000	0.0670	0.432	0.440
131	Lignite	1,650	1,000	0.1422	0.498	0.635
132	Lignite	1,650	1,000	0.0863	0.405	0.487
133	Lignite	1,650	1,000	0.0850	0.438	0.486
134	Lignite	1,650	1,000	0.0823	0.476	0.479
135A	Lignite	1,650	1,000	0.0899	0.545	0.496
135B	Lignite	1,650	1,000	0.0560	0.494	0.411

5.4 PREDICTION OF CARBON CONVERSION IN THE PERC REACTOR

A number of observations suggest that the carbon conversion in the PERC reactor is controlled by the thermodynamic equilibrium between the carbon in the coal (or char) and the reaction products. These observations are:

- The gas residence times employed in the PERC reactor are extremely large, ranging from 75 to 220 seconds (see Table 4-5). Particle residence times may also be large, because of reported backmixing in the reactor. For this condition, the kinetic component of the proposed model (Equations 2 and 3) will increase towards unity
- The values of X^* for the PERC tests are small (see Table 5-1) because of the low hydrogen-to-coal ratios employed. From Equation 6, it is expected that a reduction in X^* results in a further increase towards unity in the kinetic component of the proposed model
- There is essentially no reported higher hydrocarbon product other than methane. This condition is required at thermodynamic equilibrium (see Subsection 5.3)
- The reported carbon conversions are generally higher for subbituminous and lignite coals than for bituminous coals. This condition is predicted at equilibrium (see Subsection 5.3 and Figures 5-1 and 5-2)

To test the equilibrium hypothesis, the measured carbon conversions and predicted (PEP) equilibrium carbon conversions listed in Table 5-1 are compared in Figure 5-4. Within the accuracy of the data, the results suggest a strong correlation between the measured and equilibrium conversions.

It should be noted that the measured conversions compared in Figure 5-4 were taken as the average of the conversion based on char analysis and the conversion based on gas analysis (see Table 4-5). It should also be noted that in the predicted equilibrium conversions, it is assumed that the carbon present is β-graphite and not amorphous. As mentioned previously, if the carbon is amorphous, the predicted equilibrium values should be higher than those shown in Figure 5-4.

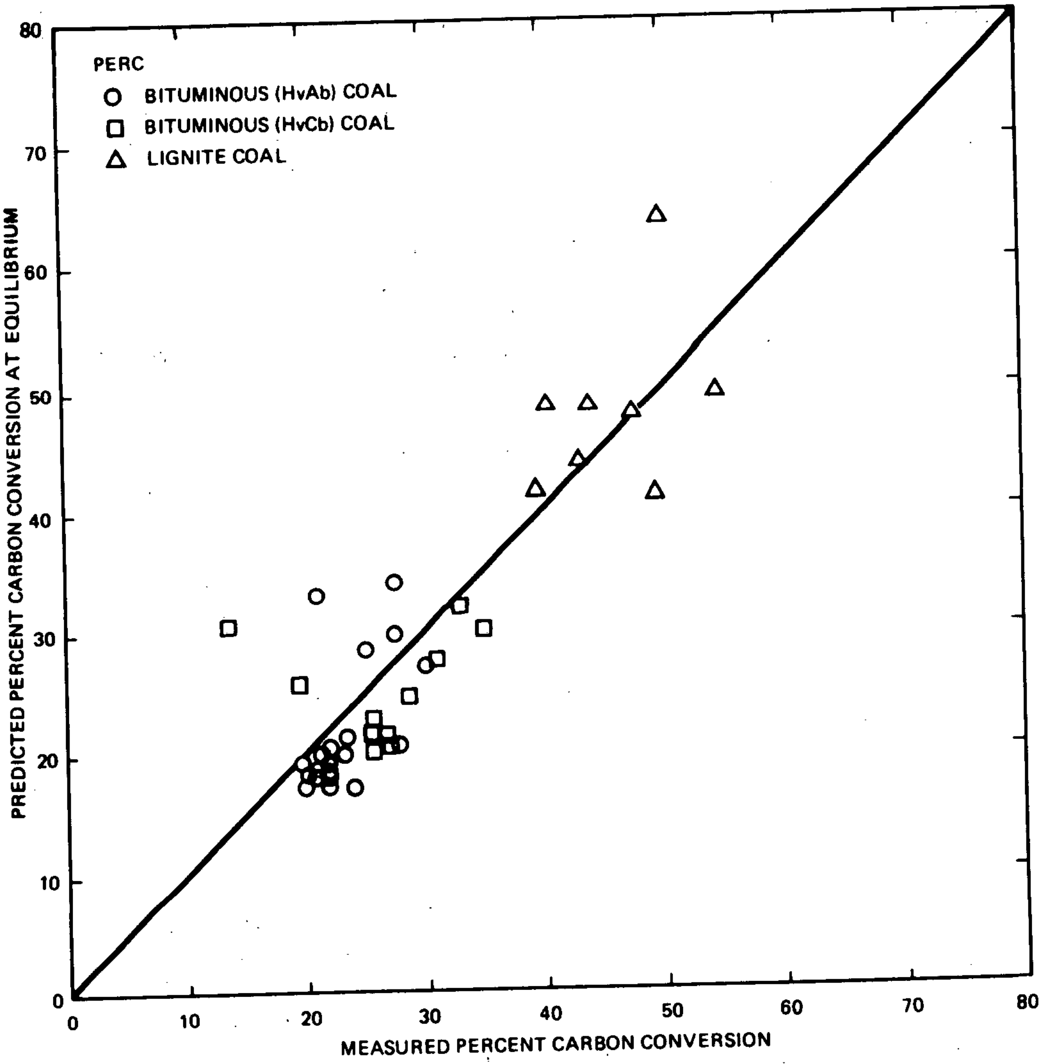

Figure 5-4. Comparison of Measured and Predicted Overall Carbon Conversion for the PERC Reactor

5.5 PREDICTION OF CARBON CONVERSION TO PRODUCTS FOR BITUMINOUS COAL

In this subsection, the Rocketdyne partial liquefaction and hydrogasification data for bituminous coal have been fitted to the model proposed for predicting overall carbon conversion and carbon conversion to gas. Computer listings of the correlated variables for the partial liquefaction and hydrogasification data are presented in Tables 4-1 and 4-2, respectively. Runs 011-7, 8, 9, and 10 have not been included in the analyses because of uncertainties in the reported values of carbon conversion for these tests (see Subsection 4.1.2).

It should be noted that for the range of variables studied in the Rocketdyne reactor systems, the predicted equilibrium overall conversion of carbon and the equilibrium conversion to gas are unity for all data points (see Subsection 5.3). For these conditions, Equations 2, 3, and 7 simplify, with $X^* = X_G^* = 1$.

5.5.1 Overall Carbon Conversion

A statistical analysis of the fitted Rocketdyne partial liquefaction and hydrogasification bituminous coal data showed that overall carbon conversion was a significant function of only maximum gas temperature. Carbon conversion was not significantly affected by particle (or gas) residence time, hydrogen partial pressure, total pressure, coal type, reactor size, hydrogen-to-coal ratio, or coal particle size. The correlation fitted to the carbon conversion data is:

$$X = 1 - \exp\left[-8.02 \exp(-4{,}840/T_G)\right] \tag{11}$$

where T_G is in ^{o}R.

As Equation 11 indicates, overall carbon conversion increases with increasing gas temperature. The fact that overall carbon conversion for bituminous coal is not affected by residence time suggests that nearly all of the carbon conversion occurs through devolatilization within a short period of time (less than 50 milliseconds) in the reactor; i.e., there is little direct hydrogenation of the char.

Equation 11 has a standard error of estimate of 3.2 percent in the predicted percent carbon conversion. Measured and predicted percent carbon conversions are shown in Figure 5-5. The statistics and Figure 5-5 indicate that the Rocketdyne 1/4- and 1-ton/hr reactor systems achieve similar carbon conversions under comparable operating conditions within the region investigated.

In Figure 5-6, predicted carbon conversion from Equation 11 is plotted against maximum gas temperature. From the figure, an overall carbon conversion of 50 ± 3 percent is predicted for a gas temperature of 1,520°F.

5.5.2 Carbon Conversion and Selectivity to Gas

A statistical analysis of the bituminous data showed that carbon conversion to gas was a significant function of particle (or gas) residence time and maximum gas temperature. Within the region investigated, conversion to gas was not significantly affected by hydrogen partial pressure, total pressure, coal type, reactor size, hydrogen-to-coal ratio, or coal particle size. The correlation fitted to the data is:

$$X_G = 1 - \exp\left[-2.88(t_R)^{0.323}\exp(-8{,}320/T_G)\right] \qquad (12)$$

where t_R is in milliseconds and T_G is in $^{\circ}$R.

As Equation 12 indicates, conversion to gas increases with increasing residence time and gas temperature. Equation 12 has a standard error of estimate of 4.1 percent in the predicted percent conversion to gas. Measured and predicted conversions are shown in Figure 5-7. The statistics and Figure 5-7 indicate that the Rocketdyne 1/4- and 1-ton/hr reactors achieve similar carbon conversions under comparable operating conditions.

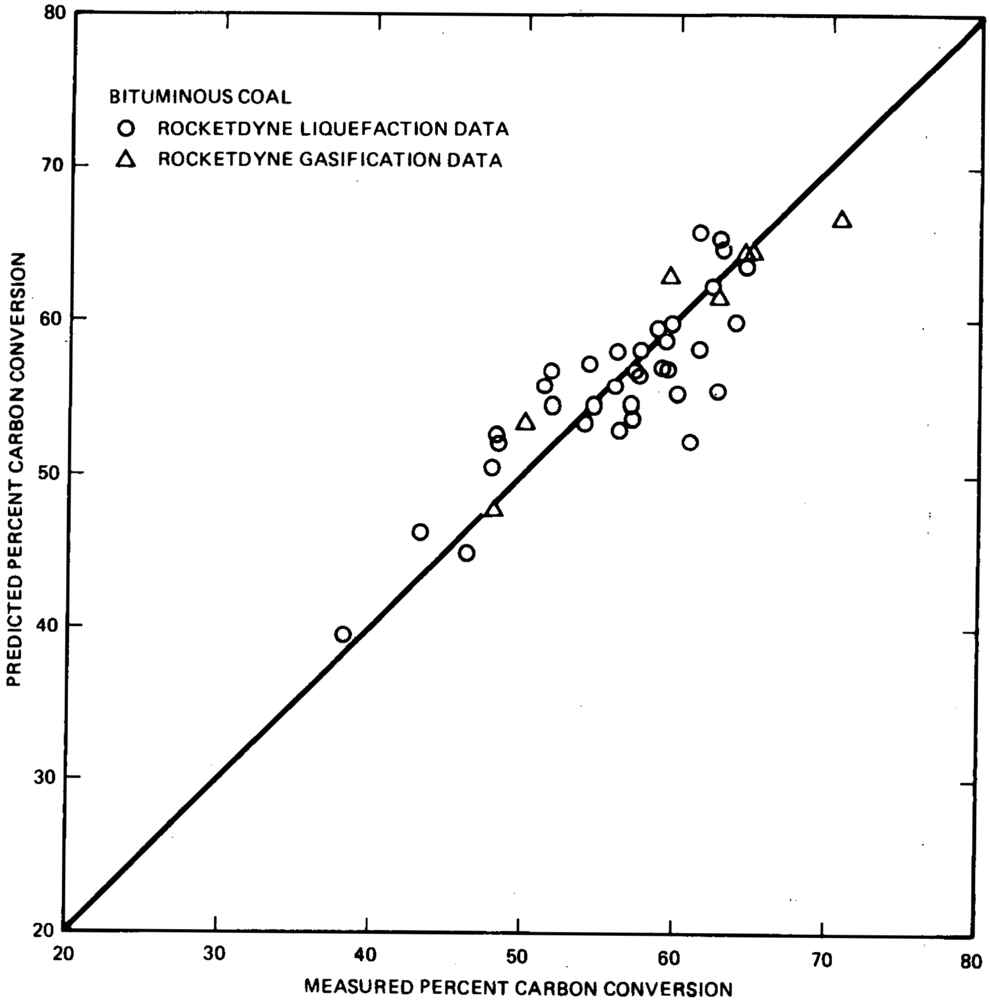

Figure 5-5. Comparison of Measured and Predicted Overall Carbon Conversion for Bituminous Coal

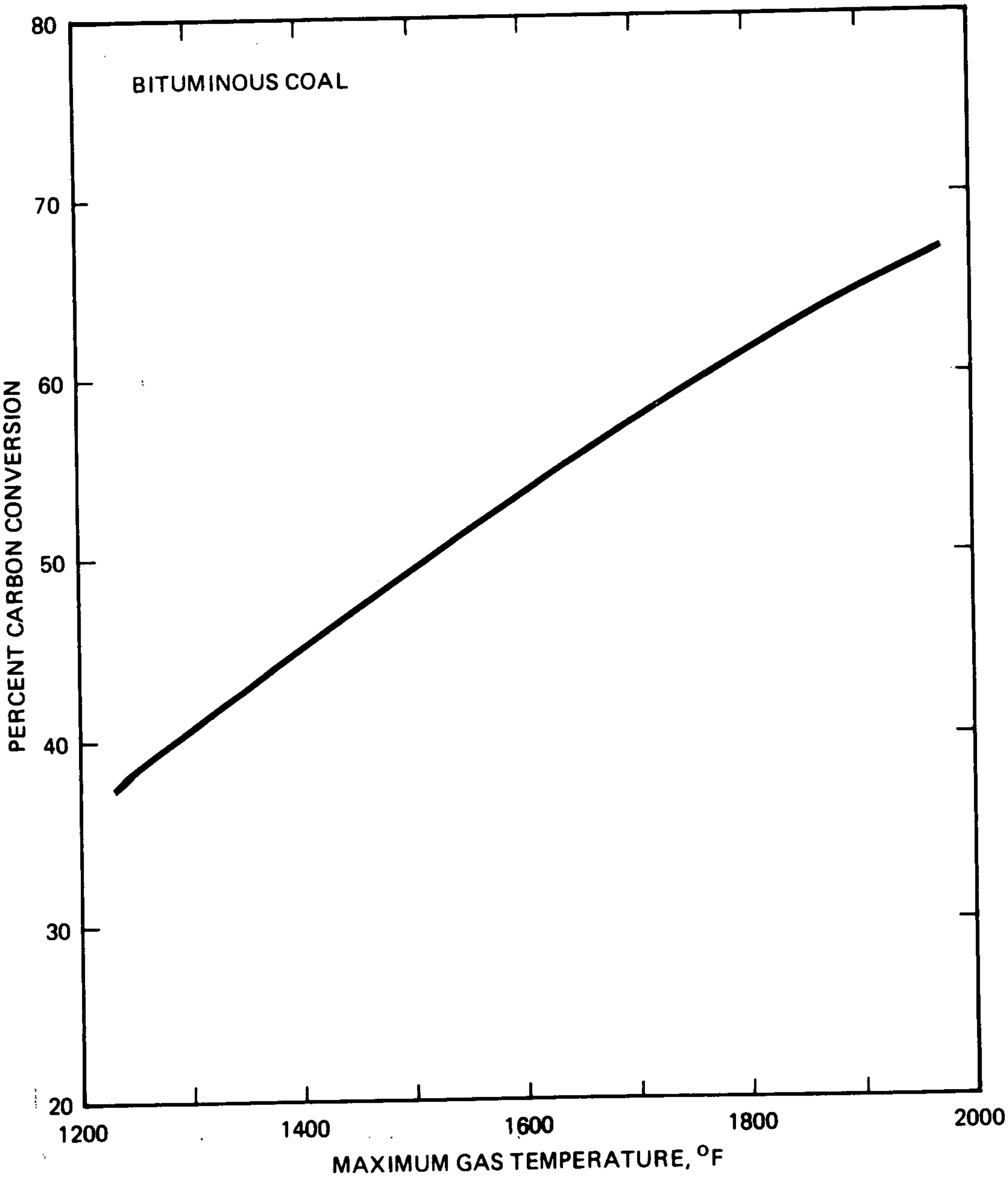

Figure 5-6. Predicted Overall Carbon Conversion for Bituminous Coal

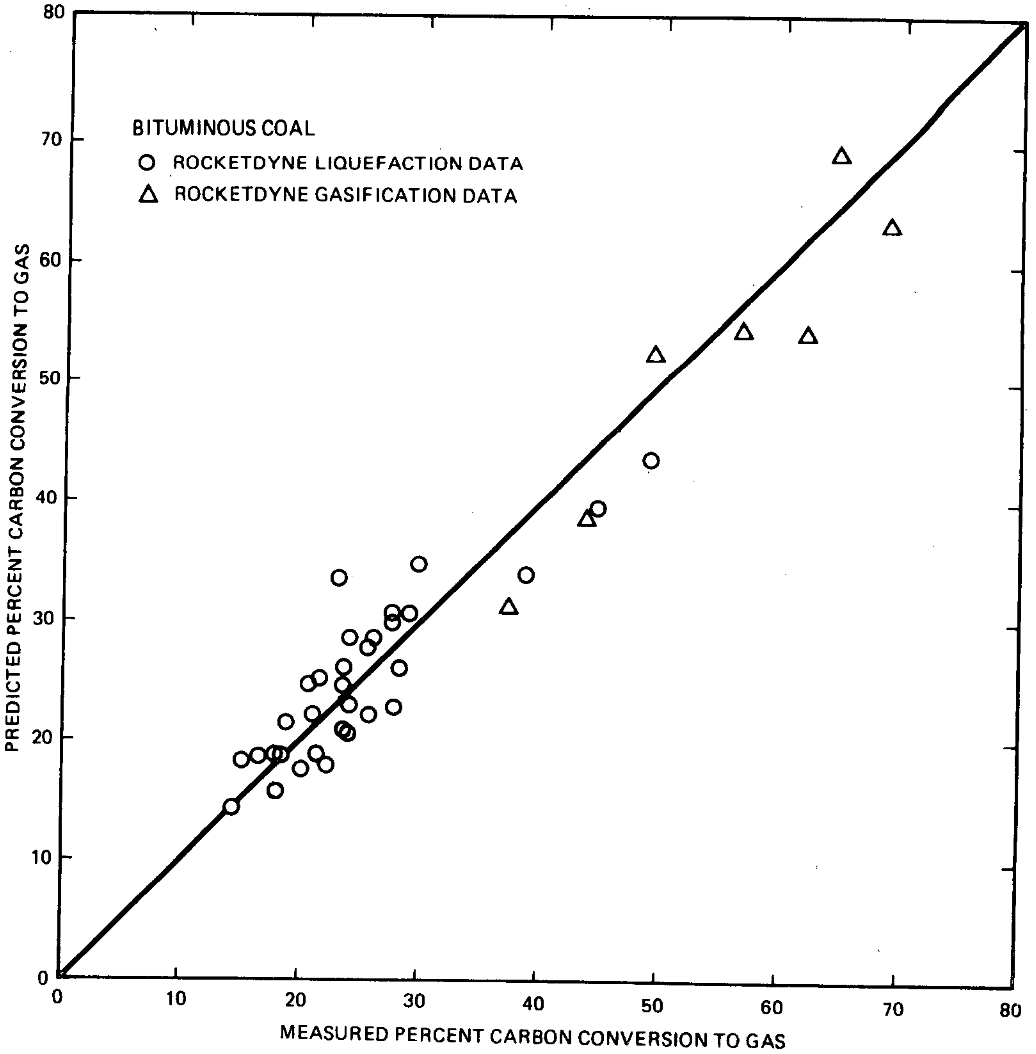

Figure 5-7. Comparison of Measured and Predicted Carbon Conversion to Gas for Bituminous Coal

In Figure 5-8, predicted values for carbon selectivity to gas from Equations 11 and 12 (i.e., $\Phi_G = X_G/X$) are shown as a function of gas temperature and residence time. As can be seen from the figure, gas selectivity increases with increasing temperature and residence time. The effect of temperature, however, is diminished at lower residence time. From the figure, a selectivity to gas of 100 percent is predicted for a gas temperature of about 1,780^{o}F at a particle residence time of 3,000 milliseconds.

The fact that carbon selectivity to gas increases with increasing residence time suggests that the intial higher (liquid) hydrocarbon products of devolatilization are continuously cracked down to lower hydrocarbon products as gas residence time increases.

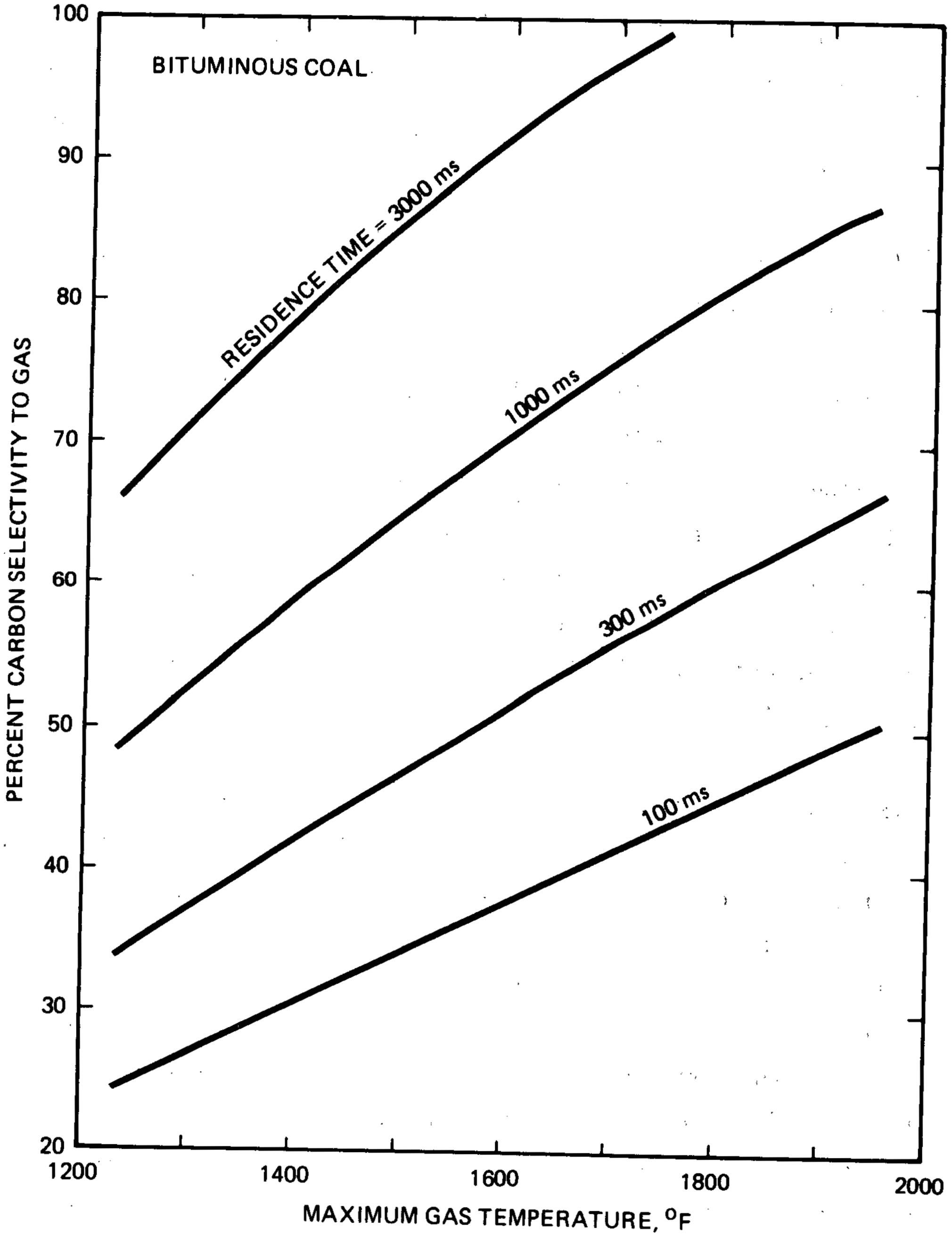

Figure 5-8. Predicted Carbon Selectivity to Gas for Bituminous Coal

5.6 PREDICTION OF CARBON CONVERSION TO PRODUCTS FOR SUBBITUMINOUS COAL

In this subsection, the Rocketdyne and Cities Service hydrogasification data for subbituminous coal have been fitted to the models proposed for predicting overall carbon conversion and carbon conversion to gaseous products. Computer listings of the correlated variables for the Rocketdyne and Cities Service subbituminous data are given in Tables 4-2 and 4-4, respectively. Owing to the uncertainty in the results from Rocketdyne Runs 011-14 and 011-15 (as was discussed in Subsection 4.1.3), these runs were not included in the analyses.

As was discussed in Subsection 4.3.2, Greene[12] has presented a series of plots for the Cities Service subbituminous data. These plots revealed that at larger residence times carbon conversion increases with increasing pressure, and at smaller residence times carbon conversion decreases with increasing pressure. Greene also showed that temperature and pressure interacted in the same manner as residence time and pressure. Because of these interactions, the variables P_{H_2}/t_R and P_{H_2}/T_G have been included as fitted parameters in the proposed subbituminous coal models.

For the subbituminous data, it was not possible to determine separately the effects of both hydrogen partial pressure, P_{H_2}, and reactor pressure, P, on carbon conversion. This is because the hydrogen partial pressure was equal to reactor pressure for the 42 fitted Cities Service tests, and nearly equal to reactor pressure for the 12 fitted Rocketdyne tests; i.e., P_{H_2} and P are confounded. For convenience, the pressure variable is referred to as pressure or hydrogen partial pressure in this section. During January 1978, Cities Service obtained data for tests in which approximately 20 volume percent of methane was added to the reactor feed gas. But these data were not received in time to be incorporated into the analyses.

It should be noted that for the range of variables studied in the Rocketdyne and Cities Service reactor systems, the predicted equilibrium overall conversion of carbon, equilibrium conversion to gas, and equilibrium conversion to methane are unity for all data points (see Subsection 5.3). Therefore, Equations 2, 3, 7, and 8 simplify, with $X^* = X^*_G = X^*_M = 1$.

5.6.1 Overall Carbon Conversion

A statistical analysis of the fitted Rocketdyne and Cities Service subbituminous coal data showed that overall carbon conversion was a significant function of gas temperature, particle (or gas) residence time, and hydrogen partial pressure. Carbon conversion was not significantly affected by reactor size, hydrogen-to-coal ratio, or coal particle size within the region investigated. The correlation fitted to the carbon conversion data is:

$$X = 1 - \exp\left[-2.53 \exp(-0.175\, P_{H_2}/t_R) \exp(0.000393\, P_{H_2}) \exp(-3{,}820/T_G)\right] \qquad (13)$$

where P_{H_2} is in psig, t_R is in milliseconds, and T_G is in ^oR.

As Equation 13 indicates, X increases with increasing coal particle residence time and gas temperature. At high particle residence times, X increases with increasing hydrogen partial pressure; at low particle residence times, X decreases with increasing hydrogen partial pressure. In addition, the effect of residence time on carbon conversion increases as pressure increases. The fact that overall carbon conversion increases with residence time suggests that conversion of carbon to products occurs throughout the length of the reactor.

Equation 13 has a standard error of estimate of 3.3 percent in the predicted percent carbon conversion. The measured and predicted carbon conversions are shown in Figure 5-9. The statistics and Figure 5-9 indicate that within the experimental error, the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar carbon conversions under comparable operating conditions.

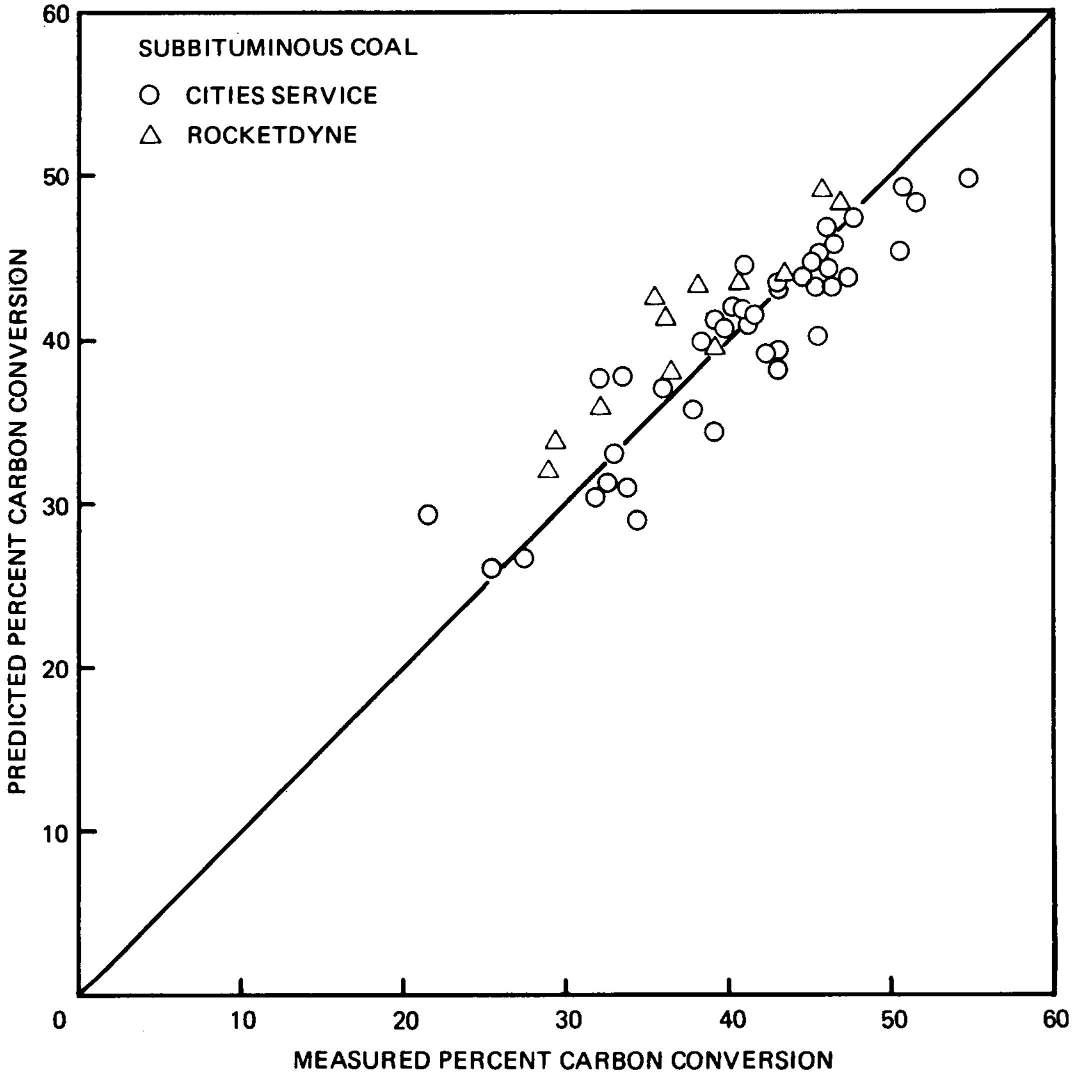

Figure 5-9. Comparison of Measured and Predicted Overall Carbon Conversion for Subbituminous Coal

As can be seen in Figure 5-9, the predictions of carbon conversion for the Rocketdyne reactor are, on the average, slightly higher than the measured values, whereas the predictions for the Cities Service reactor are, on the average, slightly lower than the measured values. With the data currently on hand, it is not possible to determine whether or not this discrepancy can be accounted for by (1) differences in the reactor sizes, (2) differences in the reactor operating conditions (e.g., the Rocketdyne feed gas contains water vapor), (3) differences in the accuracy of the values for maximum gas temperature, or (4) differences in the average levels of the hydrogen-to-coal ratio employed in the reactor systems.

In Figure 5-10, predicted overall carbon conversion from Equation 13 is plotted as a function of maximum gas temperature for selected levels of residence time and hydrogen partial pressure. Note that a carbon conversion of 50 percent is predicted for a gas temperature of about 1,880°F, a residence time of 3,000 milliseconds, and a pressure of 1,000 psig.

5.6.2 Carbon Conversion and Selectivity to Gas

A statistical analysis of the fitted Rocketdyne and Cities Service subbituminous coal data indicated that carbon conversion to gas was a significant function of particle residence time, maximum gas temperature, and hydrogen partial pressure. Carbon conversion was not significantly affected by reactor size, hydrogen-to-coal ratio, or particle size within the region investigated. The correlation fitted to the data is:

$$X_G = 1 - \exp\left[-0.277 \exp(-0.178\ P_{H_2}/t_R)\ \exp(0.00358\ P_{H_2})\ \exp(-6.57\ P_{H_2}/T_G)\right] \qquad (14)$$

where P_{H_2} is in psig, t_R is in milliseconds, and T_G is in °R.

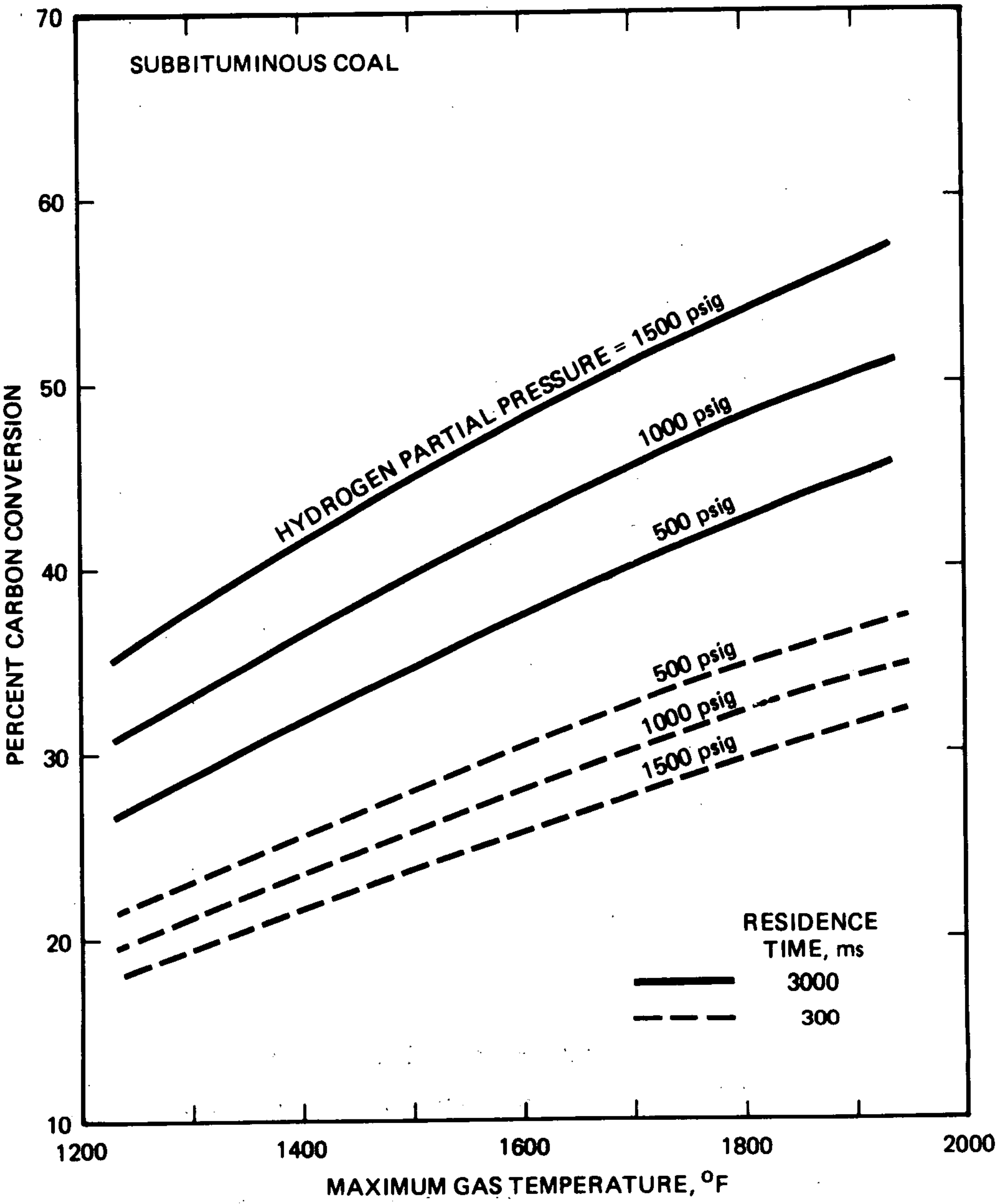

Figure 5-10. Predicted Overall Carbon Conversion for Subbituminous Coal

As can be seen from Equation 14, X_G increases with increasing residence time and gas temperature. Conversion to gas increases with increasing hydrogen partial pressure at high residence time, and decreases with increasing hydrogen partial pressure at low residence time, within the region of gas temperature investigated. In addition, the effects of residence time and gas temperature on conversion increase as hydrogen partial pressure increases.

Equation 14 has a standard error of estimate of 3.0 percent in the predicted percent carbon conversion to gas. The measured and predicted conversions are shown in Figure 5-11. The statistics and Figure 5-11 indicate that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar carbon conversions to gaseous products under comparable operation conditions within the region investigated.

In Figure 5-12, predicted values for carbon selectivity to gas obtained from Equations 13 and 14 (i.e., $\Phi_G = X_G/X$) are shown as a function of gas temperature, for selected values of hydrogen partial pressure at a residence time of 1,000 milliseconds. Note that a selectivity to gas of 100 percent is predicted at 1,900°F and 1,500 psig. Selectivity to gas is very insensitive to residence time for the subbituminous coal data.

5.6.3 Carbon Conversion and Selectivity to Methane

A statistical analysis of the fitted data indicated that carbon conversion to methane was a significant function of particle residence time, maximum gas temperature, and hydrogen partial pressure. Carbon conversion was not significantly affected by reactor size, hydrogen-to-coal ratio, or

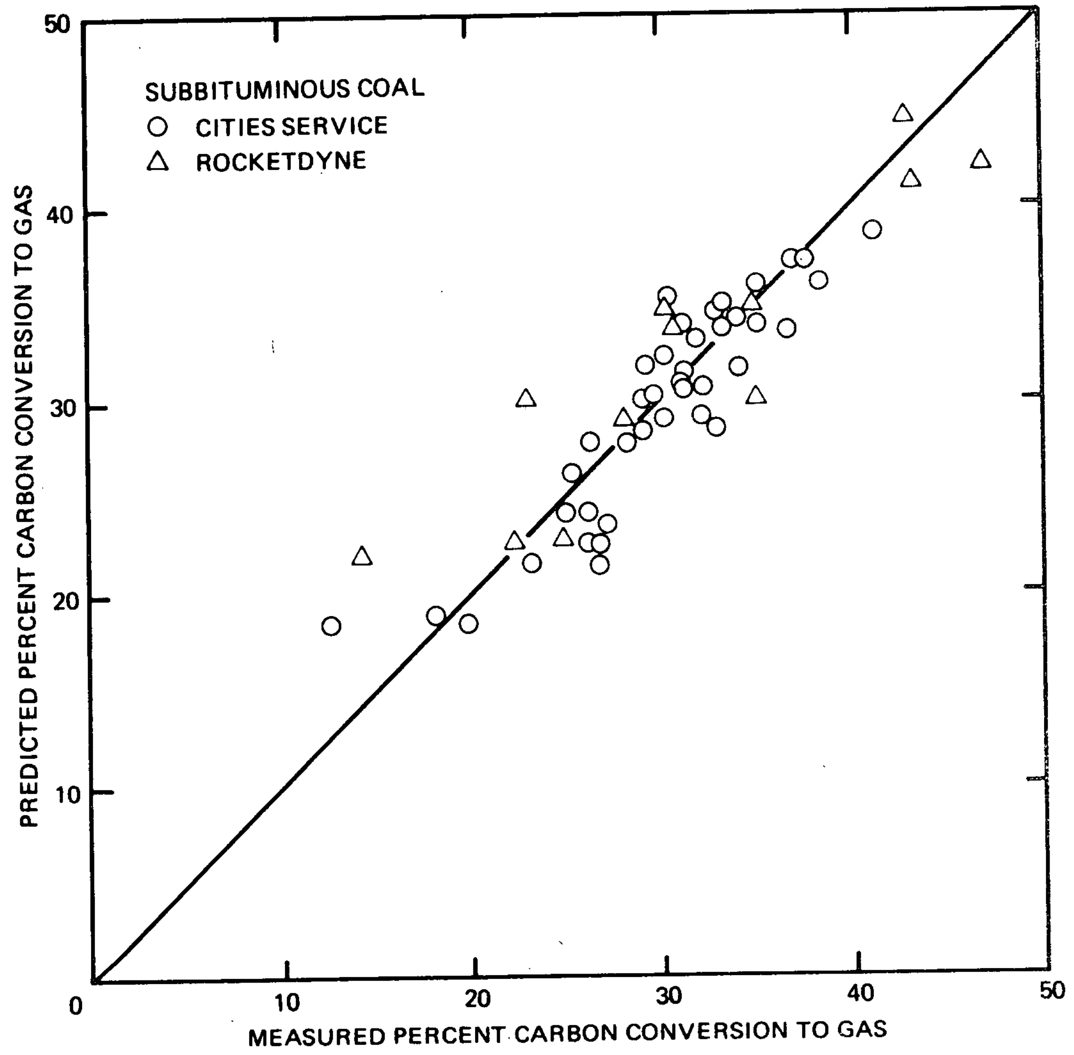

Figure 5-11. Comparison of Measured and Predicted carbon Conversion to Gas for Subbituminous Coal.

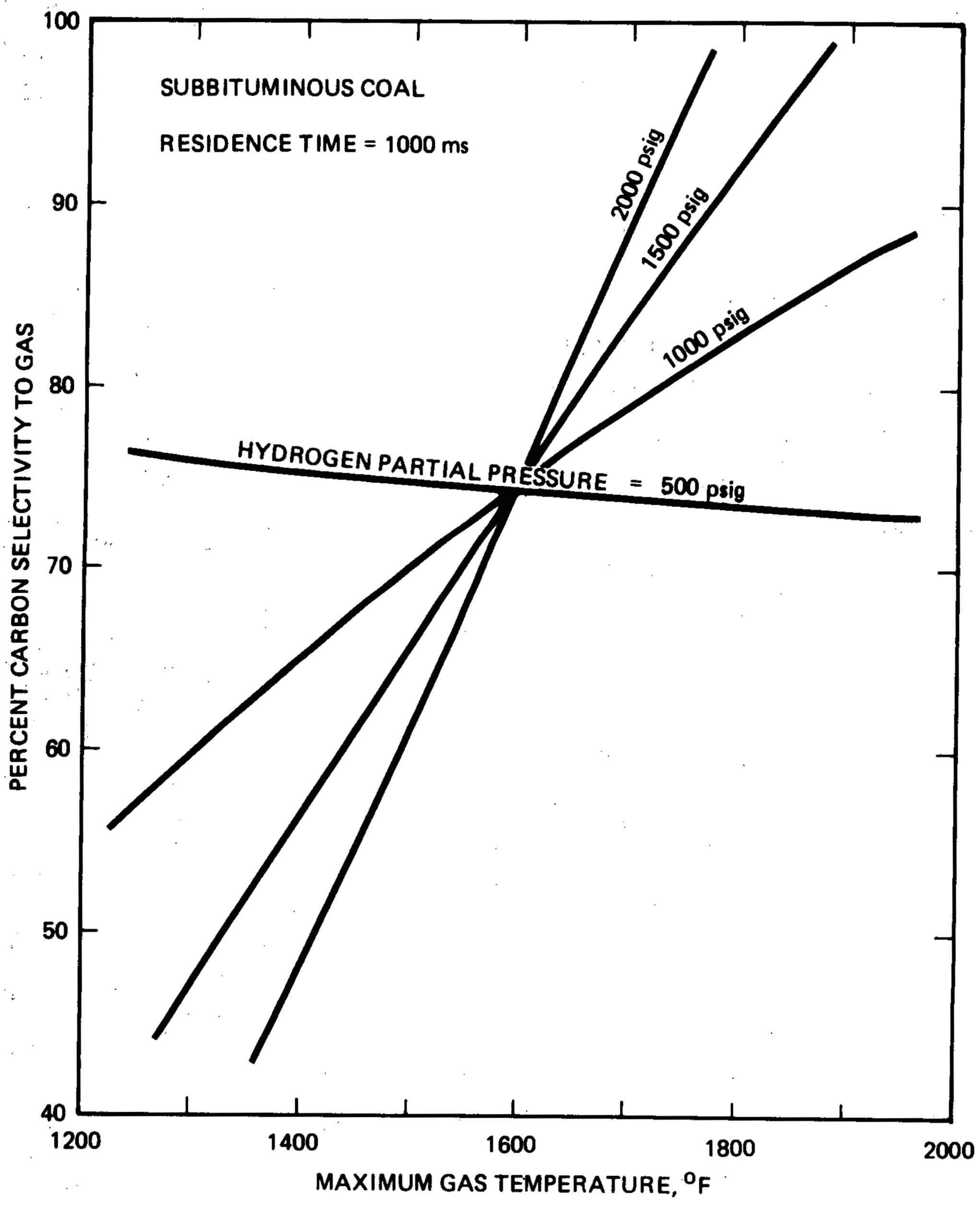

Figure 5-12. Predicted Carbon Selectivity to Gas for Subbituminous Coal

particle size within the region investigated. The correlation fitted to the data is:

$$X_M = 1 - \exp\left[-0.125 \exp(-0.286\, P_{H_2}/t_R) \exp(0.00735\, P_{H_2}) \exp(-13.9\, P_{H_2}/T_G)\right] \quad (15)$$

where P_{H_2} is in psig, t_R is in milliseconds, and T_G is in ^oR.

As can be seen from Equation 15, X_M increases with increasing particle residence time and reaction temperature. Conversion to methane increases with increasing hydrogen partial pressure at high residence time, and decreases with increasing pressure at low residence time, within the region of gas temperature investigated. In addition, the effects of residence time and gas temperature on conversion increase as hydrogen partial pressure increases.

Equation 15 has a standard error of estimate of 2.6 percent in the predicted percent conversion. The measured and predicted conversions are shown in Figure 5-13. The statistics and Figure 5-13 indicate that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar carbon conversions to methane under comparable operating conditions within the region investigated.

In Figure 5-14, predicted values for carbon selectivity to methane obtained from Equations 13 and 15 (i.e., $\Phi_M = X_M/X$) are shown as a function of gas temperature for different levels of residence time and hydrogen partial pressure. It should be noted that a selectivity to methane of 100 percent is predicted at 1,900^{o}F gas temperature, 1,000 milliseconds residence time, and 1,500 psig pressure.

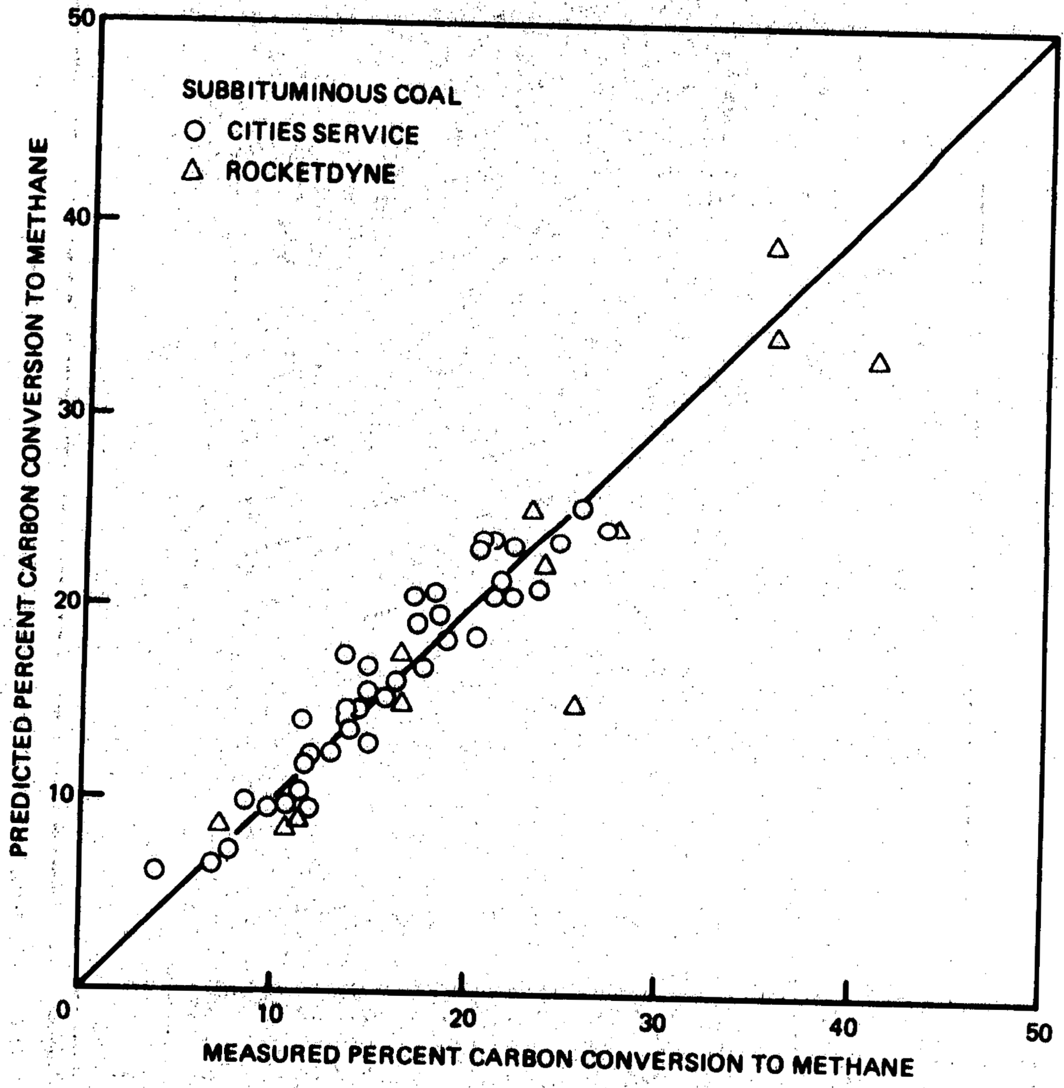

Figure 5-13. Comparison of Measured and Predicted Carbon Conversion to Methane for Subbituminous Coal

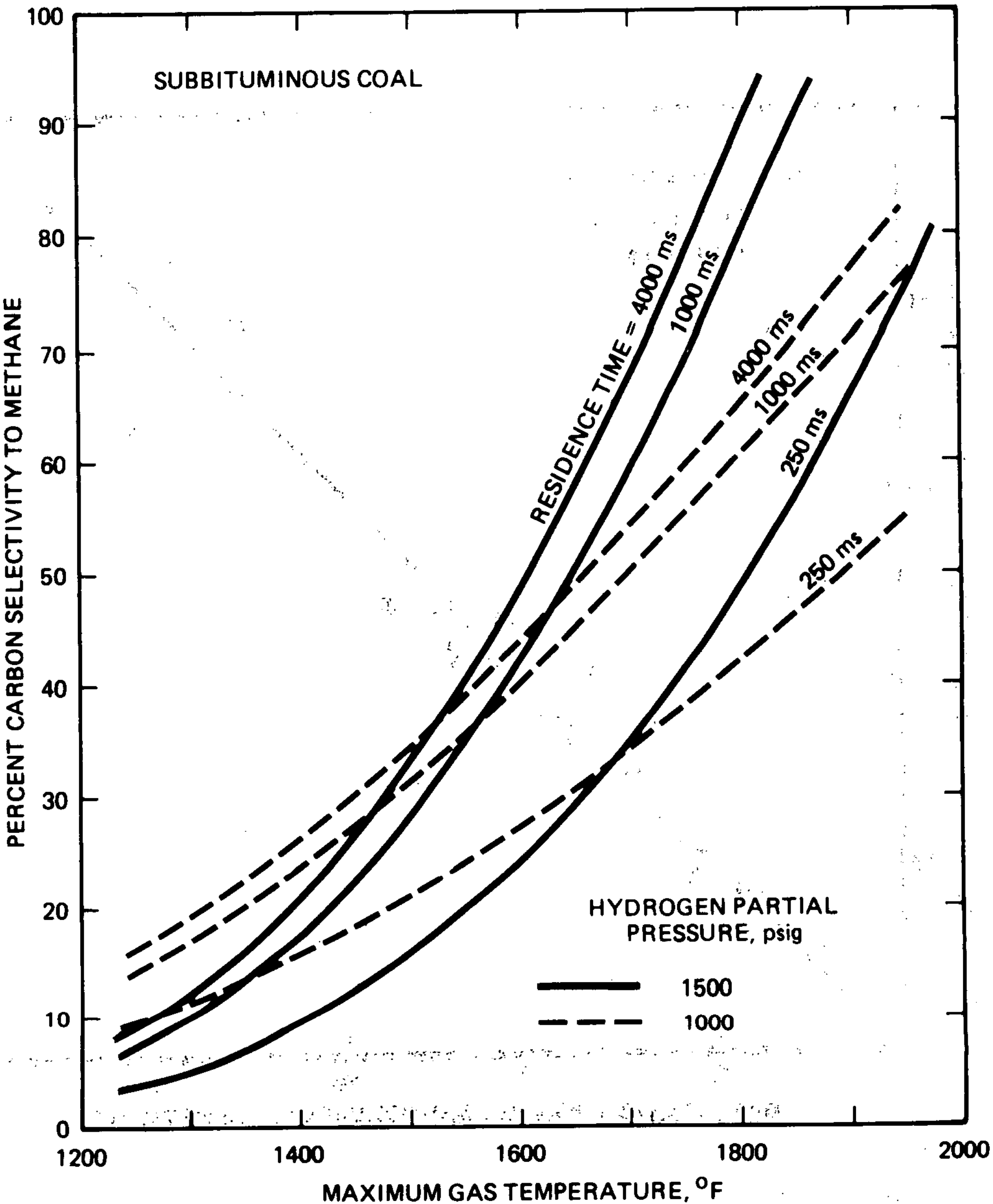

Figure 5-14. Predicted Carbon Selectivity to Methane for Subbituminous Coal

The fact that carbon selectivity to methane increases with increasing residence time suggests that the initial higher hydrocarbon products of devolatilization and, perhaps, direct char hydrogenation are cracked down to methane as gas residence time increases.

5.6.4 Carbon Conversion to Carbon Monoxide

A statistical analysis of the fitted Cities Service and Rocketdyne data indicated that carbon conversion to CO for the Montana Rosebud coal was a function of particle residence time, maximum gas temperature, hydrogen partial pressure, and hydrogen-to-coal ratio. (Cities Service Runs MR-16, 17, and 18 were excluded from the analysis since a statistical evaluation of the Cities Service subbituminous data showed that the measured conversion to CO was high for these tests.) Carbon conversion was not significantly affected by reactor size or particle size within the region investigated. The correlation fitted to the data is:

$$X_{CO} = 1 - \exp\left[-3.02\ \exp(-0.248\ P_{H_2}/t_R)\ \exp\ (0.677\ H/C)\ \exp(-8{,}380/T_G)\right] \tag{16}$$

where P_{H_2} is in psig, t_R is in milliseconds, H/C is in lb/lb, and T_G is in ^oR.

As shown in Equation 16, X_{CO} increases with increasing particle residence time, gas temperature, and hydrogen-to-coal ratio, and decreases with increasing hydrogen partial pressure. In addition, the effect of residence time on conversion increases as hydrogen partial pressure increases.

Equation 16 has a standard error of estimate of 1.3 percent in the predicted percent carbon conversion to CO. The measured and predicted carbon conversions are shown in Figure 5-15. The statistics and Figure 5-15 indicate that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar carbon conversions to CO under

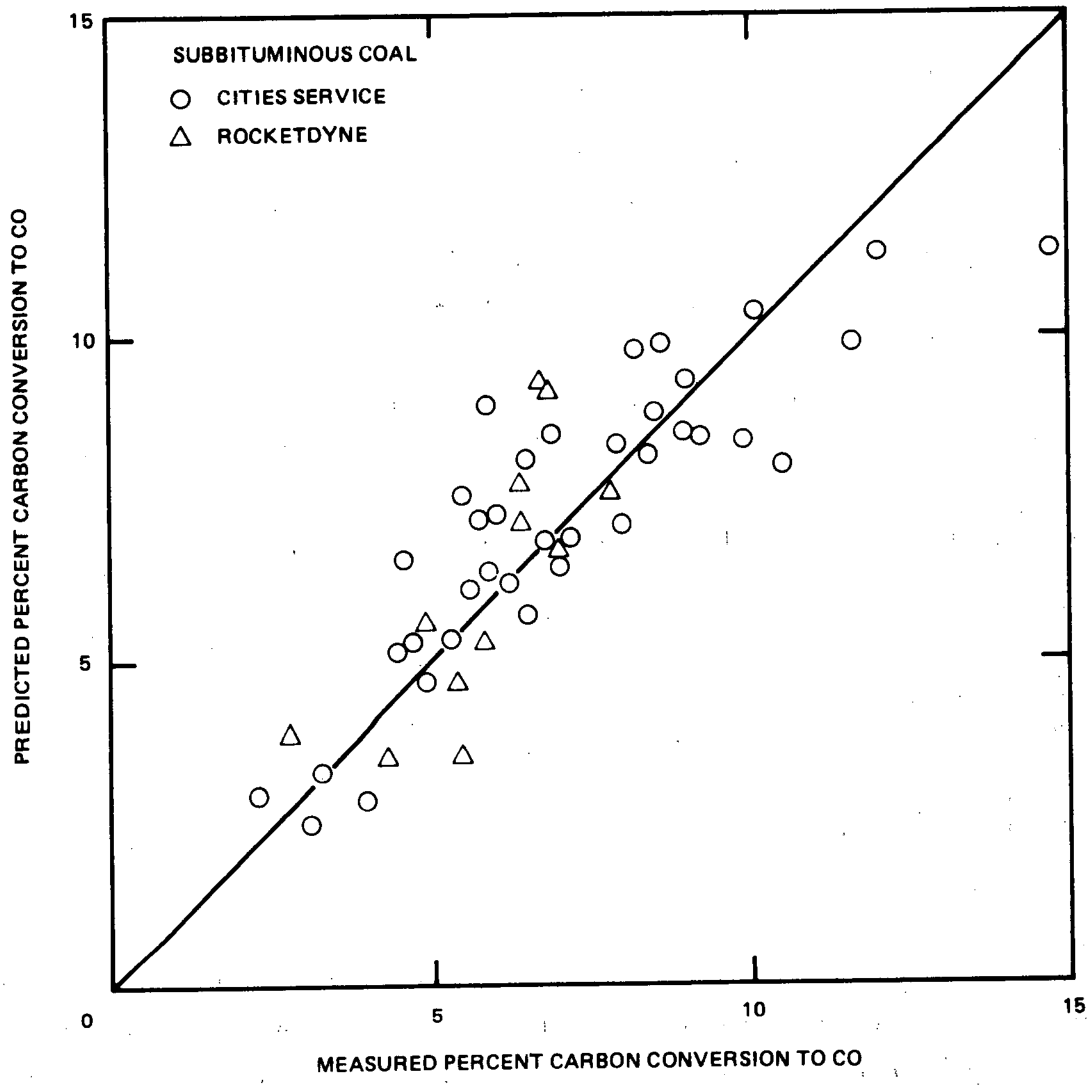

Figure 5-15. Comparison of Measured and Predicted Carbon Conversion to Carbon Monoxide for Subbituminous Coal

comparable operating conditions within the region investigated. In Figure 5-16, predicted values for carbon selectivity to CO from Equations 13 and 16 are plotted as a function of gas temperature for selected values of hydrogen partial pressure and residence times.

5.6.5 Carbon Conversion to Carbon Dioxide

A statistical analysis of the fitted data indicated that carbon conversion to CO_2 was a function of particle residence time, maximum gas temperature, hydrogen partial pressure, and hydrogen-to-coal ratio. Carbon conversion was not significantly affected by reactor size or particle size within the region investigated. The correlation fitted to the Rocketdyne and Cities Service subbituminous data is:

$$X_{CO_2} = 1 - \exp\left[-0.0231 \exp(-0.000832\, P_{H_2}) \exp(-1.36\, H/C) \exp(14{,}200/T_G)(t_R)^{-0.971}\right] \tag{17}$$

where P_{H_2} is in psig, H/C is in lb/lb, T_G is in ^oR, and t_R is in milliseconds.

As Equation 17 indicates, X_{CO_2} increases with decreasing residence time, gas temperature, hydrogen pressure, and hydrogen-to-coal ratio. Equation 17 has a standard error of estimate of 0.2 percent in the predicted percent conversion. The measured and predicted conversions are shown in Figure 5-17. The statistics and Figure 5-17 indicate that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar carbon conversions under comparable operating conditions within the region investigated. In Figure 5-18, predicted values for carbon selectivity to CO_2 from Equations 13 and 17 are shown as a function of gas temperatures for selected levels of pressure and residence time.

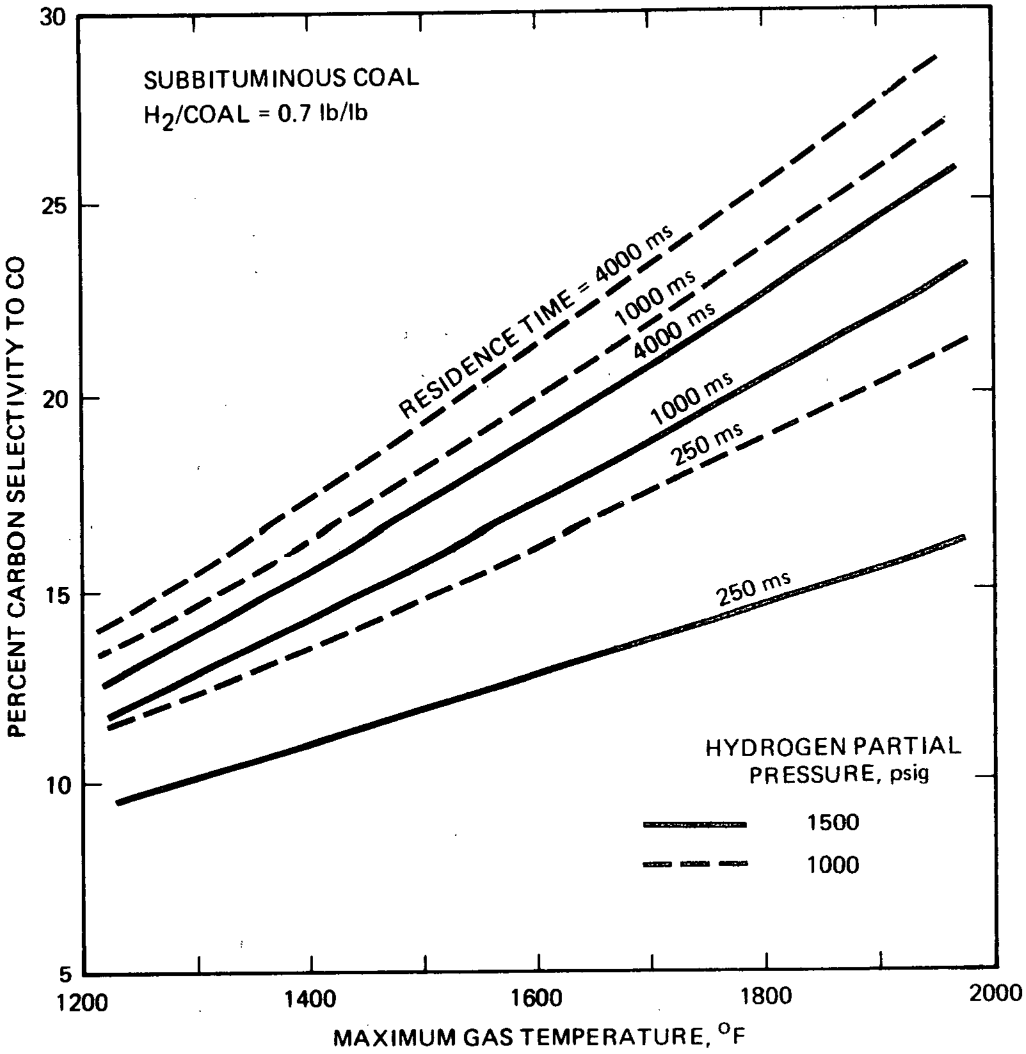

Figure 5-16. Predicted Carbon Selectivity to CO for Subbituminous Coal

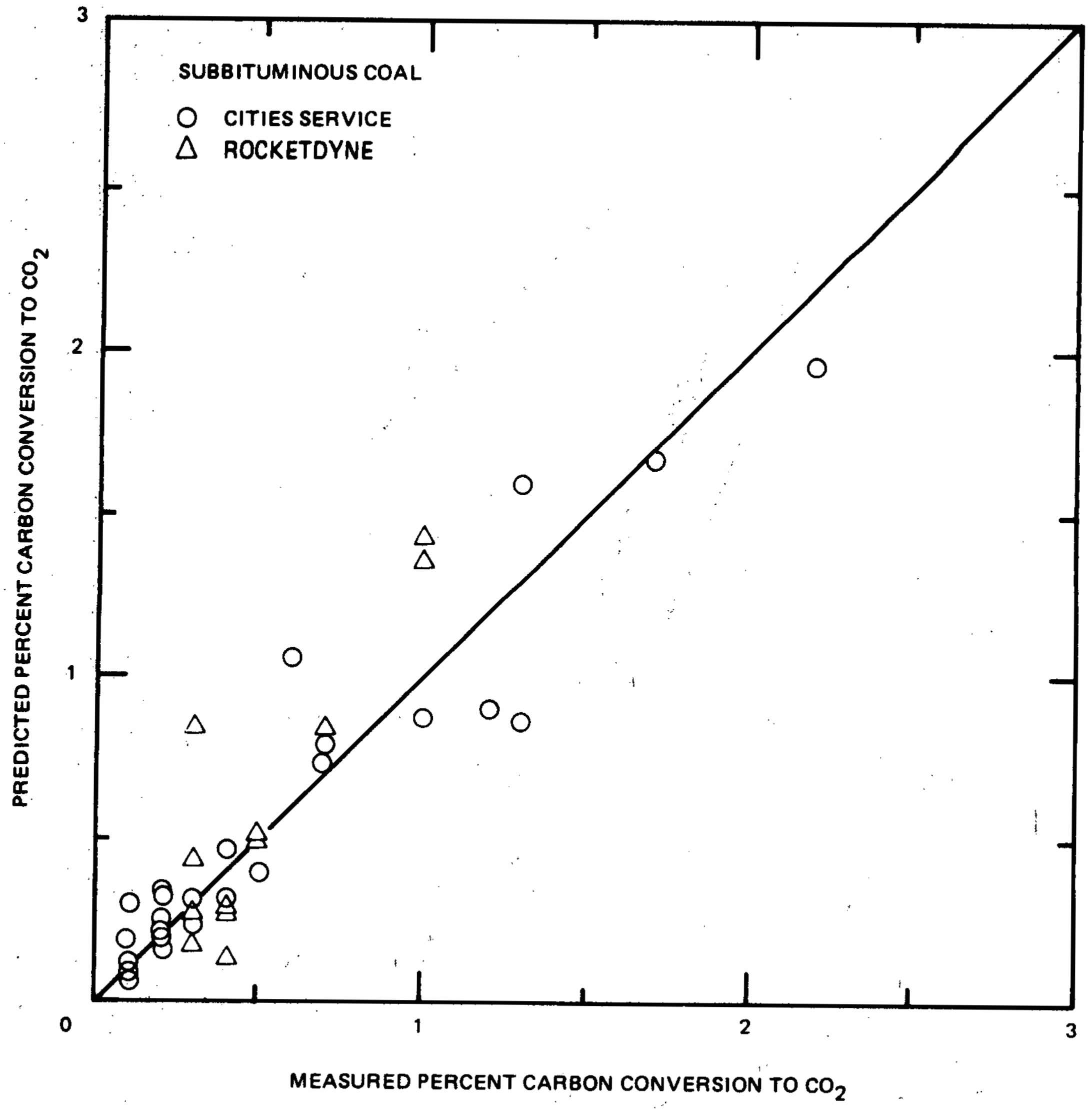

Figure 5-17. Comparison of Measured and Predicted Carbon Conversion to Carbon Dioxide for Subbituminous Coal

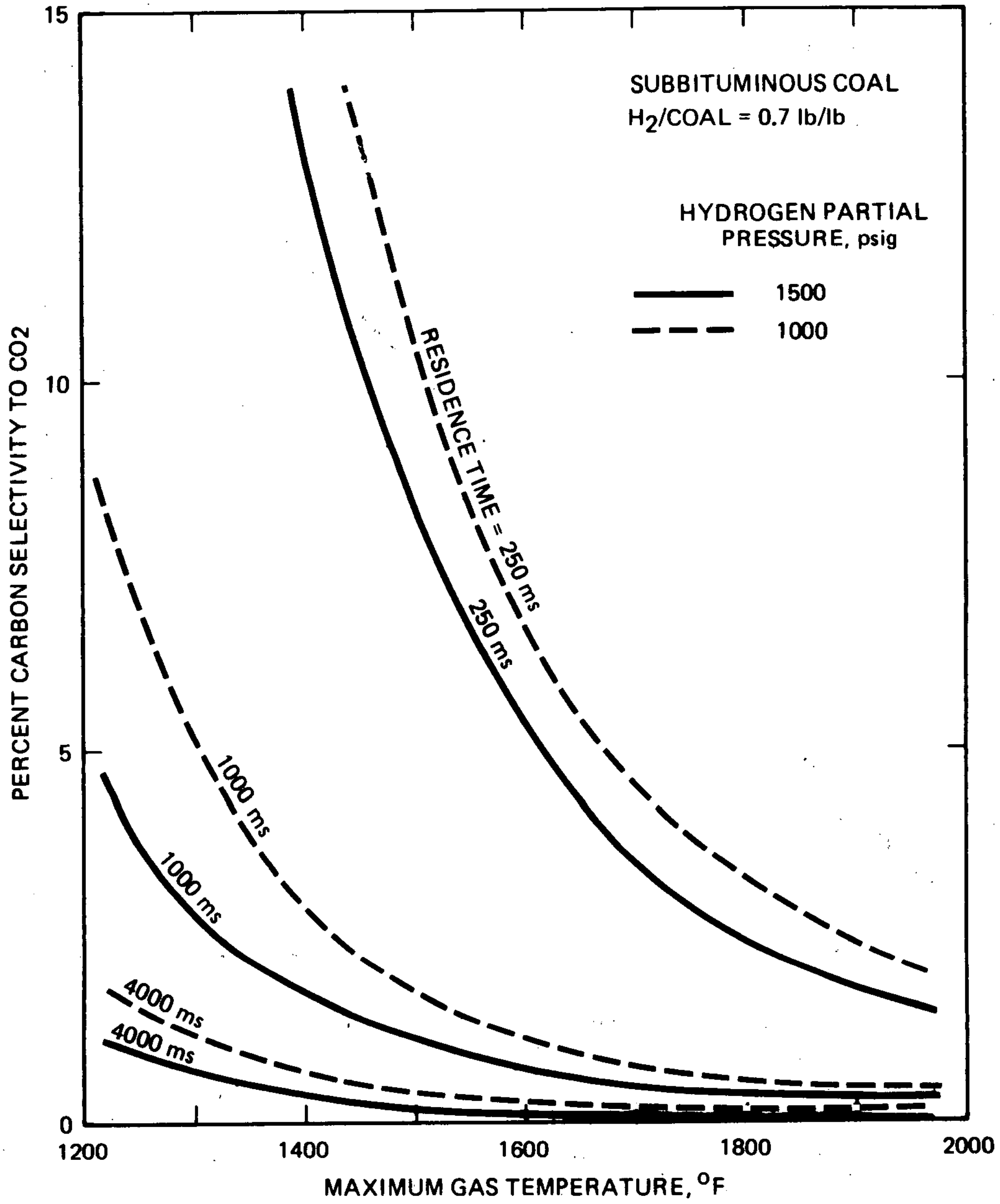

Figure 5-18. Predicted Carbon Selectivity to CO_2 for Subbituminous Coal

5.6.6 Comparison Between Predicted Values for Carbon Conversion and Selectivity to Products

In Figures 5-19 and 5-20, predicted carbon conversion to products and predicted carbon selectivity to products are shown, respectively, as functions of gas temperature for a particle residence time of 1,000 milliseconds and a hydrogen partial pressure of 1,500 psig. For these conditions of residence time and pressure, 50 percent carbon conversion and 100 percent carbon selectivity to gas are predicted for a gas temperature of approximately 1,900°F.

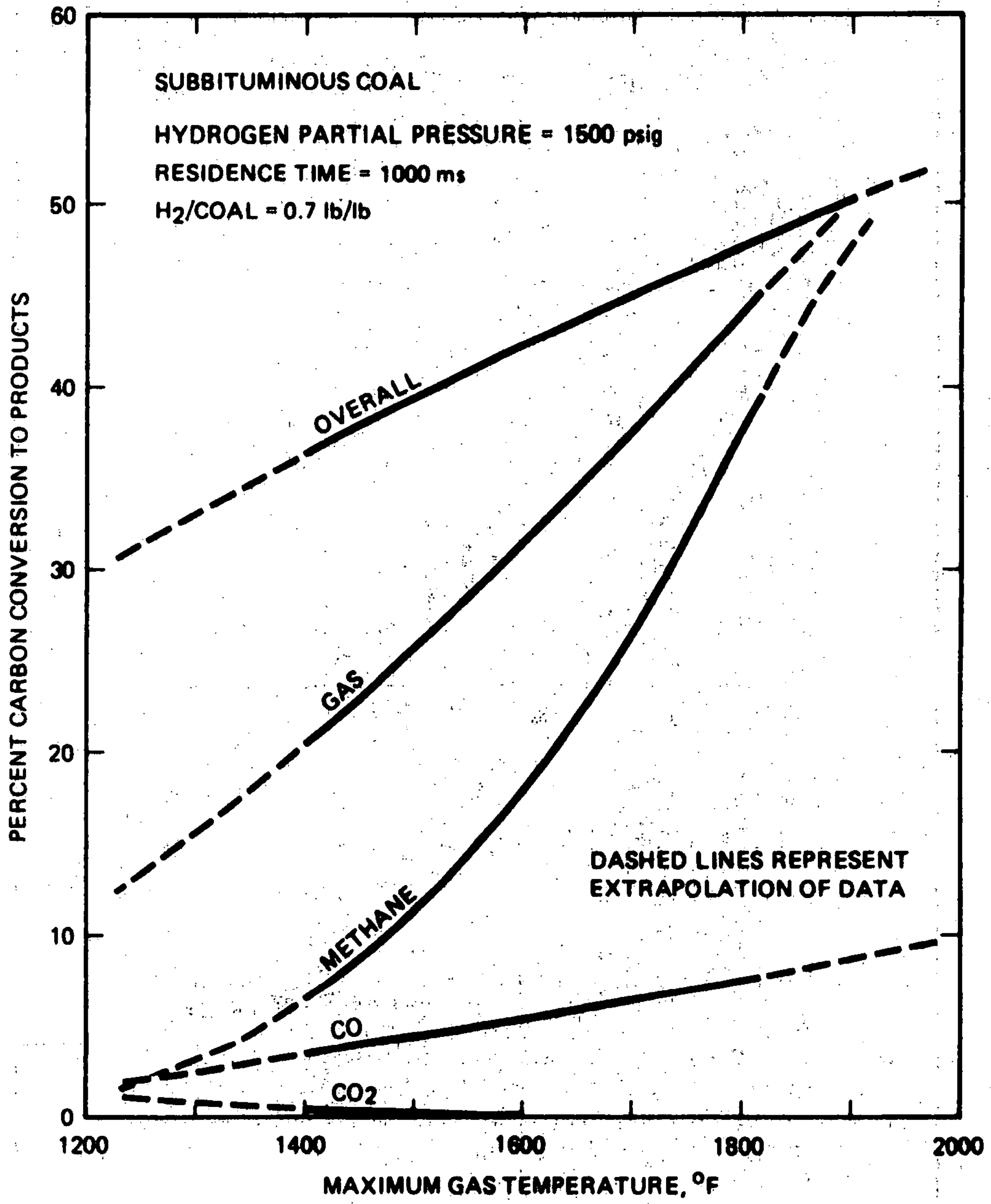

Figure 5-19. Predicted Carbon Conversion to Products for Subbituminous Coal

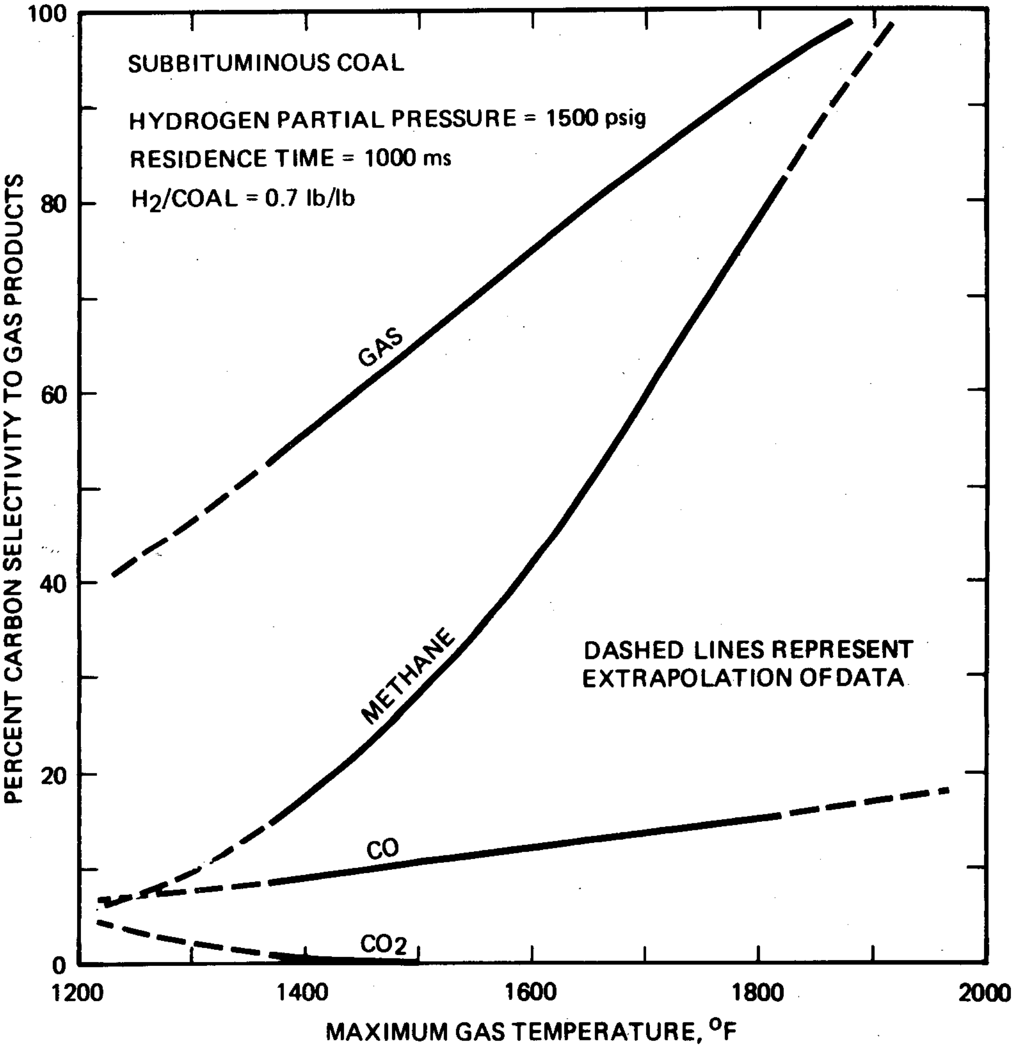

Figure 5-20. Predicted Carbon Selectivity to Gas Products for Subbituminous Coal

5.7 PREDICTION OF CARBON CONVERSION TO PRODUCTS FOR LIGNITE COAL

In this subsection, the Cities Service and Brookhaven hydropyrolysis data for lignite coal are fitted to the model proposed for predicting overall carbon conversion and carbon conversion to gas. Computer listings of the correlated variables for the Cities Service and Brookhaven lignite data are presented in Tables 4-3 and 4-6, respectively.

As discussed in Subsection 4.4, several Brookhaven tests had apparent inconsistencies in reported carbon conversion. The data from these suspect tests (Runs 16A, 16B, 16C, 17, 18A, 18B, 18C, 48, 49, 56, and 62) have been excluded from the analysis. Cities Service lignite Run 8 has also been excluded, owing to possible char accumulation on the reactor walls during the test (see Subsection 4.2.1).

Brookhaven has reported only reactor wall, and not reactor gas, temperature for its tests. Since the models for carbon conversion are correlated to gas temperature, it is assumed that the maximum gas temperature for each Brookhaven test is equal to the reported wall temperature.

It should be noted that for the range of variables studied in the Cities Service and Brookhaven reactor systems, the predicted equilibrium overall conversion of carbon and equilibrium conversion to gas are unity for all data points (see Subsection 4.3). For this condition, Equations 2, 3, and 7 simplify, with $X^* = X_G^* = 1$.

5.7.1 Overall Carbon Conversion

The Cities Service lignite test program was conducted under both entrained-flow (high gas velocity) and free-fall (low gas velocity) reactor operating conditions. For entrained-flow operation, particle residence time is approximately equal to gas residence time; for free-fall operation, particle residence time is less than gas residence time. A statistical analysis of the Cities Service lignite data showed that overall carbon conversion was a significant function of particle, rather than gas, residence time. Therefore, particle residence time was used to correlate the carbon conversion data for the combined Cities Service and Brookhaven lignite data.

A statistical analysis of the Cities Service and Brookhaven lignite coal data, with the suspect data points removed, indicated that carbon conversion was a function of particle residence time, maximum gas temperature, and hydrogen partial pressure. Carbon conversion was not significantly affected by reactor type, gas velocity, hydrogen-to-coal ratio, or particle size within the region investigated. The correlation fitted to the carbon conversion data is:

$$X = 1 - \exp\left[-5.56(t_{RP})^{0.0750} \exp(0.000327\ P_{H_2}) \exp(-6,570/T_G)\right] \qquad (18)$$

where t_{RP} is in milliseconds, P_{H_2} is in psig, and T_G is in ^{o}R.

As Equation 18 indicates, X increases with increasing coal particle residence time, hydrogen partial pressure, and gas temperature. The fact that overall carbon conversion is a relatively weak function of residence time suggests that a large fraction of the total conversion occurs through devolatilization within a short period of time and that a smaller fraction of the conversion occurs throughout the length of the reactor.

Equation 18 has a standard error of estimate of 5.2 percent in the predicted percent carbon conversion. The measured and predicted carbon conversions are shown in Figure 5-21. The statistics and Figure 5-21 indicate that the Cities Service and Brookhaven bench-scale reactors achieve similar carbon conversions under comparable operation conditions for lignite coal within the region investigated. The Brookhaven data do, however, show a poorer fit to the model than the Cities Service data.

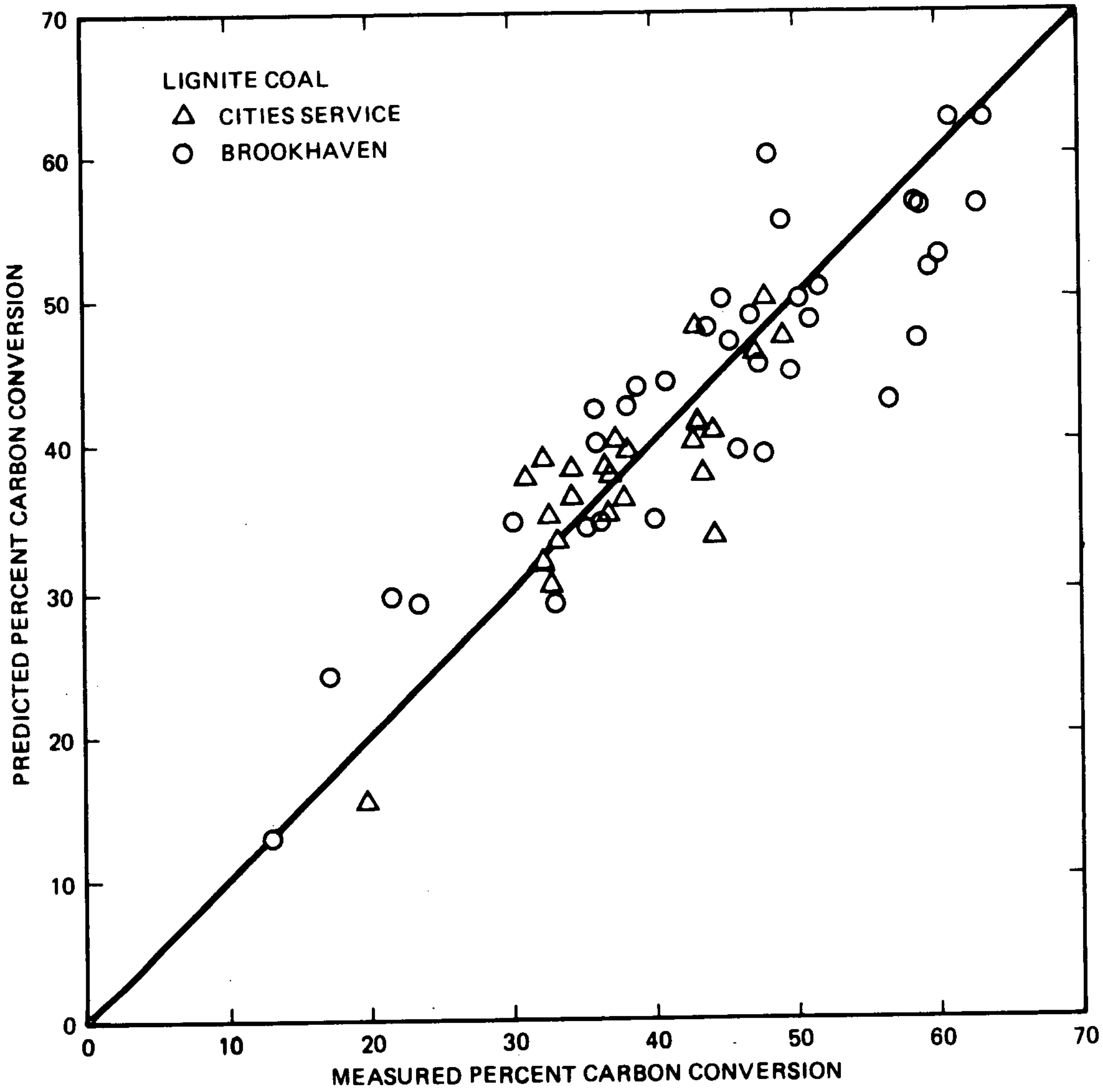

Figure 5-21. Comparison of Measured and Predicted Overall Carbon Conversion for Lignite Coal

In Figure 5-22, predicted values for overall carbon conversion from Equation 18 are shown as a function of gas temperature for selected values of pressure and particle residence time. As can be seen, conversion is a strong function of temperature and pressure, and a relatively weak function of particle residence time.

5.7.2 Carbon Conversion to Gas

A statistical analysis of the fitted Cities Service and Brookhaven lignite data indicated that carbon conversion to gas was a function of particle residence time, maximum gas temperature, and hydrogen partial pressure. Carbon conversion was not significantly affected by reactor size, hydrogen-to-coal ratio, or particle size within the region investigated. The correlation fitted to the data is:

$$X_G = 1 - \exp\left[-0.114(t_{RP})^{0.0839} \exp(0.00275\ P_{H_2}) \exp(-4.55\ P_{H_2}/T_G)\right] \qquad (19)$$

where t_{RP} is in milliseconds, P_{H_2} is in psig, and T_G is in ^{o}R.

As can be seen from Equation 19, carbon conversion increases with increasing residence time, hydrogen partial pressure, and reactor temperature. Also, the effect of temperature on gas conversion increases as pressure increases. Equation 19 has a standard error of estimate of 5.3 percent in the predicted percent carbon conversion to gas. The measured and predicted carbon conversions are illustrated in Figure 5-23. The statistics and Figure 5-23 indicate that the Cities Service and Brookhaven reactors achieve similar gas conversions under comparable operating conditions. Again, the Brookhaven data exhibit greater scatter than the Cities Service data.

In Figure 5-24, carbon selectivity to gas from Equations 18 and 19 (i.e., $\Phi_G = X_G/X$) is shown as a function of gas temperature and pressure for

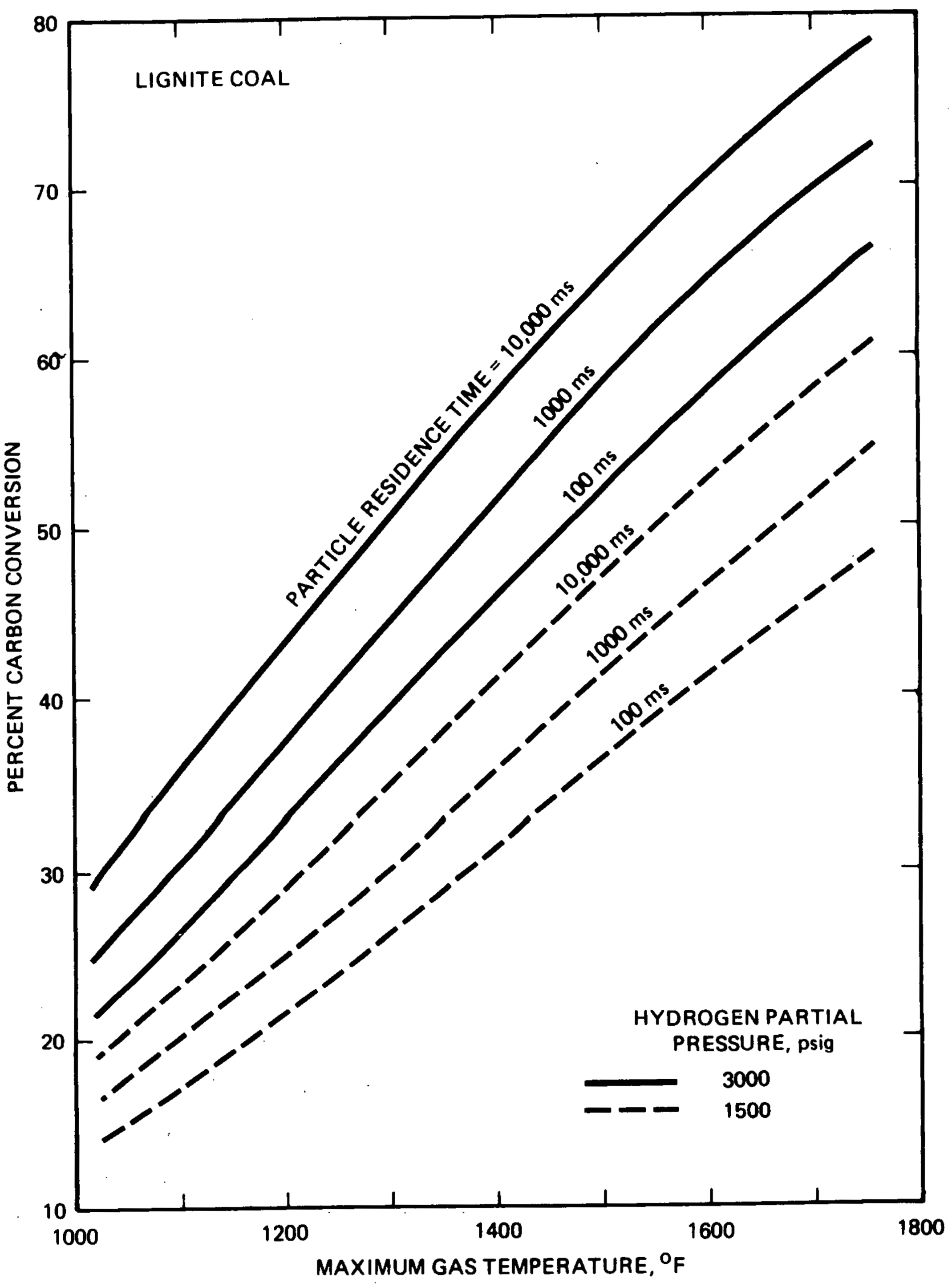

Figure 5-22. Predicted Overall Carbon Conversion for Lignite Coal

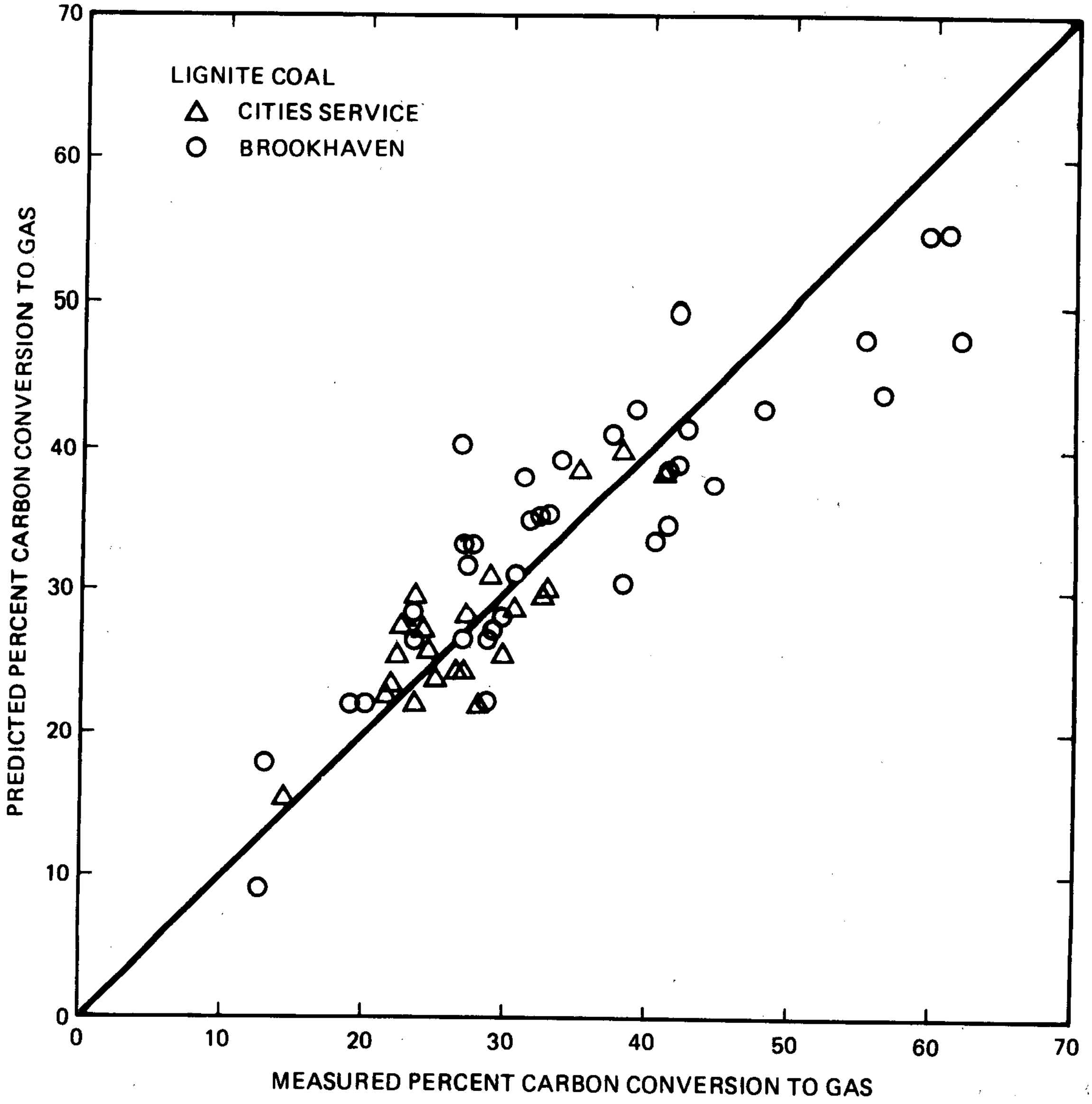

Figure 5-23. Comparison of Measured and Predicted Overall Carbon Conversion to Gas for Lignite Coal

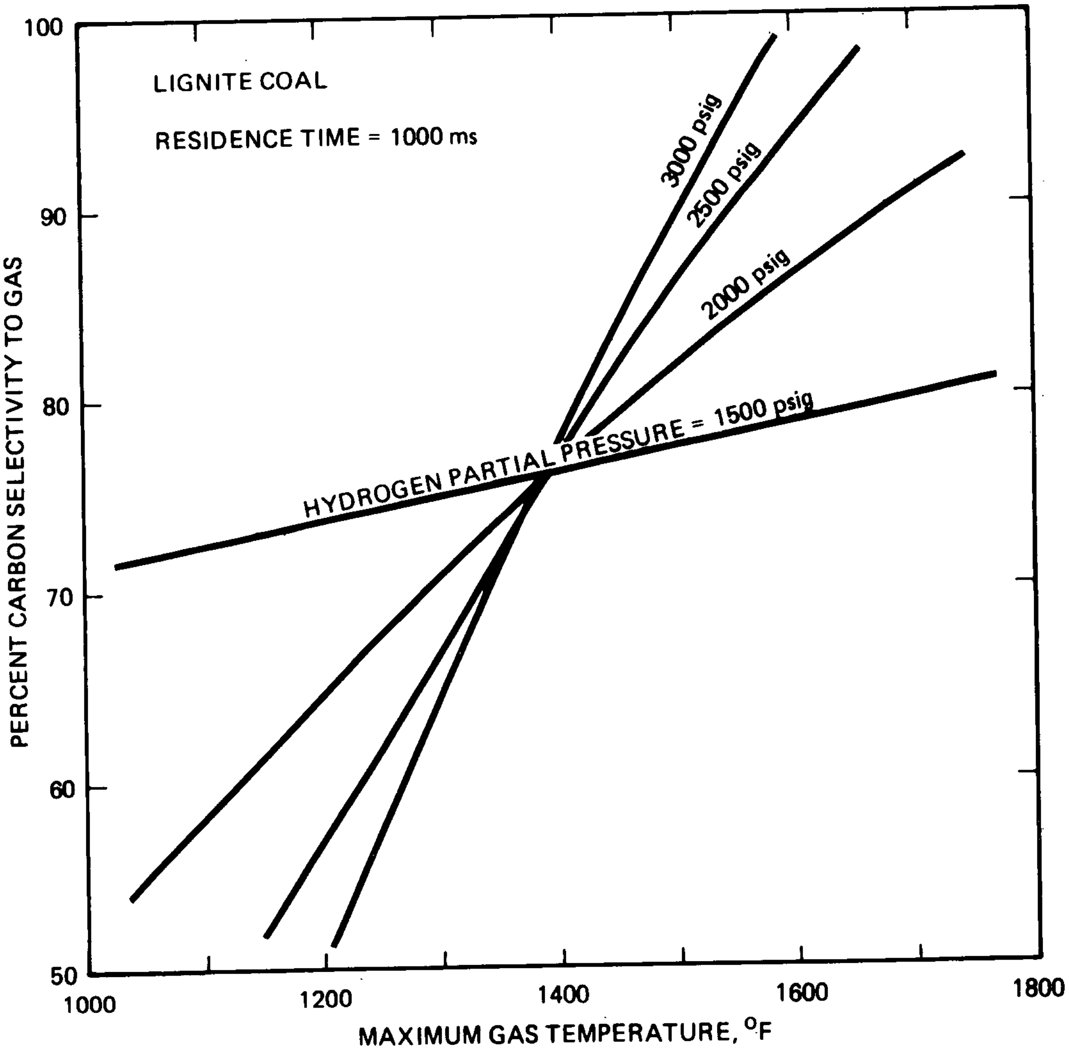

Figure 5-24. Predicted Carbon Selectivity to Gas for Lignite Coal

a particle residence time of 1,000 milliseconds. Note that gas selectivity increases with increasing pressure above 1,400°F, and decreases with increasing pressure below 1,400°F. Moreover, as predicted by Equations 18 and 19, Φ_G is a very weak function of residence time. From Figure 5-24, 100 percent selectivity to gas is predicted for a pressure of 2,500 psig and a gas temperature of approximately 1,700°F.

5.8 COMPARISON BETWEEN BITUMINOUS, SUBBITUMINOUS, AND LIGNITE COALS

The results of the data correlation have shown that predicted overall carbon conversion (or reactivity) for bituminous coal is not a statistically significant function of residence time (see Equation 11). As discussed in Subsection 5.5.1, this suggests that nearly all of the carbon conversion occurs through devolatilization within a relatively short period of time in the reactor; i.e., there is little direct methanation of char. The fact that selectivity to gas for bituminous coal is a significant function of residence time (see Equation 12) suggests that the initial higher (liquid) hydrocarbon products of devolatilization are cracked down to lower hydrocarbon products as gas residence time increases.

The fact that overall carbon conversion for subbituminous and lignite coals increases with residence time (see Equations 13 and 18) suggests that for these coals, conversion of carbon to products occurs throughout the length of the reactor.

Results from the data correlation have indicated that the predicted overall carbon conversion (or reactivity) for bituminous coal is greater than the reactivity of subbituminous and lignite coals at reduced residence time and/or pressure (see Figures 5-6, 5-10, and 5-22). The results have also shown that the reactivity of lignite coal is greater than that of subbituminous coal at increased temperature and increased pressure.

The variation in coal reactivities with temperature and particle residence time is illustrated in Figures 5-25 and 5-26. In Figure 5-25, predicted carbon conversion from Equations 11, 13, and 18 is shown as a function of temperature for a residence time of 1,000 milliseconds and a pressure of 1,500 psig. In Figure 5-26, predicted conversion is shown as a function of temperature for a residence time of 3,000 milliseconds and a pressure of 1,500 psig.

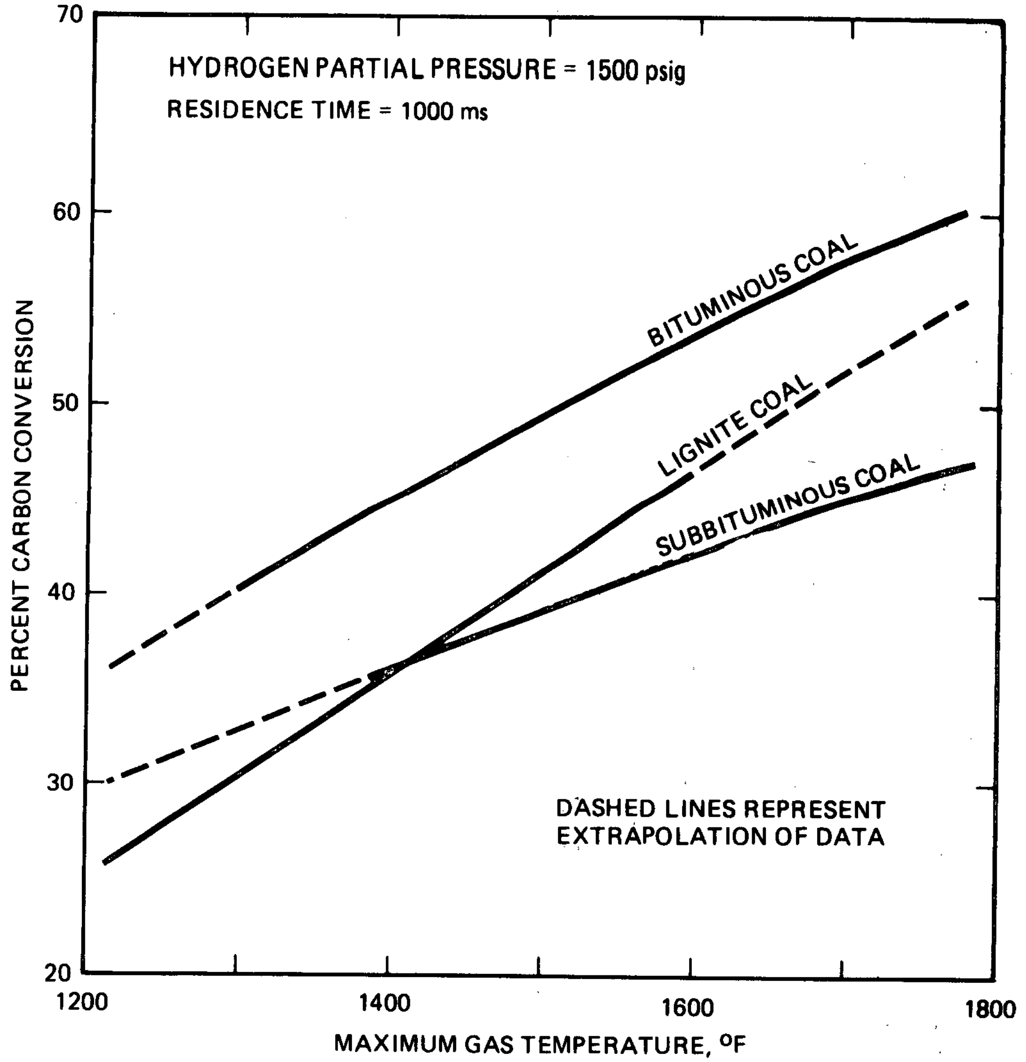

Figure 5-25. Predicted Overall Carbon Conversion for Bituminous, Subbituminous, and Lignite Coals — 1,000 Milliseconds

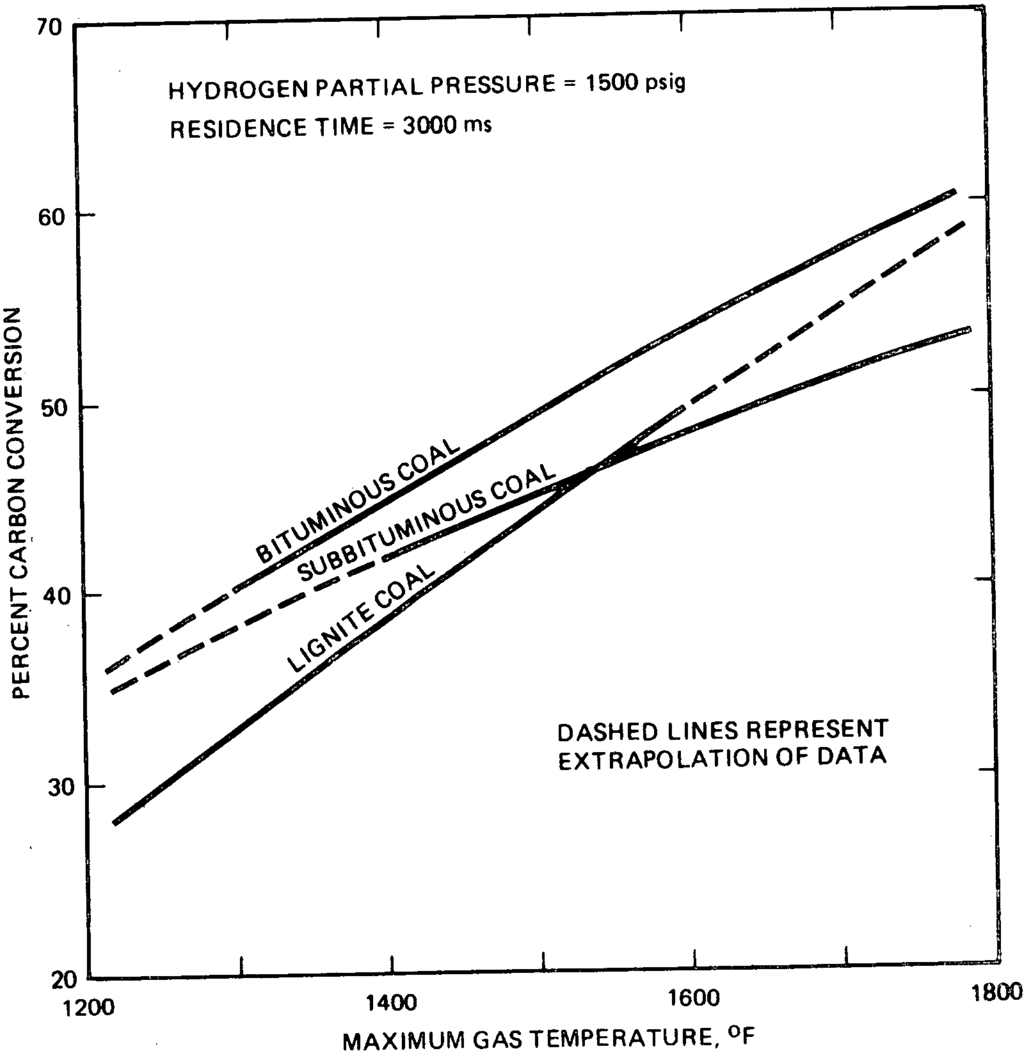

Figure 5-26. Predicted Overall Carbon Conversion for Bituminous, Subbituminous, and Lignite Coals — 3,000 Milliseconds

The variation in predicted carbon selectivity to gas with temperature and residence time is illustrated in Figures 5-27 and 5-28. For low residence times, subbituminous coal gives the highest predicted gas selectivity at higher temperatures (see Figure 5-27). At larger residence times, bituminous coal gives the highest predicted selectivity to gas throughout most of the temperature range (see Figure 5-28).

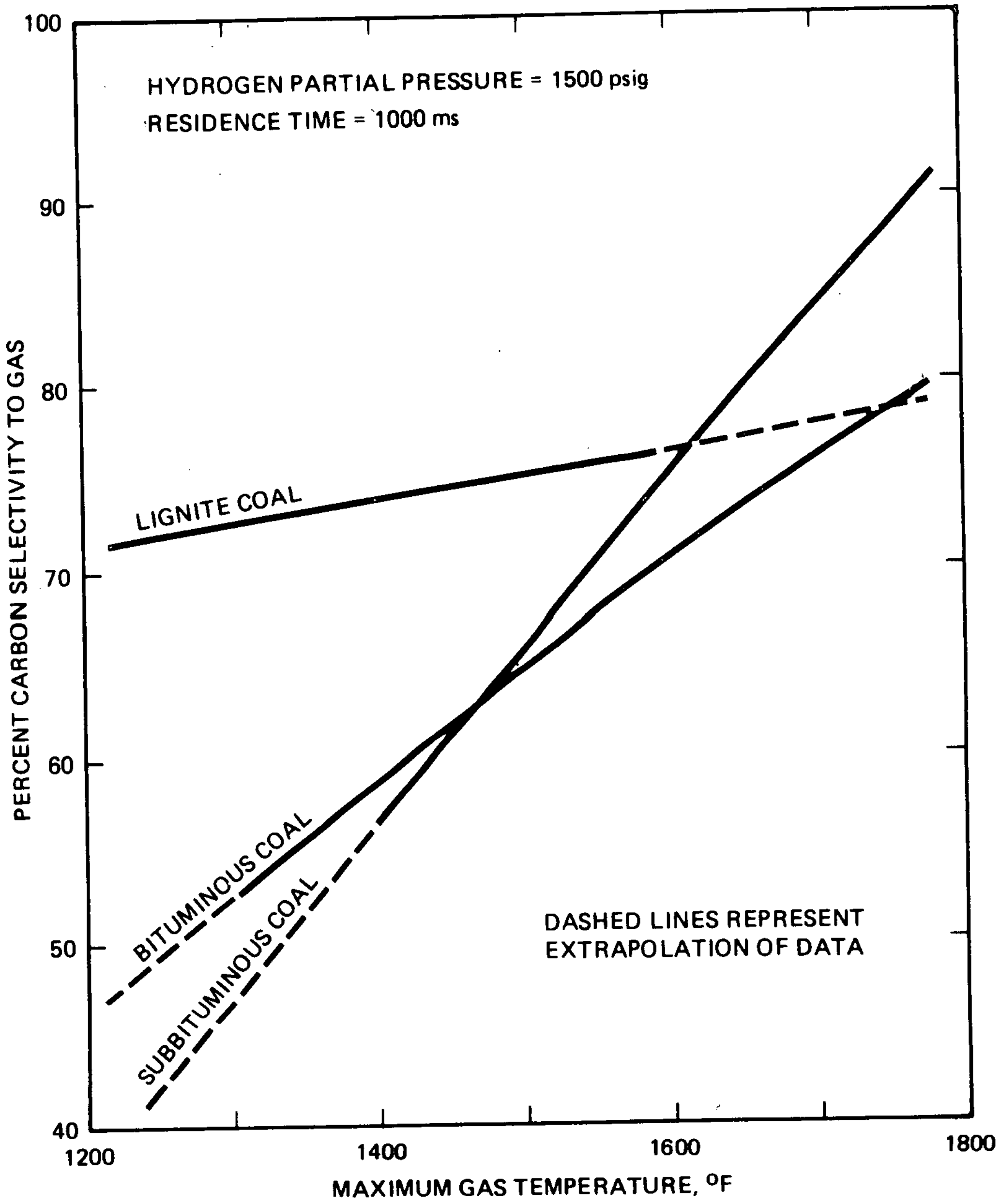

Figure 5-27. Predicted Carbon Selectivity to Gas for Bituminous, Subbituminous, and Lignite Coals — 1,000 Milliseconds

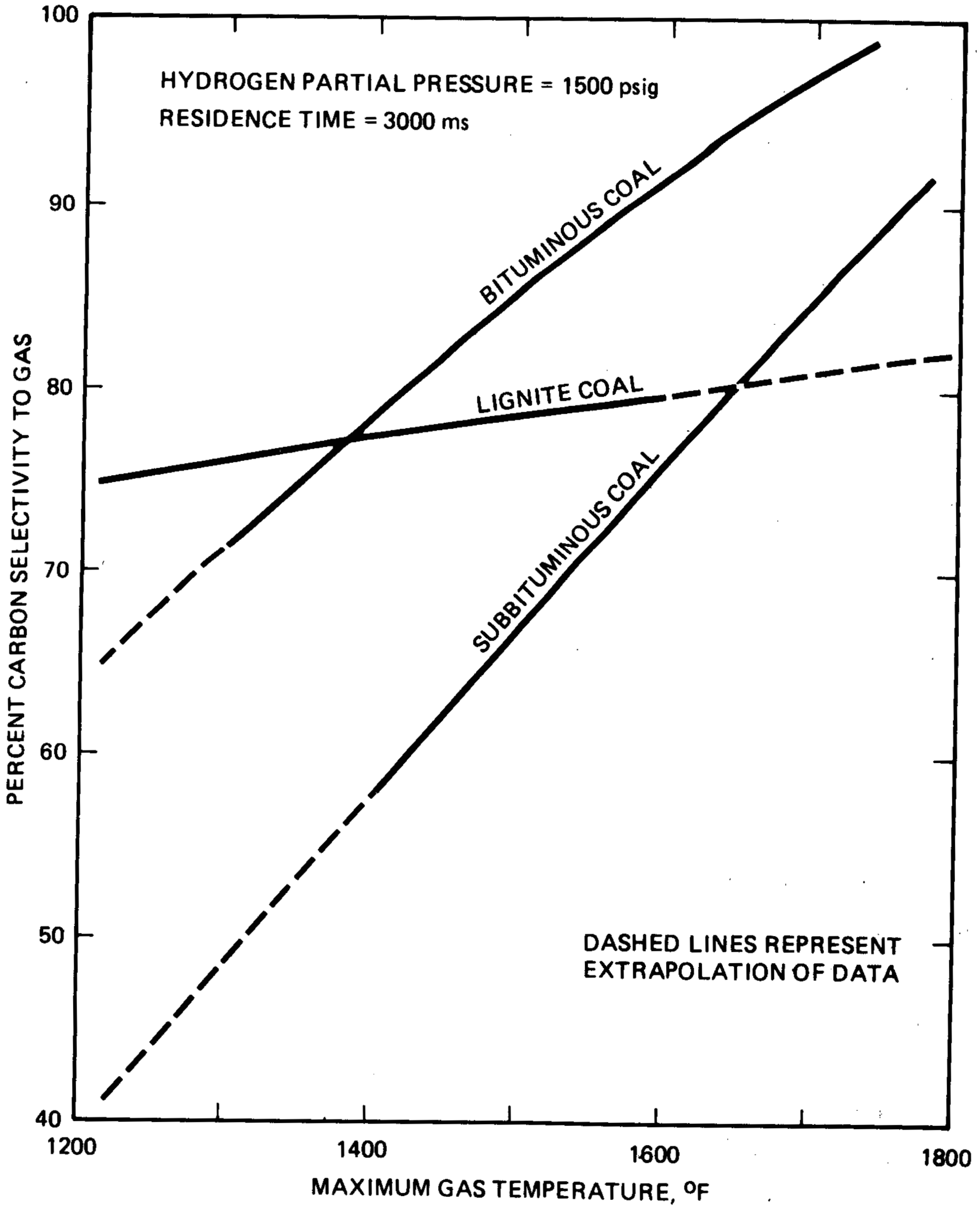

Figure 5-28. Predicted Carbon Selectivity to Gas for Bituminous, Subbituminous, and Lignite Coals — 3,000 Milliseconds

5.9 GOODNESS OF FIT FOR PROPOSED MODELS

The goodness of fit of the models proposed for carbon conversion and carbon selectivity depends primarily on three factors: (1) the accuracy of the functional form of the proposed models within the range of the data generated, (2) the experimental error associated with the generated data, and (3) the design of the experiments.

The standard error of estimate (regression error) includes both the pure experimental error and the error due to the "lack of fit" of the model.[26] The experimental error is usually determined from replicate runs. (Replicate runs have identical levels of the independent variables.) Unfortunately, replicate runs were not included in the Rocketdyne and Cities Service experimental designs. It is not possible, therefore, to separate the regression error for the fitted bituminous and subbituminous coal models into the experimental error and lack of fit components.

The design of the experiments affects the range of the independent (and dependent) variables. The statistically determined effect of an independent variable upon a dependent variable may be associated with the experimental range of the independent variable. For example, the gas temperatures for the Cities Service lignite data (see Table 4-3) are strongly concentrated between 1,480^{o}F and 1,620^{o}F, which is a difference of only 140^{o}F. There are only four data points with temperatures lower than 1,480^{o}F (at 1,460^{o}F, 1,430^{o}F, 1,320^{o}F and 1,000^{o}F), and a single data point at 1,660^{o}F. Thus, if a large experimental error exists for Run 20 at 1,000^{o}F, the calculated effect of gas temperature on conversion or selectivity will be in error at lower temperatures. Dependence of calculated effects on one (or a small number) of data points can be minimized by conducting factorial designs with a large number of runs at the independent variable extremes.

5.10 SENSITIVITY ANALYSIS FOR PROPOSED MODELS

The sensitivity (or error) of a predicted value of a depandent variable, Y, due to the uncertainty (or error) in a given independent (operating) variable, v, can be expressed as

$$\Delta Y = (\partial Y/\partial v)\ \Delta v \tag{20}$$

where ΔY is the error in the dependent variable, $\partial Y/\partial v$ is the predicted change of the dependent variable with respect to a change in the operating variable (i.e., derivative of Y with respect to v), and Δv is the error in the measured operating variable.

For this study, the dependent variables are carbon conversion and carbon selectivity, and the primary independent variables are temperature, pressure, and residence time. As can be seen from Equation 20, the error in the dependent variable increases with increasing $\partial Y/\partial v$. For the subbituminous coal data, for example, the change in carbon conversion with respect to residence time, $\partial X/\partial t_R$, is larger at smaller residence times than at larger residence times (see Equation 13 and Figure 5-10). Therefore, the error (or sensitivity) for overall carbon conversion due to errors in residence time decreases as residence time increases.

Since errors in the measurements of the independent variables or in the variations of the measurements with time (the precision) have not been reported by Rocketdyne, Cities Service, PFRC, or Brookhaven, values of Δv in Equation 20 must be assumed. Values of $\partial Y/\partial v$ can be obtained, of course, from the fitted correlations by differentiation.

Predicted errors in carbon conversion, X, and carbon selectivity to gas, Φ_G, due to assumed errors in residence time, temperature, and pressure are shown in Tables 5-2, 5-3, and 5-4, respectively. A predicted error of zero means that the independent variable has no effect on the dependent variable (e.g., from Equation 11, carbon conversion is not a function of residence time for bituminous coal). Predicted errors in gas selectivity are greater than predicted errors in carbon conversion because gas selectivity is obtained by dividing carbon conversion to gas by overall carbon conversion; i.e., $\Phi_G = X_G/X$. The error in Φ_G, therefore, is the sum of the errors in X_G and X.

Table 5-2

SENSITIVITY OF PREDICTED CARBON CONVERSION AND GAS SELECTIVITY TO ERRORS IN RESIDENCE TIME MEASUREMENT

Basis: ± 10 percent error in residence time
1,800°F gas temperature
1,500 psig pressure

Coal	Residence Time, ms	± Percent Error in Prediction	
		Carbon Conversion	Gas Selectivity
Bituminous	300	0	2.6
	3,000	0	1.9
Subbituminous	300	7.3	14.9
	3,000	0.56	1.2
Lignite	300	0.50	1.1
	3,000	0.46	1.0

Table 5-3

SENSITIVITY OF PREDICTED CARBON CONVERSION AND GAS SELECTIVITY TO ERRORS IN GAS TEMPERATURE MEASUREMENT

Basis: ± 2 percent error in gas temperature
1,000 ms residence time
1,500 psig pressure

Coal	Gas Temperature, °F	± Percent Error in Prediction	
		Carbon Conversion	Gas Selectivity
Bitiminous	1,400	3.1	9.5
	1,800	2.6	7.7
Subbituminous	1,400	2.9	11.5
	1,800	2.4	5.2
Lignite	1,400	5.1	10.7
	1,800	3.7	8.1

Table 5-4

SENSITIVITY OF PREDICTED CARBON CONVERSION
AND GAS SELECTIVITY TO ERRORS IN PRESSURE MEASUREMENT

Basis: ± 5 percent error in pressure
1,800°F gas temperature
1,000 ms residence time

Coal	Pressure, psig	± Percent Error in Prediction	
		Carbon Conversion	Gas Selectivity
Bituminous	1,000	0	0
	1,500	0	0
Subbituminous	1,000	0.80	2.8
	1,500	1.2	3.9
Lignite	1,000	1.1	4.1
	1,500	1.6	5.6

In Table 5-2, predicted errors in X and Φ_G are shown at two levels of residence time (300 and 3,000 milliseconds) for an assumed ± 10 percent error in the measurement of residence time. (At 300 and 3,000 milliseconds, the assumed measurement errors in residence time would be ± 30 and ± 300 milliseconds, respectively.) As can be seen, the subbituminous coal correlations are most sensitive to errors in residence time. At 300 milliseconds, for example, the expected errors in overall conversion and gas selectivity for subbituminous coal are ± 7 and ± 15 percent, respectively.

In Table 5-3, the predicted errors in X and Φ_G are shown at two levels of temperature (1,400°F and 1,800°F) for an assumed ± 2 percent error in the measurement of temperature. (At 1,400°F and 1,800°F, the assumed measurement errors in temperature would be ± 28°F and ± 36°F, respectively.) As can be seen, the sensitivity of predictions for X and Φ_G to errors in temperature are comparable for the three coals. The sensitivities are slightly greater at lower temperatures.

In Table 5-4, the predicted errors in X and Φ_G are shown at two levels of pressure (1,000 and 1,500 psig) for an assumed ± 5 percent measurement error in pressure. (At 1,000 and 1,500 psig, the assumed errors in pressure would be ± 50 and ± 75 psig, respectively.) As can be seen, the sensitivity of the predictions for the three coals to measurement errors in pressure is relatively small. The sensitivities are slightly larger at higher pressure.

Section 6

CONCEPTUAL DESIGN OF A FULL-SCALE HYDROGASIFICATION REACTOR

This section presents a preliminary conceptual design and design basis for the hydrogasification stage of a proposed full-scale reactor facility for converting subbituminous coal to SNG. As currently envisioned, the reactor facility will consist of a hydrogasification stage to produce methane-rich product gas from the coal, and a hydrogen production stage to produce hydrogen-rich product gas from unreacted char and coal.

The conceptual full-scale hydrogasification stage will have a configuration similar to the Rocketdyne reactor assembly, which incorporates an entrained-downflow tubular reactor chamber. Coal particles and hot hydrogen gas will be mixed inside high-efficiency injector elements, producing coal heatup rates in excess of 500,000°F/sec. The hydrogen gas will be heated first to the "preheat temperature" by heat exchange with product gas, and then to the "injected gas temperature" by partial combustion through oxygen addition in a preburner. More detailed descriptions of the Rocketdyne reactor have been given by Gray[8] and by Oberg.[9] A sketch and a description of the conceptual hydrogasification reactor are presented in Subsection 6.2.

6.1 CONCEPTUAL DESIGN BASIS

The operating levels for the full-scale hydrogasification stage have been based on predictions from the semiempirical correlations, presented in Subsection 5.6, which have been fit to the Rocketdyne and Cities Service subbituminous coal data. As mentioned in Subsection 5.6, the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar overall carbon conversions and carbon conversions to products under comparable operating conditions.

The selected and calculated operating parameters for the conceptual full-scale hydrogasification reactor stage are given below. This design basis should be considered preliminary and should be updated as more subbituminous coal data are generated by Cities Service and Rocketdyne.

Selected Operating Parameters:

Coal type	Montana Rosebud subbituminous
Coal mean particle size	40 to 50 microns
Coal feed rate	108 tons/hr
Overall carbon conversion	50 percent
Carbon selectivity to gas	100 percent
Reactor pressure	1,500 psig
Hydrogen-to-coal ratio	0.4 lb/lb

Calculated Operating Parameters:

Maximum reactor gas temperature	1,875°F
Particle (or gas) residence time	1,100 milliseconds
Carbon selectivity to methane	86 percent
Carbon selectivity to CO	13 percent
Carbon selectivity to CO_2	Negligible
Hydrogen preheat temperature	1,000°F
Oxygen-to-hydrogen ratio in preburner	0.45 lb/lb
Injected gas temperature	1,740°F
Average volumetric gas flow rate	621,000 ft^3/hr

The coal type and size chosen are those used in recent Cities Service and Rocketdyne testing; the coal properties can be found in Appendix B. The coal feed rate of 108 tons/hr is based on a recommendation by Gray[27] for a maximum coal capacity for a single injector element of 3 tons/hr and a maximum number of 36 injector elements per head.

Greene[15] has shown that an overall carbon conversion of approximately 36 percent is required to operate at the "char balance point" with Montana Rosebud subbituminous coal. At the char balance point, the quantity of unreacted char from the hydrogasification stage is just sufficient to produce the required process hydrogen in the hydrogen production (oxygasifier) stages. For conversions greater than 36 percent, additional coal is required in the oxygasifier; for conversions less than 36 percent, char from the hydrogasifier is fed to the power plant in place of coal.

Greene[28] has also shown that the cost of SNG produced from the reactor facility decreases as carbon conversion in the hydrogasification stage increases past the char balance point. An overall carbon conversion of 50 percent was selected as the reactor design basis, since that value is close to the maximum conversion obtained to date in the Cities Service and Rocketdyne subbituminous coal testing (see Tables 4-2 and 4-4 and Figure 5-9), and is above the char balance point.

A carbon selectivity to gas of 100 percent was selected as the reactor design basis by the DOE. A reactor design pressure of 1,500 psig was chosen because at pressures less than 1,500 psig, the predicted maximum reaction temperature required for 100 percent carbon selectivity to gas is greater than 1,900°F (see Figure 5-12 and Equations 13 and 14). Temperatures greater than 1,900°F are considered excessive and are outside the range of the Cities Services and Rocketdyne subbituminous coal testing.

The selected hydrogen-to-coal ratio of 0.4 lb/lb is within the lower range investigated by Rocketdyne. Note that the statistical analysis of the Cities Service and Rocketdyne subbituminous coal data revealed that carbon conversion and carbon selectivity to methane were relatively unaffected by hydrogen-to-coal ratio within the region investigated.

The maximum gas temperature of 1,875°F was calculated for the condition of 100 percent carbon selectivity to gas at a pressure of 1,500 psig. For the calculation, the predicted value for overall conversion (Equation 13) was equated to the predicted value for conversion to gas (Equation 14). Note that selectivity to gas is insensitive to residence time.

The particle (or gas) residence time of 1,100 milliseconds was computed, using Equation 14, for the condition of 50 percent overall carbon conversion, at a pressure of 1,500 psig and a temperature of 1,875°F.

The value of carbon selectivity to methane was obtained by dividing the predicted value for conversion to methane, X_M, by the predicted value for overall conversion, X, at a gas temperature of 1,875°F, a residence time of 1,100 milliseconds, a pressure of 1,500 psig, and a hydrogen-to-coal ratio of 0.4 lb/lb. The predicted value of X was obtained from Equation 13 and the predicted value of X_M from Equation 7. The kinetic component of Equation 7 was obtained from Equation 15 and the equilibrium component, X_M^*, from Figure 5-3. It should be noted that for this relatively low hydrogen-to-coal ratio and relatively high temperature, X_M^* is approximately 0.84.

The values for carbon selectivity to CO and CO_2 were calculated by dividing the predicted values for conversion to CO and CO_2 (Equations 16 and 17) by the predicted value for overall conversion at the operating conditions previously specified.

The required hydrogen preheat temperature of 1,000°F and the oxygen-to-hydrogen ratio of 0.45 lb/lb in the preburner were calculated from an overall heat balance around the hydrogen preburner inlet and the reactor outlet, assuming adiabatic operation and a coal higher heating value of 11,280 Btu/lb. For the heat balance calculation, the reactor outlet gases were assumed to be methane, CO, H_2O, and excess hydrogen.

The gas injection temperature of 1,740°F was computed from a heat balance around the hydrogen preburner, using the calculated hydrogen preheat temperature of 1,000°F and an oxygen-to-hydrogen ratio of 0.45 lb/lb.

The hydrogen mass feed rate was calculated from the given hydrogen-to-coal ratio and the coal feed rate. The calculated average volumetric gas flow rate of 621,000 ft^3/hr (172 ft^3/sec) was taken as the arithmetic average of the calculated flow rate at the reactor inlet and exit, using the ideal gas law.

The reactor dimensions are related to the nominal superficial gas velocity as follows:

$$S = V_G/u_G = 172/u_G \tag{20}$$

and

$$L = t_R u_G = 1.10\ u_G \tag{21}$$

where,

S = reactor cross-sectional area, ft^2
L = reactor length, feet
u_G = superficial gas velocity, ft/sec
V_G = average volumetric gas flow rate, ft^3/sec

For any specified gas velocity, the reactor cross-sectional area and length can be calculated using the above equations. A superficial gas velocity range of from 10 to 25 ft/sec has been selected for the reactor design, based on recommendations by Gray[27,29] and the conditions tested at Cities Service and Rocketdyne. At 10 ft/sec gas velocity, the required reactor cross-sectional area from Equation 20 is 17 ft^2 and the required reactor length from Equation 21 is 11 feet. At 25 ft/sec gas velocity, the required cross-sectional area is 7 ft^2 and the required length is 28 feet.

6.2 CONCEPTUAL DESIGN

As discussed in the previous subsection, a full-scale reactor facility will consist of a hydrogasification stage to produce methane-rich product gas from the coal, and a hydrogen production stage (char oxygasifier) to produce hydrogen-rich product gas from the unreacted char. In this subsection, a preliminary conceptual design of a full-scale hydrogasification section is presented in detail, followed by a discussion of the char gasification stage.

6.2.1 Hydrogasification Stage

A detailed sketch of the conceptual full-scale hydrogasification reactor stage is shown in Figure 6-1. The hydrogasification reactor vessel consists of two sections. The upper section of the vessel contains a shell and tube heat exchanger, and the lower section includes a hydrogasifier and a cyclone separator. As discussed in the previous subsection, the hydrogasification reactor would have a length roughly between 10 and 30 feet, depending on the gas velocity. In an alternate reactor configuration, which will not be described in this report, the heat exchanger and cyclone are placed in separate vessels.

In the hydrogasification section, hot hydrogen at 1,740°F is contacted with coal feed at 77°F in a total of 36 mixing-injection nozzles; each nozzle handles a maximum of 3 tons of coal per hour, as has been discussed in Subsection 6.1. The nozzle design is similar to that developed and used by Rocketdyne in its 1-ton/hr and 1/4-ton/hr hydrogasification reactor facilities. The mixing nozzles are arranged in single rank in a circle. Coal enters each through a central tube, and hot hydrogen enters through annular nozzles around the coal tubes.

Char and product gas flow downward in an entrained-flow manner through the annuli formed by the inner wall of the reactor vessel shell and the outer shell of a central pipe (or duct) through which the product gas

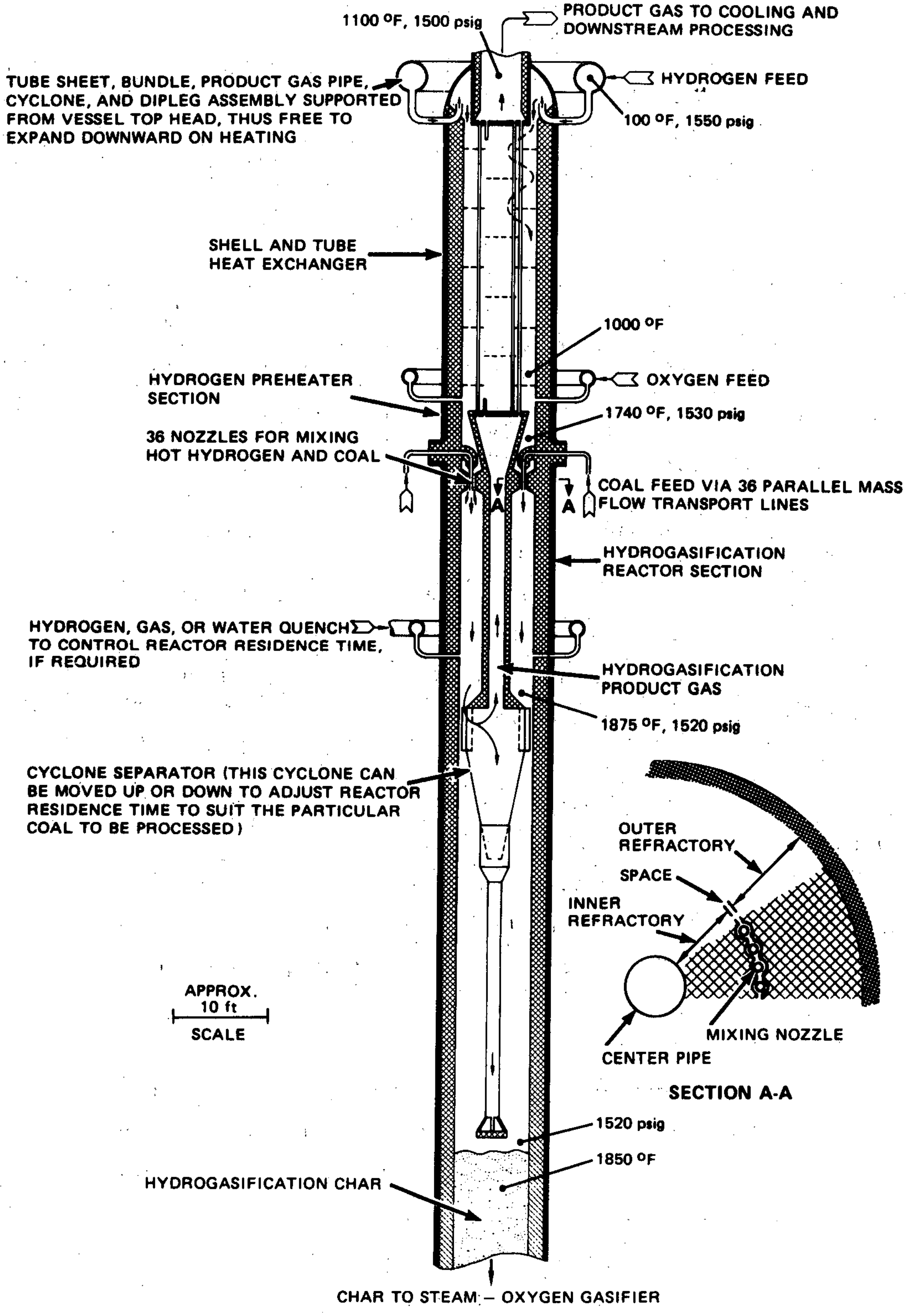

Figure 6-1. Conceptual Design of a Full-Scale Hydrogasification Reactor

leaves the hydrogasifier. The coal char solids and the gas stream are separated in a cyclone which sends the product gas stream back up through the central pipe or duct and sends the char downward through a cyclone dipleg. The char next collects in a surge volume section and is held there as a feed material for hydrogen production. The cyclone is constructed so that it can be moved vertically and hence could be used to control the residence time of char and gas inside the reactor. A gas or water quench system is also installed near the bottom of the central pipe to provide an extra or standby facility for quickly controlling the reaction, if necessary.

Product gas from the hydrogasifier cyclone flows upwards through the tube side of a shell and tube heat exchanger, where it is cooled from about 1,875°F to about 1,100°F by heat exchange with cold feed hydrogen flowing downward through the exchanger shell side. The hydrogen stream is assumed to enter at 100°F and is heated to about 1,000°F.

The hydrogen effluent from the exchanger is further heated to about 1,740°F by combustion with oxygen, which is injected into the hydrogen stream near the exchanger outlet, as shown in Figure 6-1. This hydrogen preburner section should be relatively short since combustion and heating are rapid, but if experience shows otherwise, the preheater section could be easily made longer than indicated in Figure 6-1.

The reactor vessel shell has internal refractory insulation and a bare metal shell free of external insulation. Although this "hot-wall" design is typical of catalytic cracking practice, the higher temperature (1,875°F) and pressure (1,500 psig) within the shell demand careful attention in the interest of operating reliability and overall safety. One approach would be to provide infrared scanning and hot-spot alarm instrumentation for the outer shell wall, whose surface temperature would be kept between 250°F and 400°F. A screen of louvers would shield the bare metal shell from rain and weather-induced thermal stresses. This vessel shell design will certainly require alloy lining. Other approaches to reactor vessel shell design are being considered. One approach will be to use a pressurized water jacket inside the vessel strength shell to keep the metal temperature as low as 550°F.

6.2.2 Char Gasification Stage

Efficient hydrogen generation from the hydrogasifier char product will have a major impact on process thermal efficiency and economics. Gasification of the unreacted char with steam and oxygen at temperatures of 1,800°F to 2,700°F will generally produce a gas consisting mostly of carbon monoxide and hydrogen. Further processing of this raw gas (shift, methanation, and purification) will yield the process hydrogen required for the hydrogasification stage.

The following versions of the char/oxygen/steam reactor design should be investigated:

- An entrained-downflow reactor incorporating Rocketdyne-type injectors for rapid mixing of the reactants
- A dense-phase, fluid-bed reactor similar in design to the IGT-HYGAS char gasifier
- A Texaco high-pressure, entrained-flow gasifier
- A Koppers-Totzek entrained-flow gasifier

As an example, if a dense-phase, fluid-bed reactor scheme is considered, the char solids from the hydrogasifier would normally be transferred at the hydrogasifier pressure (about 1,500 psig) to the char gasifier via a standpipe. If the fluid-bed nominal temperature equals that of the incoming char (about 1,875°F), several minutes[30] of holding time will probably be required to produce acceptable conversion of char.

Oxygen and steam would enter the char fluid bed via a gas distributor manifold near the bottom of the reactor, and the product gas would leave the reactor at the top through a cyclone separator. The entrained fines would be collected and returned to the reactor by the cyclone dipleg and the oxygen carrier stream. The spent char (mostly ash) would leave the fluid-bed reactor at the bottom and go to a quench pot, where it would be sprayed with sufficient water to make up a slurry suitable for transfer to pressure letdown and eventual disposal.

The above considerations suggest that the fluid-bed char gasifier operating at 1,875°F could be roughly 100 to 150 feet high. Higher reactor operating temperatures (2,500°F to 2,700°F) could reduce reaction time (holding time) and reactor size, but the reactor would be operating in the slagging region.

Section 7

RECOMMENDATIONS FOR ADDITIONAL EXPERIMENTS

This section (1) lists and discusses critical data that are missing from the Rocketdyne and Cities Service bituminous and subbituminous coal testing and that are required for reliable pilot plant design, (2) describes recommended experiments to acquire the necessary data, and (3) discusses the impact on the process design phase in case the necessary data cannot be experimentally determined.

The subject matter discussed in this section fulfills the contractual requirements for Task IV.

7.1 TESTS AT REDUCED HYDROGEN-TO-COAL RATIO

As discussed in Subsection 5.2, hydrogen-to-coal ratio (H/C) has a significant effect on the equilibrium conversion of carbon to products, X^*. For the high values of H/C (from 0.25 to 1.4 lb/lb) employed during the Rocketdyne and Cities Service bituminous and subbituminous coal testing, the predicted values of X^* are all unity. Therefore, the effect of X^* (or H/C) on the kinetic component of the proposed carbon conversion model (Equations 2 and 3) could not be obtained from the data, i.e., the fitted coefficient, α_9, in Equation 3 could not be determined.

To determine the effect of H/C (or X^*) on conversion, it is recommended that, if possible, the following six experiments for bituminous and subbituminous coals be conducted in the Rocketdyne and/or Cities Service reactors at a maximum gas temperature of 1,800°F, a pressure of 1,500 psig, and a residence time of 3,000 milliseconds:

For bituminous coal, H/C = 0.1, 0.2, 0.3 lb/lb

For subbituminous coal, H/C = 0.05, 0.1, 0.2 lb/lb

The predicted values of X^* for the recommended tests are all less than unity (see Figures 5-1 and 5-2). Lower values of H/C were chosen for the subbituminous tests since subbituminous coal gives higher values of predicted equilibrium conversion than bituminous coal, at the same level of H/C.

7.2 REPLICATE RUNS

The goodness of fit of the models proposed for carbon conversion and carbon selectivity depends primarily on three factors: (1) the accuracy of the functional form of the proposed models within the range of the data generated, (2) the experiemntal error associated with the generated data, and (3) the design of the experiments.

The experimental error and the variability associated with generated data are often estimated from results of replicate runs. (Replicate runs have identical levels of the independent variables.) Without replicate runs, it is not possible to separate the regression error for the model into the pure experimental error and the error due to the "lack of fit" of the model;[26] in addition, the adequacy of the model for pilot-plant design cannot be precisely determined.

Unfortunately, replicate runs were not included in the experimental designs for the Rocketdyne and Cities Service hydrogasification programs. It is recommended, therefore, that a minimum of three replicate runs be added to the Rocketdyne and Cities Service test matrices for each coal studied. If possible, the replicate runs should be distributed throughout the measured range of the dependent variable (carbon conversion).

7.3 BITUMINOUS COAL TESTS AT LOW PRESSURE

A statistical analysis of the Rocketdyne bituminous data has indicated that carbon conversion and carbon selectivity to products are not significant functions of hydrogen partial pressure over the range 480 to 1,440 psig (see Equations 11 and 12). Only 3 tests out of a total of 49, however, were conducted at pressures below 1,000 psig (see Tables 4-1 and 4-2). Since it may be advantageous to operate a commercial-scale hydrogasifier at reduced pressure, it is important to verify the results of the statistical analysis for the lower pressures. It is recommended, therefore, that additional bituminous coal tests be conducted by Rocketdyne at hydrogen partial pressures of 750 and 500 psig.

7.4 TESTS WITH ADDITION OF INERT GAS TO REACTOR RECYCLE GAS

For the Rocketdyne and Cities Service bituminous and subbituminous data, it was not possible to determine separately the effects of both hydrogen partial pressure, P_{H_2}, and reactor pressure, P, on carbon conversion. (It is expected that conversion increases with P_{H_2} and decreases with P.) This is because P_{H_2} was nearly equal to P for a majority of the tests; i.e., P_{H_2} and P are confounded. These separate effects could be determined by adding an inert gas (e.g., helium) and/or methane to the reactor recycle (feed) gas. Adding methane, however, introduces a complication, namely, that the equilibrium conversion of carbon, X^*, is changed in the reactor system, along with the hydrogen partial pressure. (Of course, in an actual full-scale system, the recycle gas will contain some quantity of methane that has not been separated from the product gas.)

Rocketdyne and Cities Service have conducted tests with 15 volume percent addition of methane into the reactor feed gas.[11,12,15] These data, however, were not available in time to be incorporated into this program.. To clearly separate the effect of methane addition on pressure and X^*, it is recommended that at least one of the Cities Service tests be duplicated with helium instead of methane addition to the reactor feed gas.

It should be noted that for a hydrogen-to-coal ratio larger than about 0.3 lb/lb, and for a small quantity of methane in the recycle gas, P and P_{H_2} are nearly equal. For these cases, the fitted models can confidently be used to predict pilot-scale performance.

Section 8

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Appendix A

COMPUTER LISTING OF HYDROPYROLYSIS DATA

This appendix presents a computer listing of the Rocketdyne, Cities Service, PERC, and Brookhaven hydrogasification and hydropyrolysis data contained in the data base. Blanks in the tables indicate data that have not been measured or data that have not been collected. The nomenclature and units in the listings are given below.

DIAM	Reactor diameter, inches
FCOAL	Coal feed rate, lb/hr
GVEL	Superficial gas velocity, ft/sec
HCONS	Hydrogen consumption, lb H_2/lb carbon feed
HCRAT	Hydrogen-to-coal ratio, lb/lb
HPRES	Hydrogen partial pressure, psig
LENGTH	Reactor length, feet
PHIC2	Weight fraction carbon selectivity to ethane
PHIG	Weight fraction carbon selectivity to gas
PHIHC	Weight fraction carbon selectivity to hydrocarbon gas
PHIM	Weight fraction carbon selectivity to methane
PSIZE	Mean coal particle size, microns
RTGAS	Gas residence time, milliseconds
RTPAR	Particle residence time, milliseconds
TGEIT	Equivalent isothermal reactor temperature, $^{\circ}$F
TGMAX	Maximum gas temperature, $^{\circ}$F
TPRES	Total pressure, psig
TWALL	Reactor wall temperature, $^{\circ}$F
X	Weight fraction overall carbon conversion
XBTX	Weight fraction carbon conversion to BTX
XCO	Weight fraction carbon conversion to CO

XCO_2	Weight fraction carbon conversion to CO_2
XC2	Weight fraction carbon conversion to ethane
XC3	Weight fraction carbon conversion to C-3 hydrocarbons
XC4.	Weight fraction carbon conversion to C-4 hydrocarbons
XGAS	Weight fraction carbon conversion to gas
XHC	Weight fraction carbon conversion to hydrocarbon gas
XM	Weight fraction carbon conversion to methane
XOIL	Weight fraction carbon conversion to light oil

The data files that constitute the data base are available from the National CSS (NCSS) on-line, time-sharing computer service. NCSS has a national computer network available through a local telephone dial-up in most major cities. For instructions concerning access and use of the data files, please contact the authors, John A. Brunner, or John K. Jacobs at Bechtel Corporation, 50 Beale Street, San Francisco, California 94941 [(415)768-1234].

Table A-1

ROCKETDYNE PARTIAL LIQUEFACTION DATA FOR BITUMINOUS COALS — DOE CONTRACT EX-76-C-01-2044

RUN	DATE	COAL*	PSIZE	LENGTH	DIAM	FCOAL	HCRAT	HCONS
5	1/31/77	BTM-1	56.	5.00	3.370	2963.00	0.250	
6	2/ 3/77	BTM-1	56.	5.00	3.370	1613.00	0.478	.0154
7	2/ 7/77	BTM-1	56.	5.00	3.370	961.00	0.775	.0393
8	2/17/77	BTM-1	56.	5.00	4.870	2020.00	0.365	.0462
9	2/22/77	BTM-1	56.	5.00	4.870	2034.00	0.365	.0998
10	3/ 1/77	BTM-1	56.	5.00	4.870	2052.00	0.314	.0961
11	3/ 4/77	BTM-1	56.	5.00	4.870	1498.00	0.334	.1216
12	3/ 9/77	BTM-1	56.	5.00	4.870	1480.00	0.333	.0513
13	3/23/77	BTM-1	56.	5.00	2.370	2650.00	0.292	.0154
14	3/25/77	BTM-1	56.	5.00	2.370	1912.00	0.397	.0487
15	3/29/77	BTM-1	56.	5.00	2.370	1883.00	0.403	.0157
16	4/ 4/77	BTM-1	56.	5.00	2.370	1642.00	0.443	.0215
17		BTM-1	56.	5.00	2.370	1490.00	0.507	.0272
18		BTM-1	56.	5.00	2.370	1814.00	0.409	.0265
19		BTM-1	56.	5.00	2.370	1796.00	0.429	.0148
20		BTM-2	52.	5.00	2.370	2153.00	0.293	.0287
21		BTM-2	52.	5.00	2.370	1602.00	0.458	.0336
22		BTM-2	52.	5.00	2.370	1188.00	0.370	.0085
23		BTM-2	36.	5.00	2.370	1620.00	0.469	.0377
24		BTM-2	36.	5.00	2.370	1404.00	0.528	.0554
25		BTM-2	36.	5.00	3.370	1159.00	0.656	
26	9/ 9/77	BTM-2	36.	5.00	3.370	1595.00	0.485	
27	9/14/77	BTM-2	36.	5.00	3.370	1631.00	0.472	
28	9/16/77	BTM-2	52.	5.00	3.370	1591.00	0.491	
29	9/21/77	BTM-2	52.	5.00	3.370	1706.00	0.418	
30	9/23/77	BTM-2	52.	5.00	3.370	1739.00	0.435	
31	9/27/77	BTM-2	52.	5.00	3.370	1397.00	0.505	
32	9/29/77	BTM-2	52.	5.00	3.370	1649.00	0.452	
34	10/ 4/77	BTM-2	52.	5.00	3.370	1858.00	0.414	
37	10/31/77	BTM-2	52.	5.00	4.870	1998.00	0.304	
38	11/ 8/77	BTM-2	52.	5.00	4.870	1958.00	0.313	
39	11/ 9/77	BTM-2	52.	5.00	4.870	2081.00	0.296	
40	11/10/77	BTM-2	52.	5.00	4.870	1498.00	0.279	
41	11/11/77	BTM-2	52.	5.00	4.870	1721.00	0.243	
42	11/14/77	BTM-2	52.	5.00	4.870	1732.00	0.249	

*BTM-1 is Kentucky #9/14 bituminous HvCb coal from the Colonial Mine of the Pittsburgh and Midway Mining Co.

BTM-2 is Kentucky #9 bituminous HvAb coal from the Hamilton No. 2 Mine of the Island Creek Coal Co.

Table A-1 (Cont'd)

RUN	GVEL	TPRES	HPRES	TWALL	TGMAX	TGEIT	RTGAS	RTPAR
5	32.30	1000.	939.	1290.	1290.		155.	155.
6	39.70	1000.	925.	1640.	1700.		126.	126.
7	42.00	1000.	921.	1900.	1950.		119.	119.
8	18.20	1000.	921.	1600.	1690.		274.	274.
9	12.20	1500.	1385.	1870.	1880.		410.	410.
10	10.20	1500.	1397.	1570.	1570.		490.	490.
11	7.90	1500.	1424.	1650.	1650.		634.	634.
12	11.80	1000.	942.	1680.	1680.		424.	424.
13	79.40	1000.	926.	1720.	1720.		63.	63.
14	51.00	1500.	1400.	1770.	1770.		98.	98.
15	111.00	700.	647.	1660.	1660.		45.	45.
16	72.50	1000.	933.	1687.	1687.		69.	69.
17	78.10	1011.	944.	1730.	1740.		64.	64.
18	74.60	999.	930.	1600.	1630.		67.	67.
19	147.00	520.	483.	1590.	1590.		34.	34.
20	63.30	1001.	928.	1590.	1600.		79.	79.
21	78.10	1001.	931.	1690.	1690.		64.	64.
22	87.70	502.	468.	1630.	1630.		57.	57.
23	79.40	1003.	934.	1640.	1640.		63.	63.
24	82.00	1002.	930.	1770.	1770.		61.	61.
25	41.30	1001.	929.	1873.	1918.		121.	121.
26	39.10	1000.	938.	1697.	1721.		128.	128.
27	37.30	1001.	946.	1579.	1609.		134.	134.
28	39.70	999.	936.	1736.	1765.		126.	126.
29	23.60	1497.	1403.	1640.	1721.		212.	212.
30	36.80	998.	941.	1568.	1627.		136.	136.
31	23.90	1496.	1401.	1826.	1938.		209.	209.
32	39.40	996.	932.	1726.	1835.		127.	127.
34	75.80	1000.	944.	1454.	1532.		66.	66.
37	19.60	999.	944.	1539.	1568.		255.	255.
38	18.50	1000.	948.	1384.	1405.		271.	271.
39	20.20	998.	944.	1614.	1661.		247.	247.
40	22.20	1004.	946.	1528.	1586.		225.	225.
41	20.90	998.	952.	1353.	1431.		239.	239.
42	23.60	1001.	946.	1590.	1687.		212.	212.

Table A-1 (Cont'd)

RUN	X	XGAS	XHC	XM	XC2	XC3	XC4
5	.382						
6	.542	.215					
7	.615	.297					
8	.596	.289					
9	.645	.490					
10	.609	.476					
11	.627	.607					
12	.576	.387					
13	.560	.187					
14	.597	.282					
15	.560	.201					
16	.573	.236					
17	.592	.257					
18	.519	.178					
19	.562	.144					
20	.540	.184					
21	.590	.238					
22	.570	.222					
23	.600	.213					
24	.638	.277					
25	.630	.230					
26	.615	.235					
27	.571	.209					
28	.587	.254					
29	.576	.275					
30	.546	.241					
31	.628	.447					
32	.622	.274					
34	.479	.181					
37	.482	.206					
38	.462	.152					
39	.513	.240					
40	.481	.234					
41	.432	.165					
42	.518	.260					

Table A-1 (Cont'd)

RUN	XCO	XCO2	XOIL	XBTX	PHIG	PHIHC	PHIM	PHIC2
5								
6				.048	.397			
7				.008	.483			
8				.053	.485			
9				.001	.760			
10				.034	.782			
11				.017	.968			
12				.071	.672			
13				.031	.334			
14				.058	.472			
15				.037	.359			
16				.033	.412			
17			.288	.049	.434			
18			.261	.037	.343			
19			.257	.019	.256			
20			.175	.046	.341			
21			.221	.078	.403			
22			.209	.027	.389			
23			.186	.072	.355			
24			.178	.110	.434			
25			.114	.097	.365			
26			.137	.075	.382			
27			.186	.054	.366			
28			.184	.072	.433			
29			.166	.087	.477			
30			.212	.053	.441			
31			.056	.085	.712			
32			.081	.086	.441			
34			.228	.034	.378			
37			.175	.040	.427			
38					.329			
39			.155	.054	.468			
40			.193	.047	.486			
41			.115	.021	.382			
42			.171	.072	.502			

Table A-2

ROCKETDYNE HYDROGASIFICATION DATA FOR BITUMINOUS COALS — DOE CONTRACT EX-77-C-01-2518

RUN	DATE	COAL *	PSIZE	LENGTH	DIAM	FCOAL	HCRAT	HCONS
011- 7	9/21/77	BTM-1		15.00	1.880	446.00	0.356	
011- 8	9/29/77	BTM-1		15.00	1.880	468.00	0.421	
011- 9	10/ 4/77	BTM-1		15.00	1.880	389.00	0.499	
011-10	10/ 7/77	BTM-1		15.00	1.880	392.00	0.506	
300- 2	1/ 6/78	BTM-3		15.00	2.830	315.00	0.643	
300- 3	1/ 9/78	BTM-3		15.00	2.830	586.00	0.342	
300- 4	1/11/78	BTM-3		15.00	2.830	396.00	0.509	
300- 5	1/16/78	BTM-3		15.00	2.830	365.00	0.548	
300- 6	1/17/78	BTM-2		15.00	2.830	429.00	0.469	
300-11	2/10/78	BTM-2		15.00	2.260	392.00	0.519	
300-12	2/16/78	BTM-2		15.00	4.260	415.00	0.489	

*BTM-1 is Kentucky #9/14 bituminous HvCb coal from the Colonial Mine of the Pittsburgh and Midway Mining Co.

BTM-2 is Kentucky #9 bituminous HvAb coal from the Hamilton No. 2 Mine of the Island Creek Coal Co.

BTM-3 is Illinois #6 bituminous HvCb coal.

Table A-2 (Cont'd)

RUN	GVEL	TPRES	HPRES	TWALL	TGMAX	TGEIT	RTGAS	RTPAR
011- 7	24.40	1003.	948.	1628.	1674.		615.	615.
011- 8	31.60	1007.	946.	1750.	1810.		475.	475.
011- 9	21.60	1504.	1416.	1881.	1955.		695.	695.
011-10	21.70	1490.	1412.	1850.	1912.		690.	690.
300- 2	10.20	1496.	1313.	1943.	1982.		1465.	1465.
300- 3	13.60	991.	871.	1464.	1603.		1100.	1100.
300- 4	14.90	997.	869.	1780.	1860.		1010.	1010.
300- 5	12.80	994.	904.	1468.	1468.		1170.	1170.
300- 6	10.00	1490.	1277.	1693.	1816.		1500.	1500.
300-11	15.90	1499.	1315.	1806.	1909.		945.	945.
300-12	4.39	1496.	1315.	1818.	1908.		3415.	3415.

Table A-2 (Cont'd)

RUN	X	XGAS	XHC	XM	XC2	XC3	XC4
011- 7	.473	.199	.171	.150	.021	.0	.0
011- 8	.535	.312	.268	.263	.005	.0	.0
011- 9	.588	.426	.386	.385	.001	.0	.0
011-10	.588	.416	.378	.378	.0	.0	.0
300- 2	.707	.688	.626	.626	.0	.0	.0
300- 3	.500	.436	.370	.324	.046	.0	.0
300- 4	.595	.492	.446	.409	.037	.0	.0
300- 5	.480	.372	.322	.229	.093	.0	.0
300- 6	.627	.566	.523	.521	.002	.0	.0
300-11	.644	.619	.569	.568	.001	.0	.0
300-12	.650	.645	.595	.595	.0	.0	.0

Table A-2 (Cont'd)

RUN	XCO	XCO2	XOIL	XBTX	PHIG	PHIHC	PHIM	PHIC2
011- 7	.024	.004			.421	.362	.317	.0444
011- 8	.039	.004			.583	.501	.492	.0093
011- 9	.036	.004			.724	.656	.655	.0017
011-10	.035	.003			.707	.643	.643	.0
300- 2	.059	.003			.973	.885	.885	.0
300- 3	.047	.009			.872	.740	.648	.0920
300- 4	.042	.004			.827	.750	.687	.0622
300- 5	.040	.009			.775	.671	.477	.1938
300- 6	.040	.004			.903	.834	.831	.0032
300-11	.046	.005			.961	.884	.882	.0016
300-12	.047	.003			.992	.915	.915	.0

Table A-3

ROCKETDYNE HYDROGASIFICATION DATA FOR SUBBITUMINOUS COAL — DOE CONTRACT EX-77-C-01-2518

RUN	DATE	COAL*	PSIZE	LENGTH	DIAM	FCOAL	HCRAT	HCONS
011- 2	8/30/77	SUBBTM		15.00	1.880	302.00	0.592	
011- 4	9/ 9/77	SUBBTM		15.00	1.880	320.00	0.512	
011- 5	9/15/77	SUBBTM		15.00	1.880	414.00	0.401	
011-11	10/14/77	SUBBTM		15.00	1.880	357.00	0.569	
011-12	10/18/77	SUBBTM		15.00	1.880	335.00	0.559	
011-13	10/21/77	SUBBTM		15.00	1.880	380.00	0.535	
011-14	10/28/77	SUBBTM		15.00	1.880	350.00	0.418	
011-15	11/ 2/77	SUBBTM		15.00	1.880	348.00	0.331	
011-16	11/21/77	SUBBTM		15.00	2.830	405.00	0.550	
011-17	11/28/77	SUBBTM		15.00	2.830	348.00	0.576	
011-22	12/14/77	SUBBTM		15.00	2.830	497.00	0.392	
011-23	12/19/77	SUBBTM		15.00	2.830	551.00	0.364	
011-24	12/21/77	SUBBTM		15.00	2.830	306.00	0.705	
300- 1	1/ 4/78	SUBBTM		15.00	2.830	328.00	0.675	

*SUBBTM is Montana Rosebud subbituminous coal.

Table A-3 (Cont'd)

RUN	GVEL	TPRES	HPRES	TWALL	TGMAX	TGEIT	RTGAS	RTPAR
011- 2	25.00	1021.	962.	1461.	1474.		600.	600.
011- 4	28.00	987.	928.	1884.	1901.		535.	535.
011- 5	26.10	995.	939.	1687.	1725.		575.	575.
011-11	22.10	1497.	1410.	1785.	1838.		680.	680.
011-12	18.60	1501.	1432.	1538.	1586.		805.	805.
011-13	19.10	1498.	1436.	1418.	1468.		785.	785.
011-14	28.47	1009.	789.	1530.	1558.		527.	527.
011-15	22.69	1128.	839.	1681.	1706.		661.	661.
011-16	10.60	1484.	1394.	1756.	1756.		1420.	1420.
011-17	8.70	1498.	1428.	1530.	1531.		1725.	1725.
011-22	13.60	999.	881.	1711.	1755.		1105.	1105.
011-23	12.90	993.	903.	1375.	1416.		1165.	1165.
011-24	15.40	1001.	891.	1793.	1801.		975.	975.
300- 1	10.60	1498.	1310.	1799.	1827.		1420.	1420.

Table A-3 (Cont'd)

RUN	X	XGAS	XHC	XM	XC2	XC3	XC4
011- 2	.289	.143	.105	.071	.034	.0	.0
011- 4	.361	.302	.233	.231	.002	.0	.0
011- 5	.364	.229	.177	.164	.013	.0	.0
011-11	.436	.432	.358	.357	.001	.0	.0
011-12	.392	.280	.221	.166	.055	.0	.0
011-13	.321	.222	.172	.106	.066	.0	.0
011-14	.278					.0	.0
011-15	.298					.0	.0
011-16	.470	.470	.410	.410	.0	.0	.0
011-17	.407	.350	.288	.255	.033	.0	.0
011-22	.354	.307	.240	.239	.001	.0	.0
011-23	.292	.248	.183	.112	.071	.0	.0
011-24	.382	.348	.277	.277	.0	.0	.0
300- 1	.459	.429	.358	.358	.0	.0	.0

Table A-3 (Cont'd)

RUN	XCO	XCO2	XOIL	XBTX	PHIG	PHIHC	PHIM	PHIC2
011- 2	.028	.010			.495	.363	.246	.1176
011- 4	.064	.005			.837	.645	.640	.0055
011- 5	.049	.003			.629	.486	.451	.0357
011-11	.070	.004			.991	.821	.819	.0023
011-12	.054	.005			.714	.564	.423	.1403
011-13	.043	.007			.692	.536	.330	.2056
011-14								
011-15								
011-16	.078	.003			1.000	.872	.872	.0
011-17	.058	.004			.860	.708	.627	.0811
011-22	.064	.003			.867	.678	.675	.0028
011-23	.055	.010			.849	.627	.384	.2432
011-24	.068	.003			.911	.725	.725	.0
300- 1	.067	.004			.935	.780	.780	.0

Table A-4

CITIES SERVICE HYDROGENATION DATA FOR LIGNITE COAL

RUN	DATE	COAL	PSIZE	LENGTH	DIAM	FCOAL	HCRAT	HCONS
1	1975-6	LIGNITE	175.	3.09	1.000	1.25	1.400	.0488
2	1975-6	LIGNITE	250.	3.04	1.000	1.25	1.300	.0599
3	1975-6	LIGNITE	200.	1.50	1.000	1.25	1.300	.0443
4	1975-6	LIGNITE	470.	3.06	1.000	1.06	1.600	.0547
5	1975-6	LIGNITE	200.	1.53	1.000	1.39	1.200	.0443
6	1975-6	LIGNITE	190.	3.08	1.000	1.60	0.900	.0676
7	1975-6	LIGNITE	190.	3.06	1.000	1.60	1.400	.1072
8	1975-6	LIGNITE	190.	2.94	1.000	1.60	1.000	.1761
9	1975-6	LIGNITE	190.	20.00	0.500	0.80	2.000	.0618
10	1975-6	LIGNITE	190.	3.12	1.000	2.30	0.480	.0588
11	1975-6	LIGNITE	56.	2.96	1.000	2.50	0.180	.0793
12	1975-6	LIGNITE	190.	3.02	1.000	1.50	0.900	.0859
13	1975-6	LIGNITE	190.	0.96	1.000	1.50	1.200	.0413
14	1975-6	LIGNITE	190.	60.00	0.250	1.90	1.200	.0546
15	1975-6	LIGNITE	190.	60.00	0.250	1.00	1.000	.0888
16	1975-6	LIGNITE	150.	60.00	0.250	0.60	1.300	.0491
17	1975-6	LIGNITE	150.	20.00	0.500	1.00	1.500	.0633
18	1975-6	LIGNITE	150.	60.00	0.250	0.70	1.600	.0653
19	1975-6	LIGNITE	109.	4.00	0.375	1.80	2.300	.0322
20	1975-6	LIGNITE	109.	4.23	1.000	3.24	0.170	.0130
21	1975-6	LIGNITE	109.	4.00	0.375	1.80	1.200	.0322
22	1975-6	LIGNITE	109.	63.00	0.375	0.75	1.500	.0395
23	1975-6	LIGNITE	161.	4.00	0.375	2.00	2.400	.0295
24	1975-6	LIGNITE	161.	4.00	0.375	0.65	1.900	.0334
25	1975-6	LIGNITE	63.	4.00	0.375	0.93	5.100	.0431

Table A-4 (Cont'd)

RUN	GVEL	TPRES	HPRES	TWALL	TGMAX	TGEIT	RTGAS	RTPAR
1	0.49	1500.	1500.	1518.	1581.		6300.	1180.
2	0.46	1500.	1500.	1540.	1502.		6600.	880.
3	0.50	1500.	1500.	1496.	1484.		3000.	430.
4	0.45	1500.	1500.	1349.	1433.		6800.	460.
5	0.90	750.	750.	1499.	1498.		1700.	350.
6	0.40	1500.	1500.	1524.	1512.		7700.	155.
7	1.70	580.	580.	1625.	1617.		1800.	880.
8	0.20	2960.	2960.	1533.	1480.		14700.	2470.
9	7.70	1000.	1000.	1554.	1533.		2400.	2400.
10	0.30	1500.	1500.	1503.	1460.		10400.	1520.
11	0.12	1500.	1500.	1538.	1543.		24700.	6290.
12	0.28	2000.	2000.	1553.	1487.		10800.	1650.
13	0.74	1000.	1000.	1556.	1508.		1300.	410.
14	77.50	1000.	1000.	1560.	1569.		800.	800.
15	24.00	1500.	1500.	1612.	1617.		2500.	2500.
16	58.30	500.	500.	1621.	1624.		1000.	1000.
17	6.70	1000.	1000.	1526.	1533.		3000.	3000.
18	23.50	1500.	1500.	1320.	1320.		2500.	2500.
19	46.60	1000.	1000.	1511.	1476.		90.	90.
20	0.17	1000.	1000.	1139.	1000.		24900.	7500.
21	48.90	1000.	1000.	1615.	1550.		70.	70.
22	44.60	300.	300.	1623.	1620.		1300.	1300.
23	58.00	1000.	1000.	1682.	1663.		70.	70.
24	13.80	1000.	1000.	1607.	1604.		290.	290.
25	57.30	1000.	1000.	1608.	1590.		70.	70.

Table A-4 (Cont'd)

RUN	X	XGAS	XHC	XM	XC2	XC3	XC4
1	.472						
2	.434						
3	.366	.236	.165	.089	.072		
4	.377	.227	.191	.104	.074		
5	.323	.215	.158	.097	.059		
6	.435	.306	.245	.150	.093		
7	.369	.270	.199	.141	.058		
8	.816	.673	.591	.518	.073		
9	.429	.325	.252	.155	.097		
10	.374	.287	.203	.143	.060		
11	.430	.350	.261	.214	.047		
12	.492	.410	.291	.237	.054		
13	.326	.223	.145	.089	.051		
14	.383	.272	.190	.129	.059		
15	.479	.379	.308	.255	.052		
16	.310	.249	.171	.131	.038		
17	.442	.328	.237	.168	.069		
18	.443	.297	.205	.113	.068		
19	.327	.235	.128	.051	.042		
20	.197	.143	.058	.019	.015		
21	.331	.219	.134	.067	.047		
22	.343	.281	.182	.154	.028		
23	.341	.244	.151	.090	.052		
24	.321	.239	.159	.098	.055		
25	.369	.266	.183	.103	.058		

Table A-4 (Cont'd)

RUN	XCO	XCO2	XOIL	XBTX	PHIG	PHIHC	PHIM	PHIC2
1			.030	.135	.650			
2								
3	.056	.015	.029	.101	.645	.451	.243	.1967
4	.002	.034	.051	.099	.602	.507	.276	.1963
5	.040	.017	.033	.075	.666	.489	.300	.1827
6	.047	.014	.044	.085	.703	.563	.345	.2138
7	.051	.020	.023	.076	.732	.540	.382	.1572
8	.082	.0	.011	.132	.825	.725	.635	.0895
9	.070	.003	.017	.087	.758	.588	.361	.2261
10	.081	.003	.030	.057	.768	.544	.382	.1604
11	.081	.008	.036	.044	.815	.608	.498	.1093
12	.079	.040	.020	.101	.834	.592	.482	.1098
13	.052	.026	.062	.041	.684	.445	.273	.1564
14	.081	.001	.039	.072	.710	.496	.337	.1540
15	.071	.0	.001	.099	.791	.643	.532	.1086
16	.077	.001	.006	.055	.803	.552	.423	.1226
17	.090	.001	.022	.092	.743	.537	.380	.1561
18	.090	.002	.098	.048	.670	.463	.255	.1535
19	.040	.067	.062	.030	.719	.391	.156	.1284
20	.020	.065	.045	.009	.726	.294	.096	.0761
21	.043	.042	.089	.023	.662	.405	.202	.1420
22	.099	.0	.008	.054	.819	.531	.449	.0816
23	.057	.036	.050	.047	.716	.443	.264	.1525
24	.056	.024	.024	.058	.745	.495	.305	.1713
25	.051	.032	.057	.046	.721	.496	.279	.1572

Table A-5

CITIES SERVICE HYDROGASIFICATION DATA FOR SUBBITUMINOUS COAL — DOE CONTRACT EX-77-C-01-2518

RUN	DATE	COAL*	PSIZE	LENGTH	DIAM	FCOAL	HCRAT	HCONS
MR- 4	6/13/77	SUBBTM	45.	31.80	0.334	1.63	1.400	
MR- 1	6/16/77	SUBBTM	45.	4.00	0.260	0.84	0.760	.0321
MR-10	6/22/77	SUBBTM	45.	4.00	0.260	2.27	0.830	.0133
MR-13	6/27/77	SUBBTM	45.	18.10	0.260	4.05	0.800	.0581
MR-14	6/29/77	SUBBTM	45.	18.10	0.260	4.24	0.740	.0705
MR-28	7/ 6/77	SUBBTM	45.	3.92	0.260	2.16	0.790	.0252
MR-29	7/ 8/77	SUBBTM	45.	3.92	0.260	1.66	0.990	.0413
MR-30	7/12/77	SUBBTM	45.	3.92	0.260	1.79	0.850	.0457
MR-11	7/15/77	SUBBTM	56.	3.92	0.26	3.16	0.780	.0299
MR-12	7/19/77	SUBBTM	56.	3.92	0.260	3.16	0.750	.0402
MR-25	7/21/77	SUBBTM	56.	18.00	0.260	2.22	0.980	.0458
MR-26	7/25/77	SUBBTM	56.	18.00	0.260	2.35	0.880	.0593
MR-27	7/27/77	SUBBTM	56.	18.00	0.260	2.14	0.930	.0642
MR-15	7/29/77	SUBBTM	56.	18.00	0.260	3.19	0.870	.0755
MR- 2	8/ 3/77	SUBBTM	56.	9.30	0.260	2.11	0.890	.0333
MR- 3	8/ 5/77	SUBBTM	56.	9.30	0.260	1.85	0.970	.0181
MR-16	8/ 8/77	SUBBTM	56.	9.30	0.260	3.03	0.910	.0265
MR-17	8/10/77	SUBBTM	56.	9.30	0.260	2.14	1.240	.0358
MR-18	8/12/77	SUBBTM	56.	9.30	0.260	2.79	0.930	.0285
MR-37	8/16/77	SUBBTM	56.	57.90	0.209	1.71	1.080	.0285
MR-38	8/18/77	SUBBTM	56.	58.10	0.209	1.30	0.970	.0515
MR-39	8/22/77	SUBBTM	56.	57.70	0.209	1.24	0.980	.0334
MR- 5	8/24/77	SUBBTM	56.	57.90	0.209	2.09	1.230	
MR-20	9/15/77	SUBBTM	56.	57.90	0.209	2.64	0.910	.0570
MR-21	9/20/77	SUBBTM	56.	58.00	0.209	2.47	0.940	.0682
MR-22	9/22/77	SUBBTM	56.	55.80	0.209	2.51	0.920	.0782
MR- 9	10/12/77	SUBBTM	56.	57.80	0.209	3.38	1.070	.0643
MR-47	10/14/77	SUBBTM	56.	57.30	0.209	2.91	1.140	.0685
MR-19	10/18/77	SUBBTM	56.	57.50	0.209	3.22	1.000	.0782
MR-35	10/20/77	SUBBTM	56.	48.80	0.209	1.52	0.990	.0635
MR-36	10/24/77	SUBBTM	56.	55.90	0.209	1.55	0.850	.0580
MR-40	10/26/77	SUBBTM	56.	55.90	0.209	1.41	0.950	.0608
MR-32	10/28/77	SUBBTM	56.	56.70	0.209	2.46	0.860	.0442
MR-33	11/ 8/77	SUBBTM	56.	56.90	0.209	2.14	0.940	.0431
MR-34	11/ 9/77	SUBBTM	56.	56.90	0.209	2.04	0.930	.0476
MR-23	11/11/77	SUBBTM	56.	17.60	0.260	1.79	0.880	.0454
MR-24	11/14/77	SUBBTM	56.	17.70	0.260	1.70	0.910	.0318
MR-31	11/16/77	SUBBTM	56.	17.70	0.260	1.54	0.940	.0371
MR- 6	11/18/77	SUBBTM	56.	17.70	0.260	2.98	0.850	.0482
MR- 8	11/21/77	SUBBTM	56.	17.70	0.260	3.10	0.770	.0555
MR- 7	11/22/77	SUBBTM	56.	17.70	0.260	2.99	0.810	.0498
MR-48	12/14/77	SUBBTM	56.	57.20	0.209	0.73	0.890	.0235

*SUBBTM is Montana Rosebud subbituminous coal.

Table A-5 (Cont'd)

RUN	GVEL	TPRES	HPRES	TWALL	TGMAX	TGEIT	RTGAS	RTPAR
MR- 4	20.90	500.	500.		1520.	1475.	1530.	1530.
MR- 1	9.00	500.	500.		1517.	1467.	433.	433.
MR-10	9.40	1500.	1500.		1497.	1455.	423.	423.
MR-13	16.60	1500.	1500.		1526.	1490.	1090.	1090.
MR-14	17.00	1500.	1500.		1630.	1597.	1060.	1060.
MR-28	12.80	1000.	1000.		1527.	1481.	307.	307.
MR-29	12.80	1000.	1000.		1631.	1580.	307.	307.
MR-30	12.30	1000.	1000.		1714.	1660.	321.	321.
MR-11	13.00	1500.	1500.		1605.	1563.	303.	303.
MR-12	12.60	1500.	1500.		1662.	1610.	312.	312.
MR-25	16.60	1000.	1000.		1517.	1483.	1090.	1090.
MR-26	16.50	1000.	1000.		1622.	1582.	1090.	1090.
MR-27	16.40	1000.	1000.		1698.	1660.	1100.	1100.
MR-15	16.40	1500.	1500.		1658.	1622.	1100.	1100.
MR- 2	29.40	500.	500.		1613.	1575.	318.	318.
MR- 3	29.50	500.	500.		1709.	1676.	317.	317.
MR-16	14.31	1500.	1500.		1515.	1482.	653.	653.
MR-17	14.30	1500.	1500.		1604.	1573.	654.	654.
MR-18	14.20	1500.	1500.		1642.	1611.	656.	656.
MR-37	25.20	750.	750.		1540.	1504.	2300.	2300.
MR-38	20.10	765.	765.		1650.	1599.	2860.	2860.
MR-39	20.70	750.	750.		1730.	1688.	2770.	2770.
MR- 5	63.50	500.	500.		1631.	1592.	910.	910.
MR-20	18.10	1600.	1600.		1517.	1485.	3190.	3190.
MR-21	17.80	1600.	1600.		1591.	1555.	3250.	3250.
MR-22	17.60	1600.	1600.		1612.	1573.	3160.	3160.
MR- 9	27.10	1600.	1600.		1518.	1487.	2130.	2130.
MR-47	25.20	1600.	1600.		1569.	1527.	2268.	2268.
MR-19	24.90	1600.	1600.		1605.	1563.	2310.	2310.
MR-35	17.60	1000.	1000.		1553.	1500.	2780.	2780.
MR-36	15.90	1000.	1000.		1636.	1582.	3508.	3508.
MR-40	16.60	1000.	1000.		1694.	1643.	3365.	3365.
MR-32	24.40	1000.	1000.		1536.	1490.	2320.	2320.
MR-33	24.50	1000.	1000.		1654.	1596.	2320.	2320.
MR-34	23.70	1000.	1000.		1688.	1629.	2400.	2400.
MR-23	11.50	1000.	1000.		1542.	1506.	1540.	1540.
MR-24	12.70	1000.	1000.		1649.	1609.	1400.	1400.
MR-31	12.20	1000.	1000.		1721.	1689.	1450.	1450.
MR- 6	12.30	1600.	1600.		1514.	1486.	1450.	1450.
MR- 8	12.10	1600.	1600.		1599.	1574.	1460.	1460.
MR- 7	12.10	1600.	1600.		1558.	1532.	1470.	1470.
MR-48	16.40	500.	500.		1746.	1695.	3486.	3486.

Table A-5 (Cont'd)

RUN	X	XGAS	XHC	XM	XC2	XC3	XC4
MR- 4	.390						
MR- 1	.319	.267	.192	.085	.069	.029	.009
MR-10	.214	.127	.091	.039	.032	.017	.003
MR-13	.397	.282	.231	.147	.083	.001	.0
MR-14	.431	.351	.286	.221	.063	.002	.0
MR-28	.275	.199	.149	.068	.056	.020	.005
MR-29	.344	.266	.205	.117	.081	.006	.001
MR-30	.324	.250	.198	.130	.066	.001	.001
MR-11	.255	.183	.142	.076	.057	.008	.001
MR-12	.321	.233	.186	.106	.074	.005	.001
MR-25	.359	.255	.204	.119	.084	.001	.0
MR-26	.382	.298	.240	.175	.065	.0	.0
MR-27	.402	.319	.258	.235	.023	.0	.0
MR-15	.453	.351	.291	.245	.046	.0	.0
MR- 2	.339	.261	.189	.111	.076	.001	.001
MR- 3	.330	.263	.152	.116	.036	.0	.0
MR-16	.379	.271	.164	.097	.065	.002	.0
MR-17	.430	.329	.203	.137	.066	.0	.0
MR-18	.430	.323	.191	.136	.055	.0	.0
MR-37	.334	.262	.169	.113	.056	.0	.0
MR-38	.414	.312	.229	.202	.027	.0	.0
MR-39	.455	.368	.220	.216	.004	.0	.0
MR- 5	.418						
MR-20	.460	.341	.268	.162	.106	.0	.0
MR-21	.507	.375	.290	.222	.068	.0	.0
MR-22	.548	.413	.313	.258	.055	.0	.0
MR- 9	.456	.313	.252	.158	.094	.0	.0
MR-47	.478	.341	.271	.182	.089	.0	.0
MR-19	.516	.369	.289	.212	.077	.0	.0
MR-35	.412	.292	.226	.148	.078	.0	.0
MR-36	.473	.332	.246	.211	.035	.0	.0
MR-40	.506	.384	.282	.270	.012	.0	.0
MR-32	.456	.322	.240	.141	.099	.0	.0
MR-33	.465	.312	.220	.180	.039	.0	.001
MR-34	.462	.304	.217	.204	.013	.0	.0
MR-23	.426	.290	.220	.138	.082	.0	.0
MR-24	.409	.303	.211	.173	.038	.0	.0
MR-31	.447	.334	.217	.207	.010	.0	.0
MR- 6	.432	.301	.234	.138	.095	.001	.0
MR- 8	.465	.330	.259	.170	.087	.001	.001
MR- 7	.410	.292	.235	.147	.087	.0	.001
MR-48	.392	.312	.191	.189	.002	.0	.0

Table A-5 (Cont'd)

RUN	XCO	XCO2	XOIL	XBTX	PHIG	PHIHC	PHIM	PHIC2
MR- 4								
MR- 1	.053	.022	.011	.034	.837	.602	.266	.2163
MR-10	.023	.013	.064	.020	.593	.425	.182	.1495
MR-13	.047	.004	.052	.053	.710	.582	.370	.2091
MR-14	.062	.003	.028	.052	.814	.664	.513	.1462
MR-28	.033	.017	.058	.018	.724	.542	.247	.2036
MR-29	.049	.012	.034	.043	.773	.596	.340	.2355
MR-30	.045	.007	.018	.056	.772	.611	.401	.2037
MR-11	.031	.010	.043	.029	.718	.557	.298	.2235
MR-12	.040	.007	.040	.050	.726	.579	.330	.2305
MR-25	.046	.005	.039	.064	.710	.568	.331	.2340
MR-26	.055	.003	.002	.083	.780	.628	.458	.1702
MR-27	.059	.002	.0	.083	.794	.642	.585	.0572
MR-15	.058	.002	.001	.098	.775	.642	.541	.1015
MR- 2	.059	.013	.028	.053	.770	.558	.327	.2242
MR- 3	.105	.006	.017	.049	.797	.461	.352	.1091
MR-16	.103	.004	.057	.048	.715	.433	.256	.1715
MR-17	.124	.002	.030	.071	.765	.472	.319	.1535
MR-18	.131	.001	.021	.082	.751	.444	.316	.1279
MR-37	.092	.001	.011	.060	.784	.506	.338	.1677
MR-38	.082	.001	.0	.101	.754	.553	.488	.0652
MR-39	.147	.001	.0	.084	.809	.484	.475	.0088
MR- 5								
MR-20	.072	.001	.016	.101	.741	.583	.352	.2304
MR-21	.084	.001	.004	.128	.740	.572	.438	.1341
MR-22	.099	.001	.001	.133	.754	.571	.471	.1004
MR- 9	.060	.001	.044	.096	.686	.553	.346	.2061
MR-47	.069	.001	.031	.106	.713	.567	.381	.1862
MR-19	.079	.001	.016	.131	.715	.560	.411	.1492
MR-35	.065	.001	.033	.086	.709	.549	.359	.1893
MR-36	.085	.001	.022	.118	.702	.520	.446	.0740
MR-40	.101	.001	.001	.120	.759	.557	.534	.0237
MR-32	.080	.002	.035	.098	.706	.526	.309	.2171
MR-33	.090	.002	.010	.143	.671	.473	.387	.0839
MR-34	.086	.001	.003	.153	.658	.470	.442	.0281
MR-23	.068	.002	.012	.124	.681	.516	.324	.1925
MR-24	.090	.002	.022	.082	.741	.516	.423	.0929
MR-31	.116	.001	.020	.083	.747	.485	.463	.0224
MR- 6	.065	.002	.055	.070	.697	.542	.319	.2199
MR- 8	.070	.001	.042	.091	.710	.557	.366	.1871
MR- 7	.056	.001	.031	.085	.712	.573	.359	.2122
MR-48	.120	.001	.009	.070	.796	.487	.482	.0051

Table A-6

PERC HYDROGASIFICATION DATA FOR BITUMINOUS AND LIGNITE COALS

RUN	DATE	COAL*	PSIZE	LENGTH	DIAM	FCOAL	HCRAT	HCONS
1	1974	BTM-1		5.00	3.260	11.7000	0.0718	.0290
2	1974	BTM-1		5.00	3.260	13.2000	0.0298	.0140
3	1974	BTM-1		5.00	3.260	12.8000	0.0320	.0200
5	1974	BTM-1	130.	5.00	3.260	12.5000	0.0319	.0190
7	1974	BTM-1		5.00	3.260	13.0000	0.0333	.0200
8	1974	BTM-1		5.00	3.260	3.9400	0.1051	.0300
9	1974	BTM-1		5.00	3.260	11.7000	0.0701	.0480
10	1974	BTM-1		5.00	3.260	12.7000	0.0321	.0200
11	1974	BTM-1		5.00	3.260	12.9000	0.0335	.0230
12	1974	BTM-1		5.00	3.260	13.0000	0.0329	.0200
13	1974	BTM-1		5.00	3.260	12.4000	0.0355	.0260
14	1974	BTM-1		5.00	3.260	6.7300	0.0547	.0310
15	1974	BTM-1		3.00	3.260	12.6000	0.0330	.0200
16	1974	BTM-1		5.00	3.260	12.4000	0.0372	.0220
17	1974	BTM-1		5.00	3.260	12.2000	0.0338	.0210
18	1974	BTM-1		5.00	3.260	24.1000	0.0374	.0210
19	1974	BTM-1	130.	5.00	3.260	12.7000	0.0695	.0510
21	1974	BTM-1		5.00	3.260	12.3000	0.0342	.0290
22	1974	BTM-1		5.00	3.260	12.9000	0.0727	.0230
23	1974	BTM-1		5.00	3.260	12.6000	0.0366	.0270
24	1974	BTM-1		5.00	3.260	12.3000	0.0374	.0290
25	1974	BTM-1		5.00	3.260	12.6000	0.0352	.0270
26	1974	BTM-1		5.00	3.260	12.5000	0.0368	.0190
27	1974	BTM-2		5.00	3.260	12.0000	0.0501	.0040
28	1974	BTM-2		5.00	3.260	12.2000	0.0411	.0080
29	1974	BTM-2		5.00	3.260	10.5000	0.0432	.0220
30	1974	BTM-2		5.00	3.260	11.8000	0.0373	.0220
31	1974	BTM-2		5.00	3.260	12.3000	0.0326	.0210
32	1974	BTM-2		5.00	3.260	12.8000	0.0343	.0240
120	1976	LIGNITE	75.	5.00	3.260	18.0000	0.0578	.0520
122	1976	BTM-2	75.	5.00	3.260	12.3000	0.0800	.0550
124A	1976	BTM-2	75.	5.00	3.260	15.0000	0.0490	.0390
124B	1976	BTM-2	75.	5.00	3.260	15.0000	0.0420	.0390
128A	6/76	BTM-2	75.	5.00	3.260	15.0000	0.0727	.0510
128B	6/76	BTM-2	75.	5.00	3.260	10.0000	0.0640	.0540
130	12/ 7/76	LIGNITE	75.	5.00	3.260	13.7000	0.0670	.0480
131	12/ 7/76	LIGNITE	75.	5.00	3.260	10.2000	0.1422	.1060
132	1/11/77	LIGNITE	75.	5.00	3.260	11.7000	0.0863	.0860
133	3/77	LIGNITE	75.	5.00	3.260	11.5000	0.0850	.0560
134	3/77	LIGNITE	75.	5.00	3.260	12.4000	0.0823	.0610
135A	4/77	LIGNITE	75.	9.00	3.260	14.8000	0.0899	.0750
135B	4/77	LIGNITE	75.	9.00	3.260	14.8000	0.0560	.0510

*BTM-1 is Pittsburgh Seam HvAb coal.

BTM-2 is Illinois No. 6 HvCb coal.

LIGNITE is North Dakota lignite coal from the Baukol-Noonan Mine.

Table A-6 (Cont'd)

RUN	GVEL	TPRES	HPRES	TWALL	TGMAX	TGEIT	RTGAS	RTPAR
1	0.0401	1000.	853.	1472.			125000.	
2	0.0420	1000.	368.	1472.			119000.	
3	0.0447	1000.	340.	1562.			112000.	
5	0.0448	1000.	339.	1562.			112000.	
7	0.0475	1000.	347.	1562.			105000.	
8	0.0412	1000.	454.	1562.			121000.	
9	0.0416	1000.	737.	1562.			120000.	
10	0.0368	1200.	411.	1562.			136000.	
11	0.0300	1500.	516.	1562.			167000.	
12	0.0232	2000.	627.	1562.			215000.	
13	0.0228	2000.	665.	1562.			219000.	
14	0.0415	500.	361.	1652.			121000.	
15	0.0442	1000.	371.	1652.			68000.	
16	0.0463	1000.	388.	1652.			108000.	
17	0.0459	1000.	348.	1652.			109000.	
18	0.0934	1000.	393.	1652.			54000.	
19	0.0458	1000.	680.	1652.			109000.	
21	0.0422	1100.	369.	1652.			118000.	
22	0.0380	1100.	783.	1652.			132000.	
23	0.0399	1200.	436.	1652.			125000.	
24	0.0310	1500.	509.	1652.			162000.	
25	0.0240	2000.	640.	1652.			209000.	
26	0.0241	2000.	671.	1652.			207000.	
27	0.0437	1000.	561.	1202.			115000.	
28	0.0435	1000.	494.	1337.			115000.	
29	0.0482	1000.	397.	1652.			104000.	
30	0.0431	1200.	409.	1652.			116000.	
31	0.0322	1500.	488.	1652.			155000.	
32	0.0248	2000.	670.	1652.			202000.	
120	0.0595	1000.	679.	1652.			84000.	
122	0.0525	1000.	736.	1652.			95000.	
124A	0.0404	1000.	669.	1652.			124000.	
124B	0.0338	1000.	601.	1652.			148000.	
128A	0.0402	1000.	705.	1652.			124000.	
128B	0.0345	1000.	655.	1652.			145000.	
130	0.0533	1000.	738.	1652.			94000.	
131	0.0660	1000.	752.	1652.			76000.	
132	0.0515	1000.	714.	1652.			97000.	
133	0.0565	1000.	755.	1652.			89000.	
134	0.0570	1000.	748.	1652.			88000.	
135A	0.0752	1000.	708.	1652.			120000.	
135B	0.0481	1000.	664.	1652.			187000.	

Table A-6 (Cont'd)

RUN	X	X	XGAS	XHC	XM	XC2	XC3	XC4
1	.281	.135	.133	.125	.118	.007	.0	.0
2	.250	.141	.139	.132	.122	.010	.0	.0
3	.250	.168	.165	.144	.139	.005	.0	.0
5	.240	.173	.168	.150	.148	.002	.0	.0
7	.220	.182	.178	.161	.159	.002	.0	.0
8	.362	.189	.187	.170	.170	.0	.0	.0
9	.308	.240	.238	.225	.223	.002	.0	.0
10	.256	.162	.160	.145	.144	.001	.0	.0
11	.242	.180	.180	.166	.165	.001	.0	.0
12	.300	.208	.221	.200	.199	.001	.0	.0
13	.280	.185	.182	.177	.176	.001	.0	.0
14	.334	.221	.224	.205	.205	.0	.0	.0
15	.314	.164	.162	.152	.150	.002	.0	.0
16	.250	.189	.184	.161	.157	.004	.0	.0
17	.256	.182	.177	.162	.159	.003	.0	.0
18	.260	.144	.143	.129	.127	.002	.0	.0
19	.332	.269	.267	.242	.242	.0	.0	.0
21	.242	.160	.194	.183	.180	.003	.0	.0
22	.233	.269	.180	.166	.165	.001	.0	.0
23	.250	.192	.213	.205	.204	.001	.0	.0
24	.242	.196	.194	.183	.180	.003	.0	.0
25	.250	.214	.213	.205	.204	.001	.0	.0
26	.240	.200	.168	.150	.148	.002	.0	.0
27	.191	.081	.076	.069	.057	.012	.0	.0
28	.251	.137	.129	.115	.086	.029	.0	.0
29	.298	.237	.225	.211	.211	.0	.0	.0
30	.278	.262	.247	.226	.226	.0	.0	.0
31	.278	.233	.217	.201	.201	.0	.0	.0
32	.263	.248	.243	.221	.219	.002	.0	.0
120	.409	.379	.393	.254	.244	.010	.0	.0
122	.337	.321	.322	.292	.281	.011	.0	.0
124A	.316	.256	.256	.225	.212	.013	.0	.0
124B	.272	.240	.242	.212	.209	.003	.0	.0
128A	.360	.337	.336	.297	.297	.0	.0	.0
128B	.298	.321	.318	.281	.281	.0	.0	.0
130	.434	.430	.359	.231	.231	.0	.0	.0
131	.332	.663	.554	.382	.382	.0	.0	.0
132	.317	.493	.411	.267	.267	.0	.0	.0
133	.330	.546	.390	.313	.313	.0	.0	.0
134	.442	.509	.365	.288	.288	.0	.0	.0
135A	.440	.650	.542	.321	.321	.0	.0	.0
135B	.507	.481	.401	.230	.230	.0	.0	.0

Table A-6 (Cont'd)

RUN	XCO	XCO2	XOIL	XBTX	PHIG	PHIHC	PHIM	PHIC2
1	.008	.0			.473	.445	.420	.0249
2	.006	.001			.556	.528	.488	.0400
3	.017	.004			.660	.576	.556	.0200
5	.014	.004			.700	.625	.617	.0083
7	.014	.003			.809	.732	.723	.0091
8	.015	.002			.517	.470	.470	.0
9	.011	.002			.773	.731	.724	.0065
10	.012	.003			.625	.566	.563	.0039
11	.011	.003			.744	.686	.682	.0041
12	.017	.004			.737	.667	.663	.0033
13	.004	.001			.650	.632	.629	.0036
14	.019	.0			.671	.614	.614	.0
15	.008	.002			.516	.484	.478	.0064
16	.017	.006			.736	.644	.628	.0160
17	.015	.0			.691	.633	.621	.0117
18	.012	.002			.550	.496	.488	.0077
19	.023	.002			.804	.729	.729	.0
21	.008	.003			.802	.756	.744	.0124
22	.011	.003			.773	.712	.708	.0043
23	.006	.002			.852	.820	.816	.0040
24	.008	.003			.802	.756	.744	.0124
25	.006	.002			.852	.820	.816	.0040
26	.014	.004			.700	.625	.617	.0083
27	.006	.001			.398	.361	.298	.0628
28	.010	.004			.514	.458	.343	.1155
29	.010	.004			.755	.708	.708	.0
30	.016	.005			.888	.813	.813	.0
31	.012	.004			.781	.723	.723	.0
32	.014	.008			.924	.840	.833	.0076
120	.086	.053			.961	.621	.597	.0245
122	.027	.003			.955	.866	.834	.0326
124A	.023	.008			.810	.712	.671	.0411
124B	.022	.008			.890	.779	.768	.0110
128A	.036	.003			.933	.825	.825	.0
128B	.034	.003			1.067	.943	.943	.0
130	.073	.055			.827	.532	.532	.0
131	.091	.081			1.669	1.151	1.151	.0
132	.072	.072			1.297	.842	.842	.0
133	.074	.003			1.182	.948	.948	.0
134	.074	.003			.826	.652	.652	.0
135A	.151	.070			1.232	.730	.730	.0
135B	.102	.069			.791	.454	.454	.0

Table A-7

BROOKHAVEN HYDROPYROLYSIS DATA FOR LIGNITE COAL

RUN	DATE	COAL	PSIZE	LENGTH	DIAM	FCOAL	HCRAT	HCONS
5	1976	LIGNITE		8.00	1.000	0.2100	3.3810	
7	1976	LIGNITE		8.00	1.000	0.5400	1.3889	
8	1976	LIGNITE		8.00	1.000	0.2500	5.8000	
9	1976	LIGNITE		8.00	1.000	0.6600	2.1970	
10	1976	LIGNITE		8.00	1.000	0.5000	1.4800	
11	1976	LIGNITE		8.00	1.000	0.4000	3.6250	
12	1976	LIGNITE		8.00	1.000	0.2600	4.8462	
13A	1976	LIGNITE		8.00	1.000	0.2400	5.6250	
13B	1976	LIGNITE		8.00	1.000	1.3900	0.8993	
14	1976	LIGNITE		8.00	1.000	0.6000	2.3333	
15	1976	LIGNITE		8.00	1.000	0.5000	2.8000	
16A	1976	LIGNITE		8.00	1.000	1.3200	0.9848	
16B	1976	LIGNITE		8.00	1.000	0.9300	1.3978	
16C	1976	LIGNITE		8.00	1.000	0.8500	1.5294	
17	1976	LIGNITE		8.00	1.000	1.3200	0.9470	
18A	1976	LIGNITE		8.00	1.000	0.9400	1.2766	
18B	1976	LIGNITE		8.00	1.000	1.2200	0.9836	
18C	1976	LIGNITE		8.00	1.000	1.2700	0.9449	
21	11/ 5/76	LIGNITE		8.00	1.000	0.7000	1.2429	.0200
22	1/13/77	LIGNITE		8.00	1.000	0.8200	1.3171	.1330
23	1/25/77	LIGNITE		8.00	1.000	0.6300	1.4603	.0740
24	1/27/77	LIGNITE		8.00	1.000	0.2900	3.6207	.1580
25	1/28/77	LIGNITE		8.00	1.000	0.4900	2.2449	.0520
26	1/31/77	LIGNITE		8.00	1.000	0.5000	2.2000	.0290
27	2/ 2/77	LIGNITE		8.00	1.000	0.5900	1.8644	.0480
28	2/ 3/77	LIGNITE		8.00	1.000	0.4800	2.2917	.1210
29	2/ 3/77	LIGNITE		8.00	1.000	0.5200	1.9231	.0480
46	4/26/77	LIGNITE		8.00	1.000	2.6400	0.4167	.1040
47	4/27/77	LIGNITE		8.00	1.000	0.9300	1.1290	.0920
48	5/ 6/77	LIGNITE		8.00	1.000	1.7500	0.6571	.0620
49	5/ 9/77	LIGNITE		8.00	1.000	1.0300	0.9709	.1860
50A	5/12/77	LIGNITE		8.00	1.000	1.1900	0.9076	.0560
50B	5/12/77	LIGNITE		8.00	1.000	1.0200	1.0392	.2200
51A	5/13/77	LIGNITE		8.00	1.000	0.9300	1.0753	.1340
51B	5/13/77	LIGNITE		8.00	1.000	0.7700	1.2597	.2600
52	5/16/77	LIGNITE		8.00	1.000	1.2200	0.8852	.1670
53	5/17/77	LIGNITE		8.00	1.000	0.7700	1.3247	.1390
55	6/ 7/77	LIGNITE		8.00	1.000	1.8000	0.5056	.2180
56	6/15/77	LIGNITE		8.00	1.000	0.9600	0.8854	.0490
57	6/16/77	LIGNITE		8.00	1.000	0.7300	1.2329	.0970
58	6/20/77	LIGNITE		8.00	1.000	1.5200	0.5263	.1100
59	6/21/77	LIGNITE		8.00	1.000	1.4500	0.6069	.0810
60A	6/23/77	LIGNITE		8.00	1.000	1.3400	0.6343	.2630
60B	6/23/77	LIGNITE		2.00	1.000	1.3400	0.6343	.2130
61A	6/27/77	LIGNITE		8.00	1.000	1.3200	0.6212	.1390
61B	6/27/77	LIGNITE		2.00	1.000	1.3200	0.6212	.0990
62	6/28/77	LIGNITE		8.00	1.000	1.3800	0.5797	.1890
63	6/29/77	LIGNITE		8.00	1.000	1.4400	0.6042	.0230

Table A-7 (Cont'd)

RUN	GVEL	TPRES	HPRES	TWALL	TGMAX	TGEIT	RTGAS	RTPAR
5	0.2264	1500.	1500.	1290.			35300.	
7	0.2392	1500.	1500.	1290.			33400.	
8	0.4625	1500.	1500.	1290.			17300.	
9	0.4387	1500.	1500.	1200.			18200.	
10	0.1770	2000.	2000.	1290.			45200.	
11	0.4149	1500.	1500.	1110.			19300.	
12	0.3089	1500.	1500.	885.			25900.	
13A	0.4084	1500.	1500.	1200.			19600.	
13B	0.3782	1500.	1500.	1200.			21200.	
14	0.4810	1500.	1500.	1425.			16600.	
15	0.5001	1500.	1500.	1500.			16000.	
16A	0.4466	1500.	1500.	1425.			17900.	
16B	0.4466	1500.	1500.	1425.			17900.	
16C	0.4466	1500.	1500.	1425.			17900.	
17	0.4260	1500.	1500.	1410.			18800.	
18A	0.2859	2100.	2100.	1370.			28000.	
18B	0.2859	2100.	2100.	1370.			28000.	
18C	0.2859	2100.	2100.	1370.			28000.	
21	0.2135	2000.	2000.	1335.			37500.	8600.
22	0.2716	2000.	2000.	1380.			29500.	11400.
23	0.2396	2000.	2000.	1445.			33400.	12200.
24	0.2784	2000.	2000.	1480.			28700.	11500.
25	0.2699	2000.	2000.	1335.			29600.	11100.
26	0.2631	2000.	2000.	1290.			30400.	11300.
27	0.2729	2000.	2000.	1355.			29300.	11200.
28	0.2824	2000.	2000.	1418.			28300.	11200.
29	0.3423	1500.	1500.	1418.			23400.	10500.
46	0.2842	2000.	2000.	1430.			28200.	9900.
47	0.2734	2000.	2000.	1445.			29300.	8300.
48	0.3961	1500.	1500.	1430.			20200.	6500.
49	0.3454	1500.	1500.	1435.			23200.	6800.
50A	0.3799	1500.	1500.	1470.			21100.	6800.
50B	0.2237	2500.	2500.	1470.			35800.	8800.
51A	0.2638	2000.	2000.	1470.			30300.	8100.
51B	0.1706	3000.	3000.	1470.			46900.	9500.
52	0.1811	3000.	3000.	1380.			44200.	9500.
53	0.1757	3000.	3000.	1430.			45500.	9500.
55	0.1600	3000.	3000.	1470.			50000.	9500.
56	0.1425	3000.	3000.	1380.			56100.	10000.
57	0.1497	3000.	3000.	1365.			53500.	9900.
58	0.2012	2000.	2000.	1380.			39800.	8700.
59	0.2951	1500.	1500.	1380.			27100.	7400.
60A	0.1794	2500.	2500.	1470.			44600.	9200.
60B	0.1794	2500.	2500.	1470.			11100.	2300.
61A	0.1650	2500.	2500.	1380.			48500.	9600.
61B	0.1650	2500.	2500.	1380.			12100.	2400.
62	0.1341	3000.	3000.	1380.			59600.	2500.
63	0.4376	1000.	1000.	1380.			18300.	6400.

Table A-7 (Cont'd)

RUN	X	XGAS	XHC	XM	XC2	XC3	XC4
5	.365	.269	.182	.122	.060	.0	.0
7	.301	.235	.138	.094	.044	.0	.0
8	.398	.287	.135	.135	.0	.0	.0
9	.215	.189	.089	.057	.032	.0	.0
10	.459	.298	.182	.119	.063	.0	.0
11	.171	.130	.043	.027	.016	.0	.0
12	.129	.126	.031	.020	.011	.0	.0
13A	.330	.286	.131	.085	.046	.0	.0
13B	.234	.200	.109	.070	.039	.0	.0
14	.566	.405	.300	.219	.081	.0	.0
15	.586	.445	.315	.263	.052	.0	.0
16A	.444	.321	.235	.177	.058	.0	.0
16B	.396	.283	.209	.156	.053	.0	.0
16C	.580	.409	.314	.237	.077	.0	.0
17	.692	.492	.367	.275	.092	.0	.0
18A	.860	.596	.458	.316	.142	.0	.0
18B	.822	.571	.428	.291	.137	.0	.0
18C	.888	.624	.465	.319	.146	.0	.0
21	.428	.307	.225	.149	.076	.0	.0
22	.475	.323	.249	.169	.080	.0	.0
23	.448	.267	.214	.165	.049	.0	.0
24	.595	.390	.335	.279	.056	.0	.0
25	.381	.272	.193	.128	.065	.0	.0
26	.360	.233	.153	.099	.054	.0	.0
27	.388	.270	.187	.123	.064	.0	.0
28	.438	.311	.235	.170	.065	.0	.0
29	.358	.276	.191	.135	.056	.0	.0
46	.511	.418	.334	.275	.059	.0	.0
47	.467	.337	.266	.167	.099	.0	.0
48	.325	.260	.195	.137	.058	.0	.0
49	.637	.512	.421	.355	.066	.0	.0
50A	.407	.317	.248	.193	.055	.0	.0
50B	.591	.552	.498	.453	.045	.0	.0
51A	.503	.426	.364	.317	.047	.0	.0
51B	.634	.611	.566	.508	.058	.0	.0
52	.587	.480	.422	.326	.096	.0	.0
53	.482	.419	.397	.310	.087	.0	.0
55	.611	.595	.543	.538	.005	.0	.0
56	.384	.304	.256	.183	.073	.0	.0
57	.492	.373	.313	.211	.102	.0	.0
58	.497	.413	.329	.274	.055	.0	.0
59	.478	.382	.308	.240	.068	.0	.0
60A	.627	.618	.565	.546	.019	.0	.0
60B	.601	.564	.524	.503	.021	.0	.0
61A	.518	.419	.351	.269	.082	.0	.0
61B	.454	.328	.273	.202	.071	.0	.0
62	.663	.535	.471	.379	.092	.0	.0
63	.353	.291	.202	.143	.059	.0	.0

Table A-7 (Cont'd)

RUN	XCO	XCO2	XOIL	XBTX	PHIG	PHIHC	PHIM	PHIC2
5	.087	.0		.057	.737	.499	.334	.1644
7	.086	.011		.040	.781	.458	.312	.1462
8	.130	.022		.066	.721	.339	.339	.0
9	.076	.024		.015	.879	.413	.265	.1484
10	.109	.007		.061	.649	.397	.259	.1373
11	.057	.030		.025	.760	.251	.158	.0936
12	.049	.046		.002	.977	.240	.155	.0853
13A	.138	.017		.027	.867	.397	.258	.1394
13B	.081	.010		.020	.855	.466	.299	.1667
14	.105	.0		.097	.716	.530	.387	.1431
15	.130	.0		.085	.759	.538	.449	.0887
16A	.084	.002		.075	.722	.529	.399	.1306
16B	.073	.001		.068	.714	.528	.394	.1338
16C	.094	.001		.103	.705	.541	.409	.1328
17	.123	.002		.120	.711	.530	.397	.1329
18A	.136	.002		.163	.693	.533	.367	.1651
18B	.141	.002		.152	.695	.521	.354	.1667
18C	.157	.002		.163	.703	.524	.359	.1644
21	.080	.002	.046	.074	.717	.526	.348	.1776
22	.074	.0	.067	.083	.680	.524	.356	.1684
23	.053	.0	.111	.069	.596	.478	.368	.1094
24	.055	.0	.127	.078	.655	.563	.469	.0941
25	.079	.0	.046	.063	.714	.507	.336	.1706
26	.075	.005	.080	.046	.647	.425	.275	.1500
27	.081	.002	.052	.067	.696	.482	.317	.1649
28	.076	.0	.038	.089	.710	.537	.388	.1484
29	.085	.0	.020	.062	.771	.534	.377	.1564
46	.078	.006	.001	.091	.818	.654	.538	.1155
47	.071	.0	.029	.102	.722	.570	.358	.2120
48	.061	.004	.011	.054	.800	.600	.422	.1785
49	.089	.002	.008	.117	.804	.661	.557	.1036
50A	.068	.001	.015	.074	.779	.609	.474	.1351
50B	.053	.001	.004	.035	.934	.843	.766	.0761
51A	.062	.0	.002	.075	.847	.724	.630	.0934
51B	.045	.0	.002	.020	.964	.893	.801	.0915
52	.058	.0	.011	.096	.818	.719	.555	.1635
53	.022	.0	.0	.062	.869	.824	.643	.1805
55	.050	.003	.008	.007	.975	.888	.881	.0737
56	.047	.001	.007	.074	.792	.667	.477	.1901
57	.060	.0	.018	.100	.758	.636	.429	.2073
58	.081	.003	.007	.076	.831	.662	.551	.1107
59	.070	.004	.002	.007	.799	.644	.502	.1423
60A	.052	.001	.002	.007	.986	.901	.871	.0303
60B	.038	.002	.0	.037	.938	.872	.837	.0349
61A	.066	.002	.009	.090	.809	.678	.519	.1583
61B	.052	.003	.048	.077	.722	.601	.445	.1564
62	.062	.002	.047	.081	.807	.710	.572	.1388
63	.086	.003	.0	.062	.824	.572	.405	.1671

Appendix B

TYPICAL ANALYSES OF COALS TESTED IN REACTOR SYSTEMS

Typical analyses of coals tested in reactor systems are shown in Table B-1.

Table B-1

TYPICAL ANALYSES OF COALS TESTED IN REACTOR SYSTEMS

	North Dakota Lignite	Montana Rosebud Subbituminous	Kentucky #9/14 Bituminous HvCb(b)	Kentucky #9 Bituminous HvAb(c)	Illinois #6 Bituminous HvCb(d)	Pittsburgh Seam Bituminous HvAb(e)
Proximate analysis,(a) wt %						
Moisture	7.8	5.6	1.9	5.0	6.8	1.2
Volatile matter	39.7	36.3	36.9	36.5	33.6	36.4
Fixed carbon	46.9	48.1	50.4	49.3	50.3	56.7
Ash	5.6	10.0	10.8	9.2	9.3	5.7
Ultimate analysis(a) (dry basis), wt %						
Carbon	64.0	64.8	69.8	72.9	73.6	79.1
Hydrogen	4.3	4.6	4.9	5.0	4.9	5.2
Nitrogen	1.2	1.1	1.5	0.9	1.0	1.6
Sulfur	1.4	1.0	4.3	2.8	1.8	1.1
Oxygen by difference	23.0	17.9	8.5	8.5	8.5	7.2
Ash	6.1	10.6	11.0	9.9	10.2	5.8

(a) As fed to the reactor system
(b) From Pittsburgh and Midway Coal Mining Co., Colonial Mine
(c) From Island Creek Coal Co., Hamilton No. 2 Mine
(d) From Freeman Coal Co., Orient #3 Mine
(e) From the U.S. Bureau of Mines experimental mine, Bruceton, Pa.