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AN ANALYSIS OF COAL HYDROGASIFICATION PROCESSES

Quarterly Technical Progress Report for the Period 1 December 1977 - 28 February 1978

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MASTER

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ABSTRACT

This Quarterly Technical Progress Report covers work performed during the period 1 December 1977 to 28 February 1978 for a program entitled "An Analysis of Coal Hydrogasification Processes." This program is being performed in four sequential tasks: Task I — Data Collection; Task II — Data Analysis; Task III — Process Modeling and Reactor Design; and Task IV — Identification of Additional Data and Recommended Experimental Programs.

Substantial progress was made on Tasks I, II, and III. Data from 15 recent Rocketdyne hydrogasification tests with subbituminous and bituminous coals and 24 Rocketdyne partial liquefaction tests with bituminous coals were entered into the computerized data base. Data from 17 recent Cities Service hydrogasification tests with subbituminous coal were also entered into the data base. The Cities Service, Rocketdyne, and PERC data bases were expanded to include values for the following: carbon selectivity to BTX (Cities Service); carbon selectivity to methane, ethane, and BTX (Rocketdyne); and gas velocity, gas residence time, and carbon selectivity to gas, methane, and ethane (PERC).

Semiempirical correlations for predicting overall carbon conversion and carbon conversion to gas, methane, CO, and CO_2 were fitted to the Cities Service and Rocketdyne subbituminous coal data. The analysis showed that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor give similar values of overall carbon conversion and carbon conversion to gaseous products under comparable operating conditions. A semiempirical correlation for predicting overall carbon conversion was fitted to the Brookhaven lignite hydropyrolysis data. Because of inconsistencies in the Brookhaven data, 11 of the 48 runs were not used in the correlation. An improved semiempirical correlation was developed for predicting overall carbon conversion for the reactor systems. The improved correlation accounts for thermodynamic equilibrium between the carbon in the coal and the reaction products.

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Section 1

OBJECTIVES AND SCOPE

This report is the fourth Quarterly Technical Progress Report for a program entitled, "An Analysis of Coal Hydrogasification Processes." The program is being performed for DOE by Bechtel Corporation under DOE Contract No. EF-77-A-01-2565. Work on this program was initiated on February 1, 1977.

The major objective of the program is "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 have been established.

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

The primary objective of Task II is to perform a detailed analysis of the data, as required to evaluate the information for a pilot plant application. Consideration will be 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, will be analyzed for potential operational problems and scaling.

Task III has two primary objectives: (1) to perform reactor model studies, where available data permit, for each of the three processes; and (2) to generate a conceptual, full-scale, optimum reactor design in consultation with DOE. The reactor model study will attempt to predict, where possible, overall carbon conversion, carbon selectivity to gas, and carbon selectivity to methane and ethane for the three processes. In conjunction with the modeling study, a sensitivity analysis will be performed that will 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 are 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 man-hours 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 2

PROGRESS SUMMARY AND OPEN ITEMS

2.1 PROGRESS SUMMARY

Figure 2-1 summarizes the program progress between February 1, 1977 (the program start date) and February 28, 1978. As shown in Figure 2-1, the contract period has been extended through April 30, 1978, to reflect contract modification A001.

During this reporting period, substantial progress was made on Tasks I, II, and III. The technical progress for each subject task is presented in Section 3. As can be seen in Figure 2-1, actual manhours expended and program progress are on schedule.

2.2 OPEN ITEMS

At the end of the February 1978 reporting period, there were no significant open items.

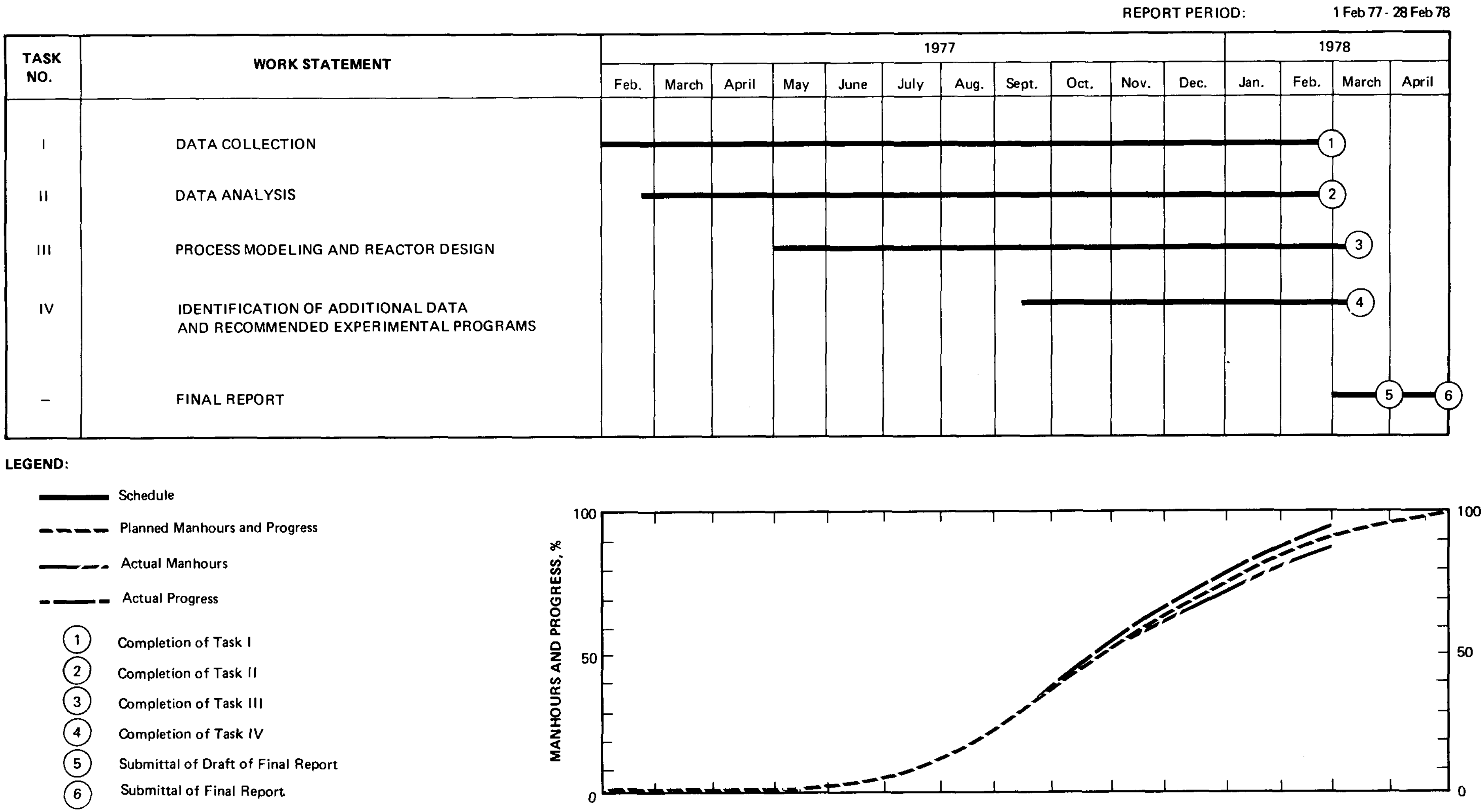

Figure 2-1. Progress and Performance Chart

Section 3

TECHNICAL PROGRESS

This section describes the technical progress for Tasks I, II, and III during the reporting period. A computer listing of all of the Rocketdyne and Cities Service subbituminous coal data contained in the data base is presented in the Appendix.

3.1 TASKS I AND II — ROCKETDYNE DATA COLLECTION AND ANALYSIS

During this reporting period, Bechtel received additional hydrogasification data from Rocketdyne[1,2,3] for 15 recently completed tests (Runs 011-14, 15, 16, 17, 22, 23, and 24, and Runs 300-1, 2, 3, 4, 5, 6, 11, and 12) conducted in Rocketdyne's 1/4-ton/hr reactor test facility. Runs 011-14 through 011-24 and Run 300-1 all used Montana Rosebud subbituminous coal feed; Runs 300-2 through 300-5 used Illinois #6 bituminous (HvCb) coal feed; and Runs 300-6 through 300-12 used Kentucky #9 bituminous (HvAb) coal feed. Bechtel also received from Rocketdyne the following: a revised set of data[1] for 10 earlier hydropyrolysis tests previously reported by Bechtel,[4] and additional data[5,6] for 24 coal partial liquefaction tests (Runs 16 through 42) conducted in Rocketdyne's 1-ton/hr reactor test facility using two Western Kentucky bituminous coal feeds (analyses of these coals are given elsewhere[5]).

All the above hydrogasification and partial liquefaction data were entered into the computerized data base. Table 3-1 gives a computer listing of selected data from the Rocketdyne subbituminous and bituminous tests. A computer listing of all of the Rocketdyne subbituminous data contained in the data base is presented in the Appendix.

Table 3-1

ROCKETDYNE HYDROPYROLYSIS DATA

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 R)	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)
5	1/31/77	BTM-1	1 TPH	.382					1750.	1000.	940.	32.30	155.	.250	56.
6	2/ 3/77	BTM-1	1 TPH	.542	0.397			.089	2160.	1000.	930.	39.70	126.	.478	56.
7	2/ 7/77	BTM-1	1 TPH	.615	0.483			.013	2410.	1000.	920.	42.00	119.	.775	56.
8	2/17/77	BTM-1	1 TPH	.596	0.485			.089	2150.	1000.	920.	18.20	274.	.365	56.
9	2/22/77	BTM-1	1 TPH	.645	0.760			.002	2340.	1500.	1390.	12.20	410.	.365	56.
10	3/ 1/77	BTM-1	1 TPH	.609	0.782			.056	2030.	1500.	1400.	10.20	490.	.314	56.
11	3/ 4/77	BTM-1	1 TPH	.627	0.968			.027	2110.	1500.	1420.	7.90	634.	.334	56.
12	3/ 9/77	BTM-1	1 TPH	.576	0.672			.123	2140.	1000.	940.	11.80	424.	.333	56.
13	3/23/77	BTM-1	1 TPH	.560	0.334			.055	2180.	1000.	930.	79.40	63.	.292	56.
14	3/25/77	BTM-1	1 TPH	.597	0.472			.097	2230.	1500.	1400.	51.00	98.	.397	56.
15	3/29/77	BTM-1	1 TPH	.560	0.359			.066	2120.	700.	650.	111.00	45.	.403	56.
16	4/ 4/77	BTM-1	1 TPH	.573	0.412			.058	2150.	1000.	930.	72.50	69.	.443	56.
17		BTM-1	1 TPH	.592	0.434			.083	2200.	1010.	940.	78.10	64.	.507	56.
18		BTM-1	1 TPH	.519	0.343			.071	2090.	1000.	930.	74.60	67.	.409	56.
19		BTM-1	1 TPH	.562	0.256			.034	2050.	520.	480.	147.00	34.	.429	56.
20		BTM-2	1 TPH	.540	0.341			.085	2060.	1000.	930.	63.30	79.	.293	52.
21		BTM-2	1 TPH	.590	0.403			.132	2150.	1000.	930.	78.10	64.	.458	52.
22		BTM-2	1 TPH	.570	0.389			.047	2090.	500.	470.	87.70	57.	.370	52.
23		BTM-2	1 TPH	.600	0.355			.120	2100.	1000.	930.	79.40	63.	.469	36.
24		BTM-2	1 TPH	.638	0.434			.172	2230.	1000.	930.	82.00	61.	.528	36.
25		BTM-2	1 TPH	.630	0.365			.154	2380.	1000.	930.	41.30	121.	.656	36.
26	9/ 9/77	BTM-2	1 TPH	.615	0.382			.122	2180.	1000.	940.	39.10	128.	.485	36.
27	9/14/77	BTM-2	1 TPH	.571	0.366			.095	2070.	1000.	950.	37.30	134.	.472	36.
28	9/16/77	BTM-2	1 TPH	.587	0.433			.123	2230.	1000.	940.	39.70	126.	.491	52.
29	9/21/77	BTM-2	1 TPH	.576	0.477			.151	2180.	1500.	1400.	23.60	212.	.418	52.
30	9/23/77	BTM-2	1 TPH	.546	0.441			.097	2090.	1000.	940.	36.80	136.	.435	52.
31	9/27/77	BTM-2	1 TPH	.628	0.712			.135	2400.	1500.	1400.	23.90	209.	.505	52.
32	9/29/77	BTM-2	1 TPH	.622	0.441			.138	2300.	1000.	930.	39.40	127.	.452	52.
34	10/ 4/77	BTM-2	1 TPH	.479	0.378			.071	1990.	1000.	940.	75.80	66.	.414	52.
37	10/31/77	BTM-2	1 TPH	.482	0.427			.083	2030.	1000.	940.	19.60	255.	.304	52.
38	11/ 8/77	BTM-2	1 TPH	.462	0.329				1870.	1000.	950.	18.50	271.	.313	52.
39	11/ 9/77	BTM-2	1 TPH	.513	0.468			.105	2120.	1000.	940.	20.20	247.	.296	52.
40	11/10/77	BTM-2	1 TPH	.481	0.486			.098	2050.	1000.	950.	22.20	225.	.279	52.
41	11/11/77	BTM-2	1 TPH	.432	0.382			.049	1890.	1000.	950.	20.90	239.	.243	52.
42	11/14/77	BTM-2	1 TPH	.518	0.502			.139	2150.	1000.	950.	23.60	212.	.249	52.

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 R)	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		2130.	1000.	950.	24.40	615.	.356	
011- 8	9/29/77	BTM-1	1/4 TPH	.535	0.583	.492	.009		2270.	1010.	950.	31.60	475.	.421	
011- 9	10/ 4/77	BTM-1	1/4 TPH	.588	0.724	.655	.002		2420.	1500.	1420.	21.60	695.	.499	
011-10	10/ 7/77	BTM-1	1/4 TPH	.588	0.707	.643	.0		2370.	1490.	1410.	21.70	690.	.506	
300- 2	1/ 6/78	BTM-3	1/4 TPH	.707	0.973	.885	.0		2440.	1500.	1310.	10.20	1465.	.643	
300- 3	1/ 9/78	BTM-3	1/4 TPH	.500	0.872	.648	.092		2060.	990.	870.	13.60	1100.	.342	
300- 4	1/11/78	BTM-3	1/4 TPH	.595	0.827	.687	.062		2320.	1000.	870.	14.90	1010.	.509	
300- 5	1/16/78	BTM-3	1/4 TPH	.480	0.775	.477	.194		1930.	990.	900.	12.80	1170.	.548	
300- 6	1/17/78	BTM-2	1/4 TPH	.627	0.903	.831	.003		2280.	1490.	1280.	10.00	1500.	.469	
300-11	2/10/78	BTM-2	1/4 TPH	.644	0.961	.882	.002		2370.	1500.	1320.	15.90	945.	.519	
300-12	2/16/78	BTM-2	1/4 TPH	.650	0.992	.915	.0		2370.	1500.	1320.	4.39	3415.	.489	
011- 2	8/30/77	SUBBTM	1/4 TPH	.289	0.495	.246	.118		1930.	1020.	960.	25.00	600.	.592	
011- 4	9/ 9/77	SUBBTM	1/4 TPH	.361	0.837	.640	.006		2360.	990.	930.	28.00	535.	.512	
011- 5	9/15/77	SUBBTM	1/4 TPH	.364	0.629	.451	.036		2190.	1000.	940.	26.10	575.	.401	
011-11	10/14/77	SUBBTM	1/4 TPH	.436	0.991	.819	.002		2300.	1500.	1410.	22.10	680.	.569	
011-12	10/18/77	SUBBTM	1/4 TPH	.392	0.714	.423	.140		2050.	1500.	1430.	18.60	805.	.559	
011-13	10/21/77	SUBBTM	1/4 TPH	.321	0.692	.330	.206		1930.	1500.	1440.	19.10	785.	.535	
011-14	10/28/77	SUBBTM	1/4 TPH	.278					2020.	1010.	790.	28.47	527.	.418	
011-15	11/ 2/77	SUBBTM	1/4 TPH	.298					2170.	1130.	840.	22.69	661.	.331	
011-16	11/21/77	SUBBTM	1/4 TPH	.470	1.000	.872	.0		2220.	1480.	1390.	10.60	1420.	.550	
011-17	11/28/77	SUBBTM	1/4 TPH	.407	0.860	.627	.081		1990.	1500.	1430.	8.70	1725.	.576	
011-22	12/14/77	SUBBTM	1/4 TPH	.354	0.867	.675	.003		2220.	1000.	880.	13.60	1105.	.392	
011-23	12/19/77	SUBBTM	1/4 TPH	.292	0.849	.384	.243		1880.	990.	900.	12.90	1165.	.364	
011-24	12/21/77	SUBBTM	1/4 TPH	.382	0.911	.725	.0		2260.	1000.	890.	15.40	975.	.705	
300- 1	1/ 4/78	SUBBTM	1/4 TPH	.459	0.935	.780	.0		2290.	1500.	1310.	10.60	1420.	.675	

*BTM-1 is Kentucky bituminous HvAb coal from the Colonial Mine of the Pittsburgh and Midway Mining Co.

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

BTM-3 is Illinois #6 bituminous HvCb coal.

**Runs 5 through 42 were conducted under DOE Contract EX-76-C-01-2044.
Runs 011-7 through 300-1 were conducted under DOE Contract EX-77-C-01-2518.

The data base was expanded during this reporting period to include data for additional operating and dependent variables. The additional variables are total reactor pressure, gas velocity, mean particle size, and carbon selectivities to methane, ethane, and BTX. Product selectivities were calculated from product gas and liquid analyses, where available, and overall carbon conversions.

The additional partial liquefaction bituminous tests shown in Table 3-1 were conducted at reactor pressures of 500 to 1,000 psig, outlet gas temperatures of 1,410°F to 1,920°F (1,870°R to 2,380°R), and gas (or particle) residence times of 34 to 271 milliseconds. Results indicate a maximum carbon conversion to gas of 45 percent (selectivity of 71 percent) at a hydrogen partial pressure of 1,400 psig, gas temperature of 1,940°F (2,400°R), and gas residence time of 209 milliseconds. Lower temperatures and/or residence times decrease the carbon conversion to gas. Maximum carbon conversion to BTX of about 10 percent (selectivity of 17 percent) was obtained at a hydrogen partial pressure of 930 psig, gas temperature of 1,770°F (2,230°R), and gas residence time of 61 milliseconds.

The recent hydrogasification data were generated in two entrained downflow reactors; one is 1.88 inches I.D. by 15 feet long and the other is 2.83 inches I.D. by 15 feet long. These data were obtained at reactor pressures of 1,000 to 1,500 psig, outlet gas temperatures of 1,420°F to 1,940°F (1,880°R to 2,400°R), and gas (or particle) residence times of approximately 530 to 3,420 milliseconds.

Overall carbon conversion for the Montana subbituminous coal ranged from 28 to 47 percent; overall carbon conversion for the Illinois and Kentucky bituminous coals ranged from 48 to 71 percent and 63 to 65 percent, respectively. Illinois bituminous coal Run 300-2 achieved the highest overall carbon conversion (71 percent) reported to date from the 1/4-ton/hr reactor tests. This conversion was obtained at a hydrogen partial pressure of 1,310 psig, outlet gas temperature of 1,980°F (2,440°R), residence time of 1,465 milliseconds, and hydrogen-to-coal ratio of 0.64.

For the Montana subbituminous coal, a maximum carbon selectivity to methane of 87 percent was achieved; for the Illinois and Kentucky bituminous coals, maximum carbon selectivities to methane were 89 to 91 percent, respectively. Almost 100 percent carbon selectivity to gaseous products was obtained in Kentucky bituminous coal Run 300-12.

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,[1] the results obtained from these two tests are uncertain. Significant fluctuations in reactant flows, particularly in Run 011-14, remains essentially unexplained.

Insufficient information was available to calculate the carbon conversion and selectivity to BTX for the 25 bituminous and subbituminous gasification tests.

3.2 TASKS I AND II — CITIES SERVICE DATA COLLECTION AND ANALYSIS

During this reporting period, Bechtel received additional hydropyrolysis data from Cities Service for 17 recently completed tests (Runs MR-22 through MR-48) using Montana Rosebud subbituminous coal.[2] A revised set of data was also received from Cities Service[2] for the 26 earlier hydropyrolysis tests previously reported by Bechtel.[7]

All the above hydropyrolysis data were entered into the computerized data base. Table 3-2 gives a computer listing of selected data from the Cities Service subbituminous tests. The Cities Service data base was expanded during this reporting period to include data for total reactor pressure and carbon selectivity to BTX. A computer listing of all of the Cities Service subbituminous data contained in the data base is presented in the Appendix.

The 17 recent subbituminous tests were conducted at reactor pressures of 500 to 1,600 psig, outlet gas temperatures of 1,510°F to 1,750°F (1,970°F to 2,210°R), and gas (or particle) residence times of 1,400 to 3,500 milliseconds. Overall carbon conversions for these tests ranged from 39 to 52 percent. Run MR-22 gave the highest carbon conversion of 55 percent at a hydrogen partial pressure of 1,600 psig, outlet gas temperature of 1,610°F (2,070°R), and gas residence time of 3,160 milliseconds.

Good carbon mass balance closures ranging from 91 to 103 percent and ash balance closures ranging from 88 to 109 percent were reported for the recently completed subbituminous tests.[2]

Table 3-2

CITIES SERVICE HYDROPYROLYSIS DATA

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 R)	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					1980.	500.	500.	20.90	1530.	1.400	45.
MR- 1	6/16/77	SUBBTM	EF	.319	0.837	.266	.216	.107	1980.	500.	500.	9.00	433.	0.760	45.
MR-10	6/22/77	SUBBTM	EF	.214	0.593	.182	.150	.093	1960.	1500.	1500.	9.40	423.	0.830	45.
MR-13	6/27/77	SUBBTM	EF	.397	0.710	.370	.209	.134	1990.	1500.	1500.	16.60	1090.	0.800	45.
MR-14	6/29/77	SUBBTM	EF	.431	0.814	.513	.146	.121	2090.	1500.	1500.	17.00	1060.	0.740	45.
MR-28	7/ 6/77	SUBBTM	EF	.275	0.724	.247	.204	.065	1990.	1000.	1000.	12.80	307.	0.790	45.
MR-29	7/ 8/77	SUBBTM	EF	.344	0.773	.340	.235	.125	2090.	1000.	1000.	12.80	307.	0.990	45.
MR-30	7/12/77	SUBBTM	EF	.324	0.772	.401	.204	.173	2170.	1000.	1000.	12.30	321.	0.850	45.
MR-11	7/15/77	SUBBTM	EF	.255	0.718	.298	.224	.114	2070.	1500.	1500.	13.00	303.	0.780	56.
MR-12	7/19/77	SUBBTM	EF	.321	0.726	.330	.231	.156	2120.	1500.	1500.	12.60	312.	0.750	56.
MR-25	7/21/77	SUBBTM	EF	.359	0.710	.331	.234	.178	1980.	1000.	1000.	16.60	1090.	0.980	56.
MR-26	7/25/77	SUBBTM	EF	.382	0.780	.458	.170	.217	2080.	1000.	1000.	16.50	1090.	0.880	56.
MR-27	7/27/77	SUBBTM	EF	.402	0.794	.585	.057	.206	2160.	1000.	1000.	16.40	1100.	0.930	56.
MR-15	7/29/77	SUBBTM	EF	.453	0.775	.541	.102	.216	2120.	1500.	1500.	16.40	1100.	0.870	56.
MR- 2	8/ 3/77	SUBBTM	EF	.339	0.770	.327	.224	.156	2070.	500.	500.	29.40	318.	0.890	56.
MR- 3	8/ 5/77	SUBBTM	EF	.330	0.797	.352	.109	.148	2170.	500.	500.	29.50	317.	0.970	56.
MR-16	8/ 8/77	SUBBTM	EF	.379	0.715	.256	.172	.127	1980.	1500.	1500.	14.30	653.	0.910	56.
MR-17	8/10/77	SUBBTM	EF	.430	0.765	.319	.153	.165	2060.	1500.	1500.	14.30	654.	1.240	56.
MR-18	8/12/77	SUBBTM	EF	.430	0.751	.316	.128	.191	2100.	1500.	1500.	14.20	656.	0.930	56.
MR-37	8/16/77	SUBBTM	EF	.334	0.784	.338	.168	.180	2000.	750.	750.	25.20	2300.	1.080	56.
MR-38	8/18/77	SUBBTM	EF	.414	0.754	.488	.065	.244	2110.	770.	770.	20.10	2860.	0.970	56.
MR-39	8/22/77	SUBBTM	EF	.455	0.809	.475	.009	.185	2190.	750.	750.	20.70	2770.	0.980	56.
MR- 5	8/24/77	SUBBTM	EF	.418					2090.	500.	500.	63.50	910.	1.230	56.
MR-20	9/15/77	SUBBTM	EF	.460	0.741	.352	.230	.220	1980.	1600.	1600.	18.10	3190.	0.910	56.
MR-21	9/20/77	SUBBTM	EF	.507	0.740	.438	.134	.252	2050.	1600.	1600.	17.80	3250.	0.940	56.
MR-22	9/22/77	SUBBTM	EF	.548	0.754	.471	.100	.243	2070.	1600.	1600.	17.60	3160.	0.920	56.
MR- 9	10/12/77	SUBBTM	EF	.456	0.686	.346	.206	.211	1980.	1600.	1600.	27.10	2130.	1.070	56.
MR-47	10/14/77	SUBBTM	EF	.478	0.713	.381	.186	.222	2030.	1600.	1600.	25.20	2268.	1.140	56.
MR-19	10/18/77	SUBBTM	EF	.516	0.715	.411	.149	.254	2070.	1600.	1600.	24.90	2310.	1.000	56.
MR-35	10/20/77	SUBBTM	EF	.412	0.709	.359	.189	.209	2010.	1000.	1000.	17.60	2780.	0.990	56.
MR-36	10/24/77	SUBBTM	EF	.473	0.702	.446	.074	.249	2100.	1000.	1000.	15.90	3508.	0.850	56.
MR-40	10/26/77	SUBBTM	EF	.506	0.759	.534	.024	.237	2150.	1000.	1000.	16.60	3365.	0.950	56.
MR-32	10/28/77	SUBBTM	EF	.456	0.706	.309	.217	.215	2000.	1000.	1000.	24.40	2320.	0.860	56.
MR-33	11/ 8/77	SUBBTM	EF	.465	0.671	.387	.084	.308	2110.	1000.	1000.	24.50	2320.	0.940	56.
MR-34	11/ 9/77	SUBBTM	EF	.462	0.658	.442	.028	.331	2150.	1000.	1000.	23.70	2400.	0.930	56.
MR-23	11/11/77	SUBBTM	EF	.426	0.681	.324	.192	.291	2000.	1000.	1000.	11.50	1540.	0.880	56.
MR-24	11/14/77	SUBBTM	EF	.409	0.741	.423	.093	.200	2110.	1000.	1000.	12.70	1400.	0.910	56.
MR-31	11/16/77	SUBBTM	EF	.447	0.747	.463	.022	.197	2180.	1000.	1000.	12.20	1450.	0.940	56.
MR- 6	11/18/77	SUBBTM	EF	.432	0.697	.319	.220	.162	1970.	1600.	1600.	12.30	1450.	0.850	56.
MR- 8	11/21/77	SUBBTM	EF	.465	0.710	.366	.187	.196	2060.	1600.	1600.	12.10	1460.	0.770	56.
MR- 7	11/22/77	SUBBTM	EF	.410	0.712	.359	.212	.207	2020.	1600.	1600.	12.10	1470.	0.810	56.
MR-48	12/14/77	SUBBTM	EF	.392	0.796	.482	.005	.179	2210.	500.	500.	16.40	3486.	0.890	56.

*Runs MR-4 through MR-48 were conducted under DOE Contract EX-77-C-01-2518.

3.3 TASKS I AND II — PERC DATA COLLECTION AND ANALYSIS

In an earlier report,[8] Bechtel presented and analyzed the data from 42 hydropyrolysis tests conducted at the Pittsburgh Energy Research Center (PERC) in a free-fall, dilute-phase (FDP) reactor using bituminous and lignite coal feeds. During this reporting period, the PERC computerized data base was expanded to include additional operating and dependent variables for the above 42 tests.

Table 3-3 gives an updated computer listing of selected data from the PERC tests. This listing presents additional data for carbon selectivities to gas, methane, and ethane; gas velocity; gas residence time; and mean particle size. Carbon selectivities to gaseous products were calculated from PERC-reported product gas analyses and overall carbon conversion;[9,10] gas velocity was calculated using the average of the reported inlet and outlet gas flow rates and the reactor cross-sectional area; and gas residence time was calculated using the reactor heated length and the gas velocity.

Insufficient data were available to calculate carbon conversions and selectivities to liquid products. Particle residence time data were also unavailable.

Table 3-3

PITTSBURGH ENERGY RESEARCH CENTER
HYDROPYROLYSIS 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 R)	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	1930.	1000.	853.	.0401	124.7	.0718
IHR-167	1974	BTM-1	.141	.250	0.556	0.488	0.040	1930.	1000.	368.	.0420	119.1	.0298
IHR-156	1974	BTM-1	.168	.250	0.660	0.556	0.020	2020.	1000.	340.	.0447	111.9	.0320
IHR-176	1974	BTM-1	.173	.240	0.700	0.617	0.008	2020.	1000.	339.	.0448	111.5	.0319
IHR-190	1974	BTM-1	.182	.220	0.809	0.723	0.009	2020.	1000.	347.	.0475	105.2	.0333
IHR-183	1974	BTM-1	.189	.362	0.517	0.470	0.0	2020.	1000.	454.	.0412	121.3	.1051
IHR-177	1974	BTM-1	.240	.308	0.773	0.724	0.006	2020.	1000.	737.	.0416	120.1	.0701
IHR-166	1974	BTM-1	.162	.256	0.625	0.563	0.004	2020.	1200.	411.	.0368	135.8	.0321
IHR-165	1974	BTM-1	.180	.242	0.744	0.682	0.004	2020.	1500.	516.	.0300	166.5	.0335
IHR-157	1974	BTM-1	.208	.300	0.737	0.663	0.003	2020.	2000.	627.	.0232	215.3	.0329
IHR-172	1974	BTM-1	.185	.280	0.650	0.629	0.004	2020.	2000.	665.	.0228	219.0	.0355
IHR-186	1974	BTM-1	.221	.334	0.671	0.614	0.0	2110.	500.	361.	.0415	120.6	.0547
IHR-173	1974	BTM-1	.164	.314	0.516	0.478	0.006	2110.	1000.	371.	.0442	67.9	.0330
IHR-147	1974	BTM-1	.189	.250	0.736	0.628	0.016	2110.	1000.	388.	.0463	108.0	.0372
IHR-146	1974	BTM-1	.182	.256	0.691	0.621	0.012	2110.	1000.	348.	.0459	109.0	.0338
IHR-182	1974	BTM-1	.144	.260	0.550	0.488	0.008	2110.	1000.	393.	.0934	53.6	.0374
IHR-181	1974	BTM-1	.269	.332	0.804	0.729	0.0	2110.	1000.	680.	.0458	109.2	.0695
IHR-151	1974	BTM-1	.160	.242	0.802	0.744	0.012	2110.	1100.	369.	.0422	118.4	.0342
IHR-153	1974	BTM-1	.269	.233	0.773	0.708	0.004	2110.	1100.	783.	.0380	131.7	.0727
IHR-149	1974	BTM-1	.192	.250	0.852	0.816	0.004	2110.	1200.	436.	.0399	125.4	.0366
IHR-160	1974	BTM-1	.196	.242	0.802	0.744	0.012	2110.	1500.	509.	.0310	161.5	.0374
IHR-158	1974	BTM-1	.214	.250	0.852	0.816	0.004	2110.	2000.	640.	.0240	208.7	.0352
IHR-154	1974	BTM-1	.200	.240	0.700	0.617	0.008	2110.	2000.	671.	.0241	207.3	.0368
IHR-192	1974	BTM-2	.081	.191	0.398	0.298	0.063	1660.	1000.	561.	.0437	114.5	.0501
IHR-191	1974	BTM-2	.137	.251	0.514	0.343	0.116	1800.	1000.	494.	.0435	115.0	.0411
IHR-161	1974	BTM-2	.237	.298	0.755	0.708	0.0	2110.	1000.	397.	.0482	103.8	.0432
IHR-164	1974	BTM-2	.262	.278	0.888	0.813	0.0	2110.	1200.	409.	.0431	116.0	.0373
IHR-162	1974	BTM-2	.233	.278	0.781	0.723	0.0	2110.	1500.	488.	.0322	155.3	.0326
IHR-163	1974	BTM-2	.248	.263	0.924	0.833	0.008	2110.	2000.	670.	.0248	201.9	.0343
120	1976	LIGNITE	.379	.409	0.961	0.597	0.024	2110.	1000.	679.	.0595	84.1	.0578
122	1976	BTM-2	.321	.337	0.935	0.834	0.033	2110.	1000.	736.	.0525	95.2	.0800
124A	1976	BTM-2	.256	.316	0.810	0.671	0.041	2110.	1000.	669.	.0404	123.6	.0490
124B	1976	BTM-2	.240	.272	0.890	0.768	0.011	2110.	1000.	601.	.0338	147.7	.0420
128A	6/76	BTM-2	.337	.360	0.933	0.825	0.0	2110.	1000.	705.	.0402	124.5	.0727
128B	6/76	BTM-2	.321	.298	1.067	0.943	0.0	2110.	1000.	655.	.0345	145.0	.0640
130	12/ 7/76	LIGNITE	.430	.434	0.827	0.532	0.0	2110.	1000.	738.	.0533	93.9	.0670
131	12/ 7/76	LIGNITE	.663	.332	1.669	1.151	0.0	2110.	1000.	752.	.0660	75.7	.1240
132	1/11/77	LIGNITE	.493	.317	1.297	0.842	0.0	2110.	1000.	714.	.0515	97.1	.0863
133	3/77	LIGNITE	.546	.330	1.182	0.948	0.0	2110.	1000.	755.	.0565	88.5	.0850
134	3/77	LIGNITE	.509	.442	0.826	0.652	0.0	2110.	1000.	748.	.0570	87.7	.0823
135A	4/77	LIGNITE	.650	.440	1.232	0.730	0.0	2110.	1000.	708.	.0752	119.7	.0899
135B	4/77	LIGNITE	.481	.507	0.791	0.454	0.0	2110.	1000.	664.	.0481	187.1	.0560

3.4 TASK III — AN IMPROVED SEMIEMPIRICAL CORRELATION FOR PREDICTING CARBON CONVERSION

This subsection presents:

- An improved semiempirical correlation that predicts overall carbon conversion efficiency and accounts for thermodynamic equilibrium effects
- Predictions of overall carbon conversion at thermo- iynamic equilibrium
- A comparison between the original and improved correlations for predicting overall carbon conversion

3.4.1 Derivation of the Improved Model

The following model was previously proposed by Bechtel[8] for correlating overall carbon conversion to the reactor operating variables:

$$X = 1 - \exp\left[-\alpha_1 (t_{RG})^{\alpha_2} (t_{RP})^{\alpha_3} (u_G)^{\alpha_4} (P)^{\alpha_5} (P_{H_2})^{\alpha_6} (H_2/\text{coal})^{\alpha_7} (d_P)^{\alpha_8} \exp(-\alpha_9/T)\right] \quad (1)$$

where,

X = weight fraction overall carbon conversion

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

t_{RG} = gas residence time

t_{RP} = particle residence time

u_G = superficial gas velocity

P_{H_2} = hydrogen partial pressure

P = total reactor pressure

H_2/coal = hydrogen-to-coal ratio

d_P = mean particle diameter

T = reaction temperature

The coefficients, α_1 through α_9, have been fitted to the data using a computerized multiple regression statistical analysis. The choice for the exponential form for Equation 1 was influenced by the similar form for an integrated, first-order, irreversible kinetic model.[8] The boundary conditions for the proposed correlation are zero carbon conversion at time zero and unity (100 percent conversion) at infinite time.

Hydropyrolysis of coal, however, is an extremely complex process, involving a number of reversible heterogeneous and homogeneous reactions.[11] Because of this reversibility, the maximum carbon conversion for a given set of operating conditions is limited by the thermodynamic equilibrium between the carbon in the coal, the oxygen, hydrogen, and reactant products. Since the overall hydropyrolysis reaction is exothermic, this equilibrium limit of carbon conversion, X^*, should decrease with increasing temperature. Furthermore, since there are fewer product gas moles than reactant gas moles, X^* should increase with increasing pressure.

To satisfy this equilibrium boundary condition, the following model has been proposed for correlating carbon conversion to the operating variables:

$$X = X^* \left\{ 1 - \exp\left[-\alpha_1 (t_{RG})^{\alpha_2} (t_{RP})^{\alpha_3} (u_G)^{\alpha_4} (P)^{\alpha_5} (P_{H_2})^{\alpha_6} (H_2/\text{coal})^{\alpha_7} (d_P)^{\alpha_8} \exp(-\alpha_9/T) \right] \right\} \quad (2)$$

where X^* is the equilibrium conversion, i.e., conversion at $t = \infty$

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. For this reaction, the analytical expression for conversion of A to B, X_A, is

$$X_A = X_A^* \left[1 - e^{-(k_1 + k_2)t} \right] \quad (3)$$

with

$$X_A^* = k_1/(k_1 + k_2) = K/(1 + K) \quad (4)$$

where,

X_A^* = equilibrium fraction conversion of A

k_1 = forward reaction rate constant

k_2 = reverse reaction rate constant

t = time

K = equilibrium constant = k_1/k_2

3.4.2 Prediction of Fraction Carbon Conversion at Equilibrium

Owing to the complexity of the coal hydropyrolysis process, a thermodynamic equilibrium computer model, PEP[12] (Propellant Evaluation Program), has been used to predict the thermodynamic equilibria. 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. The equilibrium fraction of carbon converted, X^*, for the bituminous and subbituminous coals used by Cities Service and Rocketdyne[1] are shown in Figures 3-1 through 3-6 for various levels of temperature, pressure, and hydrogen-to-coal ratio.

For both types of coal, the results from PEP indicate that methane is the major hydrocarbon product at equilibrium. Higher hydrocarbon products, such as ethane and ethylene, are present only in trace amounts. PEP predicts that significant quantities of CO and CO_2 are also present in the gas phase at equilibrium. For the bituminous coal (Figures 3-1 through 3-3), the predicted amount of CO and CO_2 present is small relative to methane. For the subbituminous coal (Figures 3-4 through 3-6), which contains higher fractions of oxygen and moisture, the predicted quantities of CO and CO_2 can be significant relative to the methane.

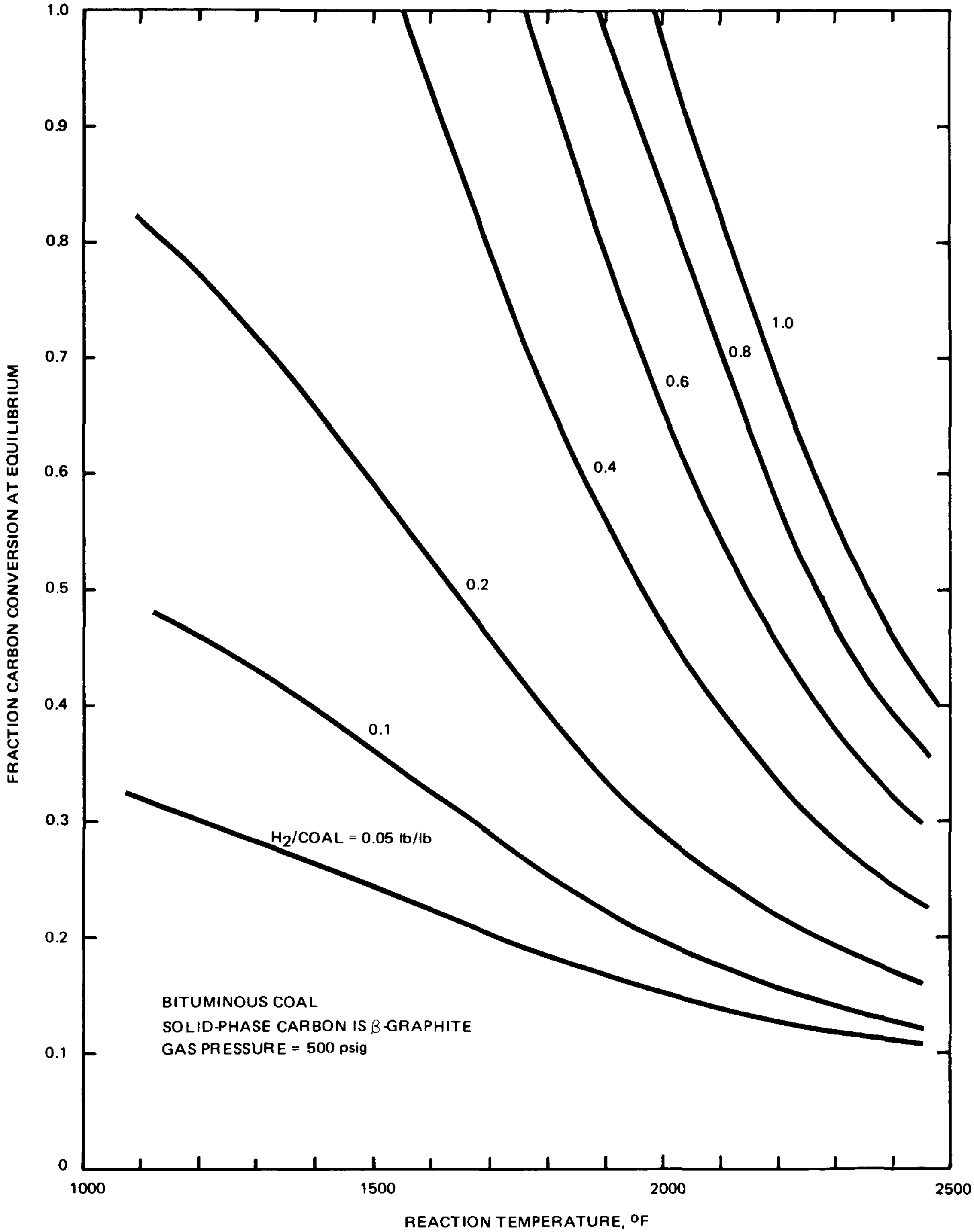

Figure 3-1. Fraction Carbon Conversion at Equilibrium — Bituminous Coal at 500 psig

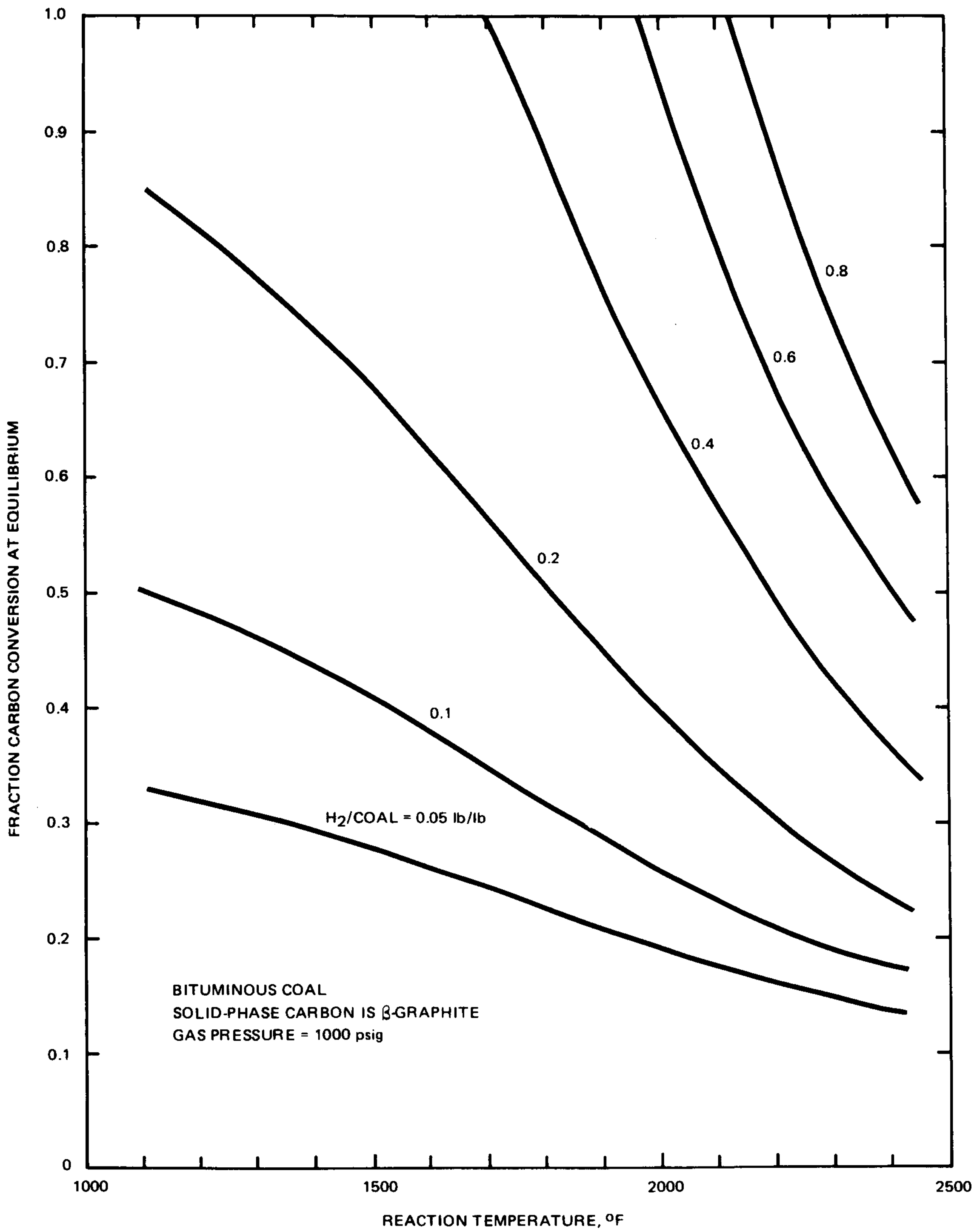

Figure 3-2. Fraction Carbon Conversion at Equilibrium — Bituminous Coal at 1,000 psig

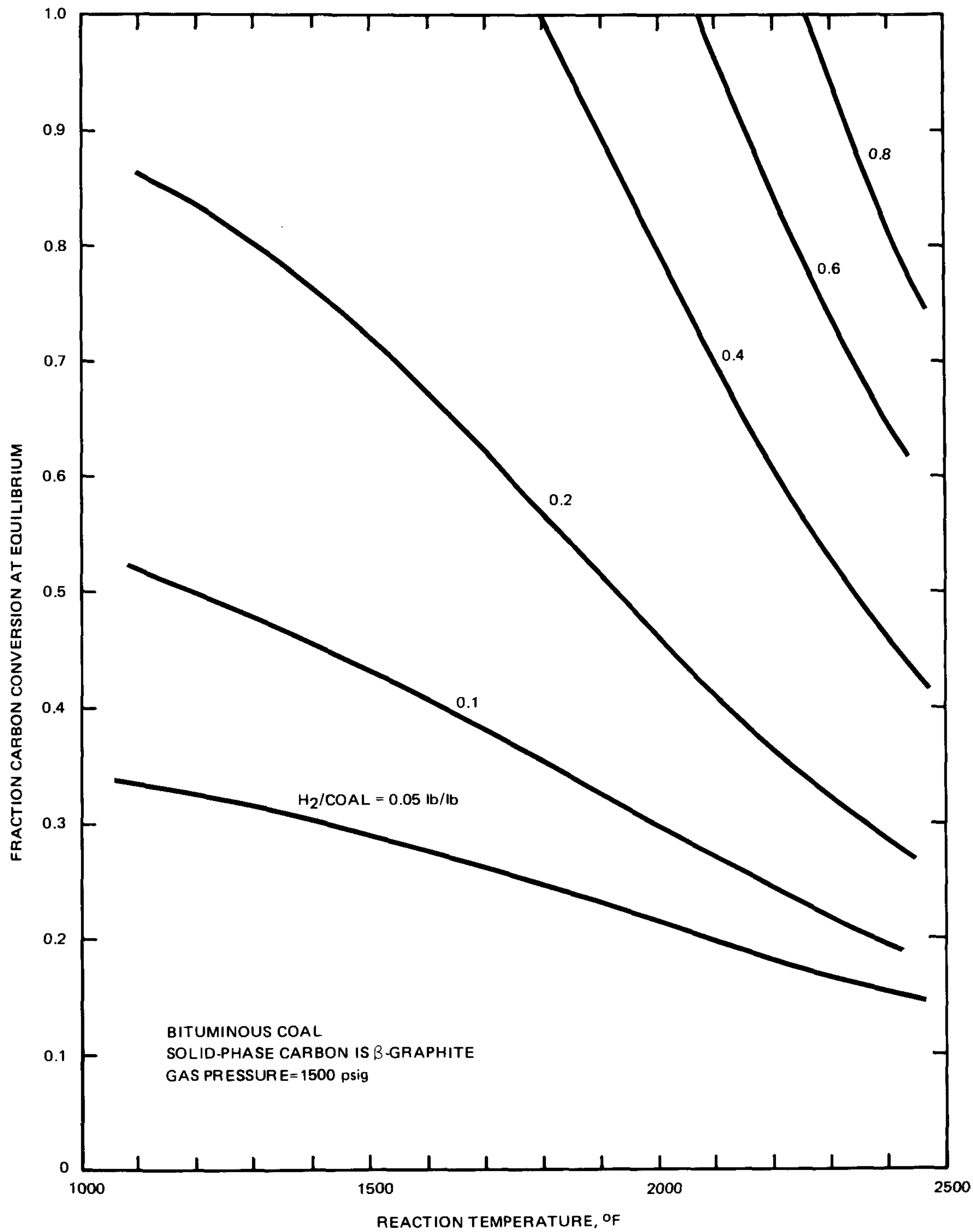

Figure 3-3. Fraction Carbon Conversion at Equilibrium — Bituminous Coal at 1,500 psig

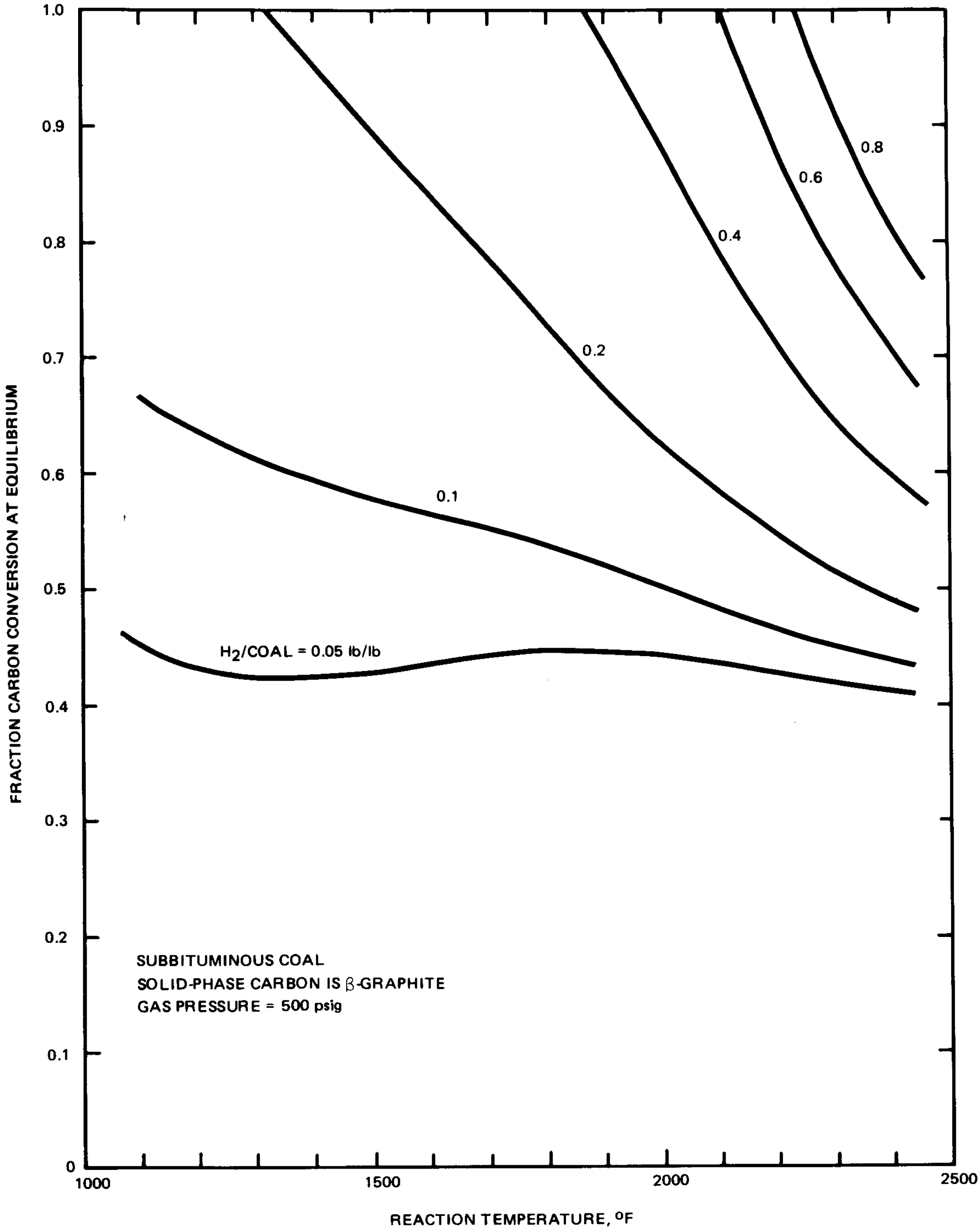

Figure 3-4. Fraction Carbon Conversion at Equilibrium — Subbituminous Coal at 500 psig

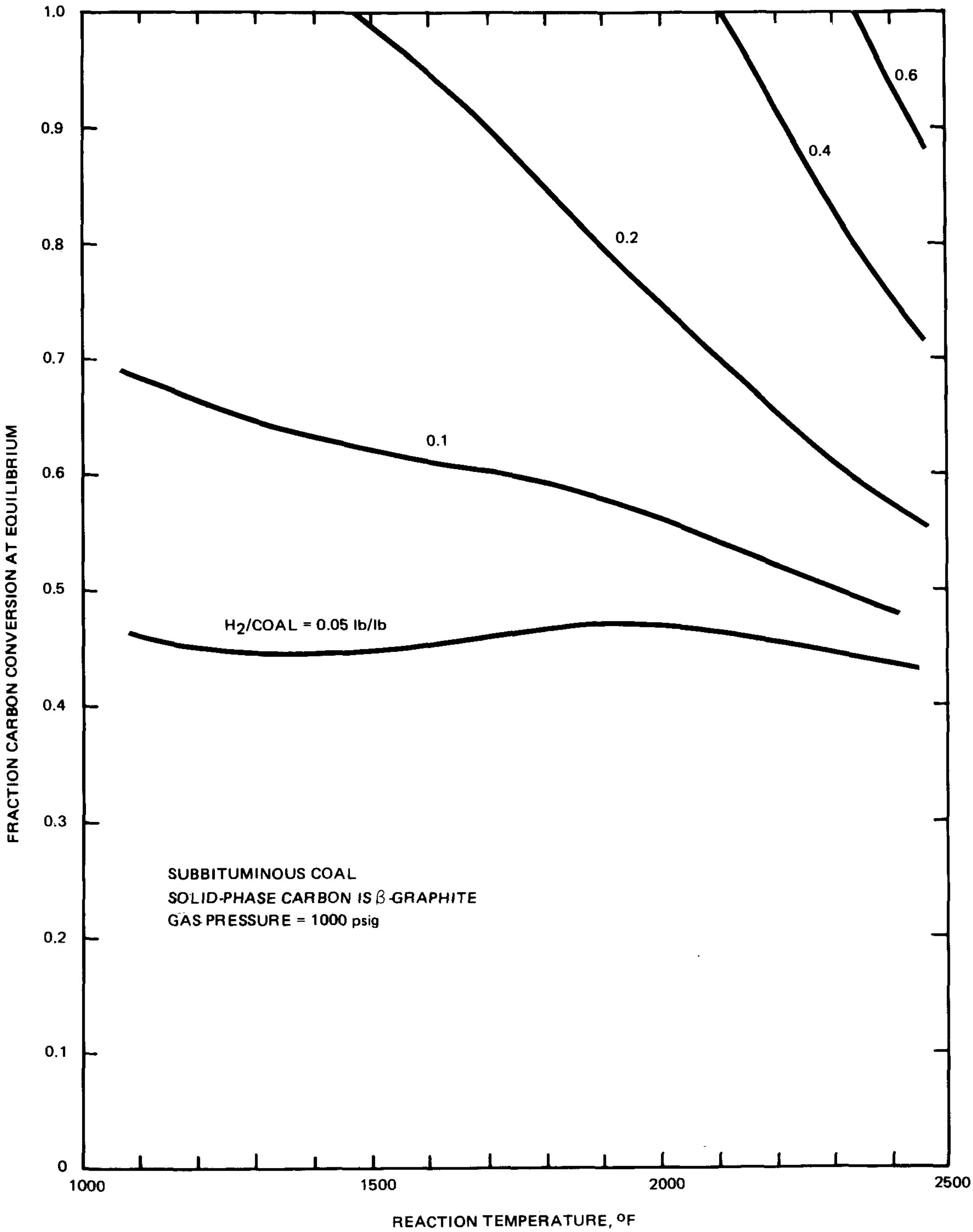

Figure 3-5. Fraction Carbon Conversion at Equilibrium — Subbituminous Coal at 1,000 psig

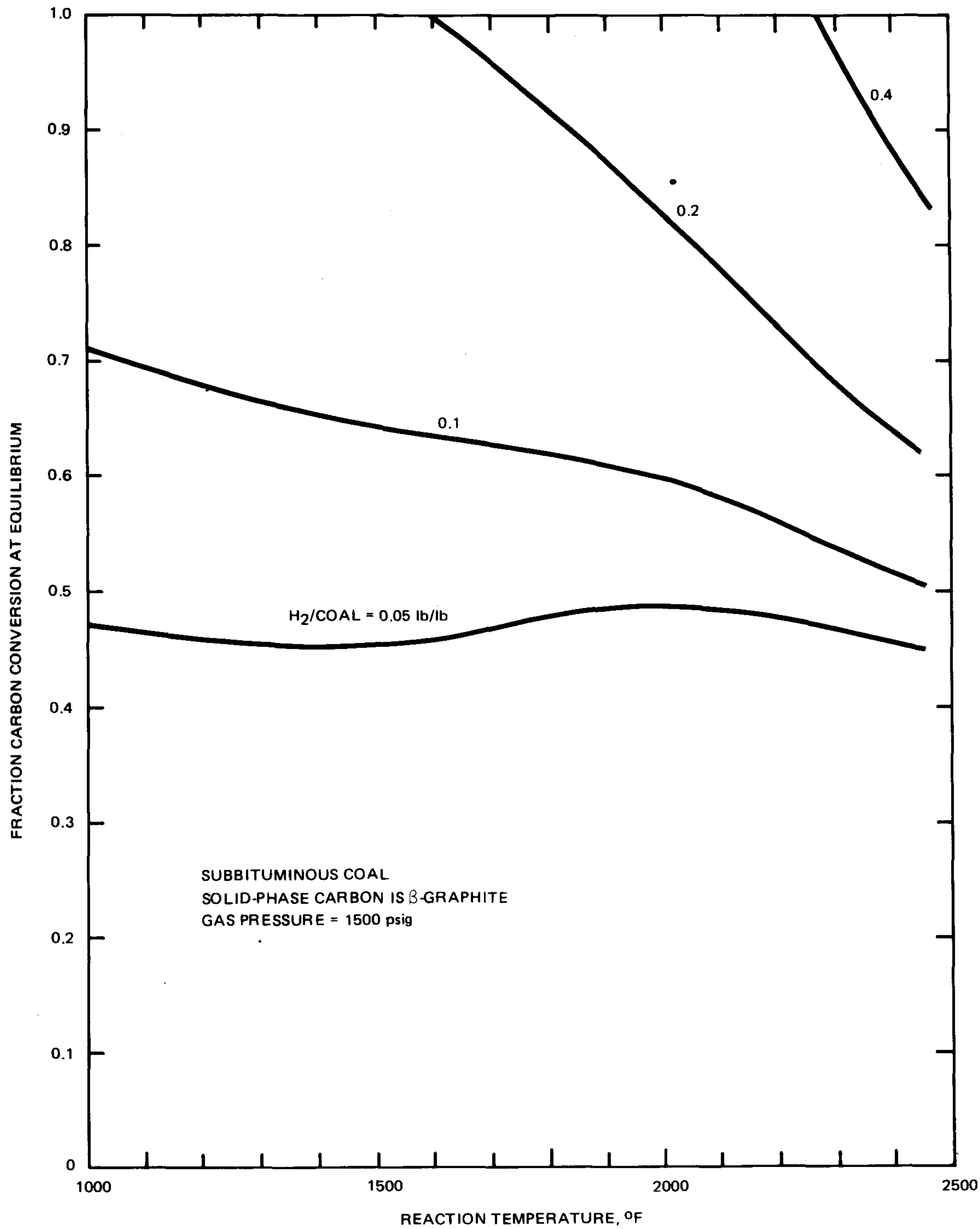

Figure 3-6. Fraction Carbon Conversion at Equilibrium — Subbituminous Coal at 1,500 psig

The equilibrium distribution of oxygen in coal to H_2O, CO, and CO_2 exhibits the following temperature dependence. At low temperatures, the oxygen in the coal reacts with hydrogen to form additional water. As the temperature increases, (1) the amount of this additional water decreases and the production of CO and CO_2 increases (indicating that the oxygen in coal preferentially reacts with carbon instead of hydrogen as the temperature is raised), and (2) CO production predominates over CO_2 production. At very high temperatures, the water present at equilibrium may be less than the water contained in the coal feed. Presumably, at these high temperatures, water reacts with carbon to form additional CO. These temperature effects are the opposite of the effects due to increasing hydrogen partial pressure or hydrogen-to-coal ratio.

As can be seen in Figures 3-1 through 3-6, the fraction carbon conversion at equilibrium is unity at low temperature, decreases below unity at higher temperatures, and increases with increasing pressure and 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
- 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

As mentioned previously, PEP assumes that the carbon present is β-graphite. Other studies[13,14,15] have indicated that the carbon present at equilibrium is amorphous carbon, which has a higher reactivity than β-graphite. Therefore, the predictions of X^* in Figures 3-1 through 3-6 should be considered as approximate, and probably on the low side.

3.4.3 Comparison Between Original and Improved Models

The Rocketdyne and Cities Service test programs have been conducted to date within a temperature range of 1,400°F to 2,000°F, a hydrogen partial pressure range of 500 to 1,600 psig, and a hydrogen-to-coal ratio range of 0.5 to 1.2 lb/lb. As shown in Figures 3-1 through 3-6, the equilibrium conversions predicted by PEP for these conditions all have a value of unity (100 percent conversion). For this case, Equation 2 reduces to Equation 1, the original proposed model. This explains why the original model, which did not take the equilibrium limitation into account, has successfully correlated the Cities Service and Rocketdyne carbon conversion data.

The equilibrium limitation, however, must be taken into consideration when extrapolating the results of the fitted Cities Service and Rocketdyne model to a commercial-scale reactor. The reason for this is that a commercial-scale reactor will operate at a hydrogen-to-coal ratio less than 0.5 lb/lb. For this reduced hydrogen-to-coal ratio, X^* may fall below unity for the normal operating levels of reactor temperature and pressure.

The equilibrium limitation must also be considered for an evaluation of the PERC hydrogasification data. This is due to the fact that the PERC reactor has operated with extremely low hydrogen-to-coal ratios, varying between 0.03 and 0.12 lb/lb (see Table 3-3). It is expected that X^* is less than 0.5 for most of the PERC data.

3.5 TASK III — CITIES SERVICE AND ROCKETDYNE REACTOR MODELING

During this reporting period, the Cities Service and Rocketdyne subbituminous data received were fitted to semiempirical models proposed by Bechtel[4] for predicting overall carbon conversion and carbon conversion to gaseous products. Computer listings of the correlated variables are given in Tables 3-1 and 3-2.

Owing to the uncertainty in the results from Rocketdyne Runs 011-14 and 011-15 (as was discussed in Subsection 3.1 of this report), these runs were not included in the analyses. It should be noted that, within the region of the Rocketdyne and Cities Service subbituminous data, the equilibrium conversion of carbon to products, X^*, is unity, i.e., the fraction carbon conversion approaches unity as particle residence time becomes large.

3.5.1 Overall Carbon Conversion

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

$$X = 1 - \exp\left[-2.53 \exp(-0.175\, P_{H_2}/t_R)\exp(0.000393\, P_{H_2}) \exp(-3{,}820/T_G)\right] \tag{5}$$

where,

X = overall carbon conversion, weight fraction

P_{H_2} = hydrogen partial pressure, psig

t_R = particle (or gas) residence time, milliseconds

T_G = maximum gas temperature, $^{\circ}R$

As Equation 5 indicates, X increases with increasing coal particle residence time and gas temperature. At high particle residence times, X increases with increasing hydrogen partial pressure, and at low particle residence times, X decreases with increasing hydrogen partial pressure.

Equation 5 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 3-7. The statistics and Figure 3-7 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.

3.5.2 Carbon Conversion to Gas

A statistical analysis of the fitted data indicated that carbon conversion to gaseous products 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, gas velocity, or particle size within the region investigated. The correlation fitted to the Rocketdyne and Cities Service subbituminous carbon conversion to gas data is:

$$X_G - 1 - \exp\left[- 0.277 \exp(-0.178\ P_{H_2}/t_R)\ \exp(0.00358\ P_{H_2})\ \exp(-6.57\ P_{H_2}/T_G) \right] \quad (6)$$

where X_G is the weight fraction carbon conversion to gas.

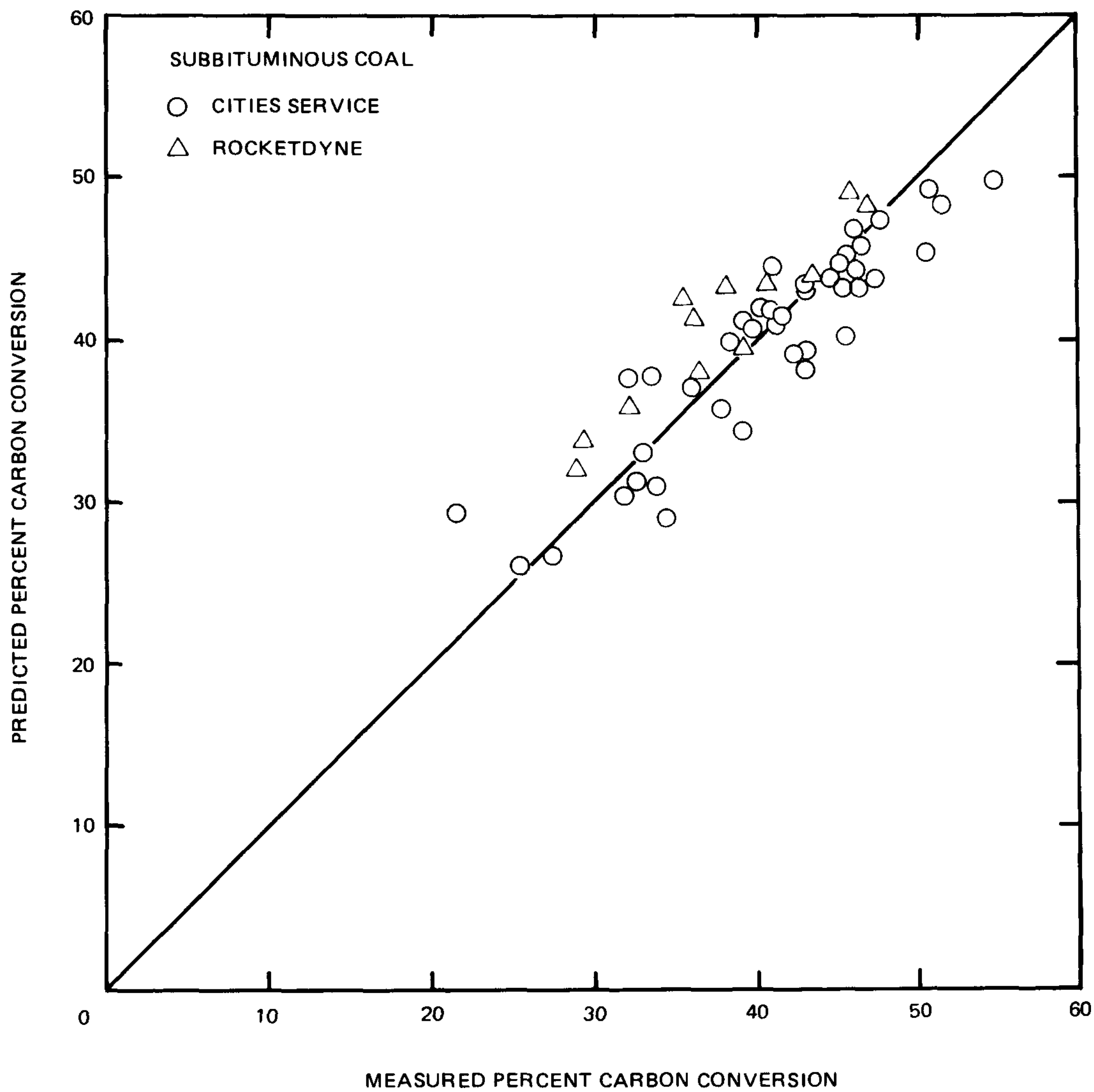

Figure 3-7. Comparison of Measured and Predicted Carbon Conversion for the Cities Service and Rocketdyne Reactors

As can be seen from Equation 6, 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.

Equation 6 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 3-8. The statistics and Figure 3-8 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.

3.5.3 Carbon Conversion to Methane

A statistical analysis of the fitted data indicated that carbon conversion to methane 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, gas velocity, or particle size within the region investigated. The correlation fitted to the Rocketdyne and Cities Service subbituminous carbon conversion to methane data is:

$$X_M = 1 - \exp\left[-0.125 \exp(-0.286\, P_{H_2}/t_R) \exp(0.00735\, P_{H_2}) \exp(-13.9\, P_{H_2}/T_G)\right] \quad (7)$$

where X_M is the weight fraction carbon conversion to methane.

As can be seen from Equation 7, 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.

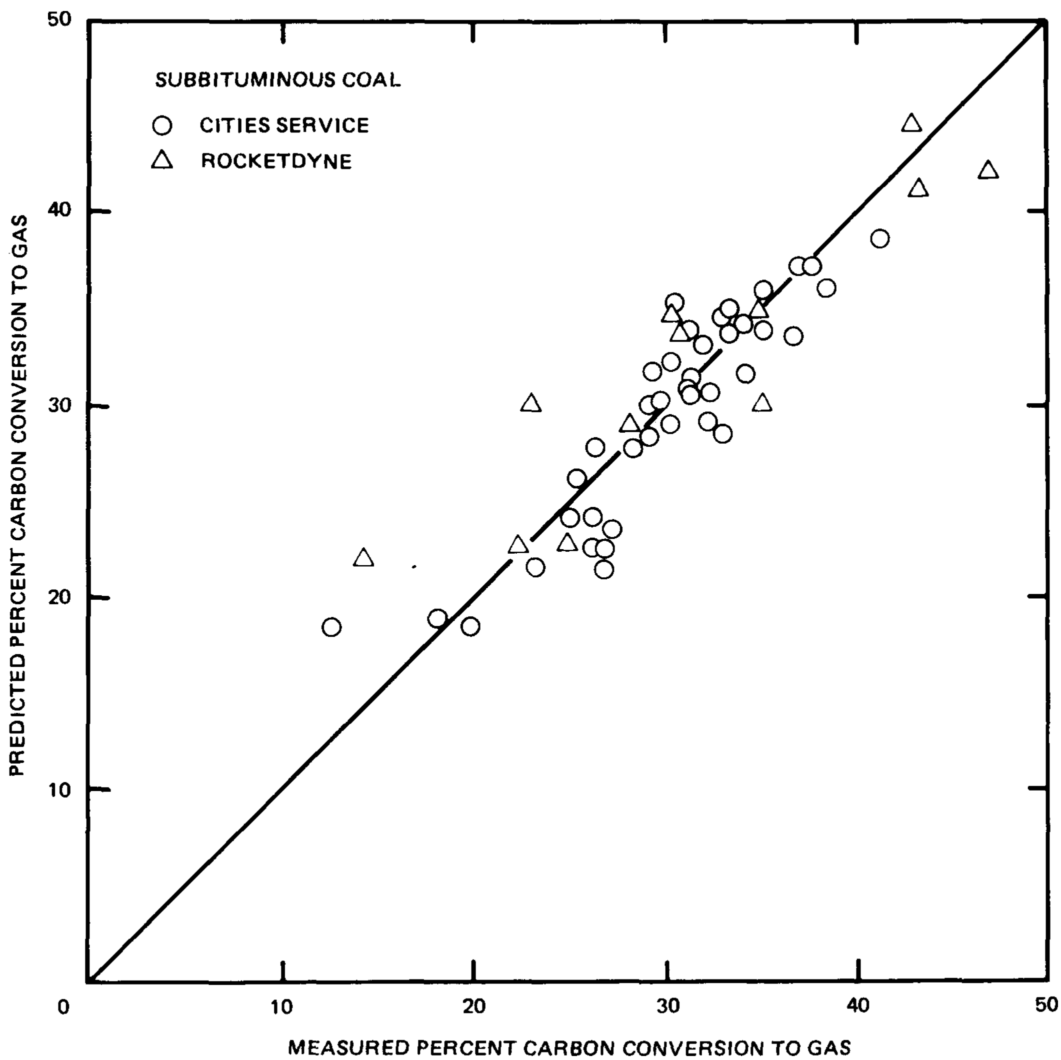

Figure 3-8. Comparison of Measured and Predicted Carbon Conversion to Gas for the Cities Service and Rocketdyne Reactors

Equation 7 has a standard error of estimate of 2.6 percent in the predicted percent conversion. The measured and predicted conversions are shown in Figure 3-9. The statistics and Figure 3-9 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.

3.5.4 Carbon Conversion to Carbon Monoxide

A statistical analysis of the fitted Cities Service and Rocketdyne data[a] 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. Carbon conversion was not significantly affected by reactor size, gas velocity, or particle size within the region investigated. The correlation fitted to the data is:

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

where X_{CO} is the weight fraction carbon conversion to CO and H/C is the hydrogen-to-coal ratio in lb/lb.

As shown in Equation 8, X_{CO} increases with increasing particle residence time, gas temperature, and hydrogen-to-coal ratio. Also, X_{CO} increases with decreasing hydrogen partial pressure.

Equation 8 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 3-10. The statistics and Figure 3-10 indicate that the Cities Service bench-scale reactor and the Rocketdyne 1/4-ton/hr reactor achieve similar carbon conversions to CO under comparable operating conditions within the region investigated.

(a) 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.

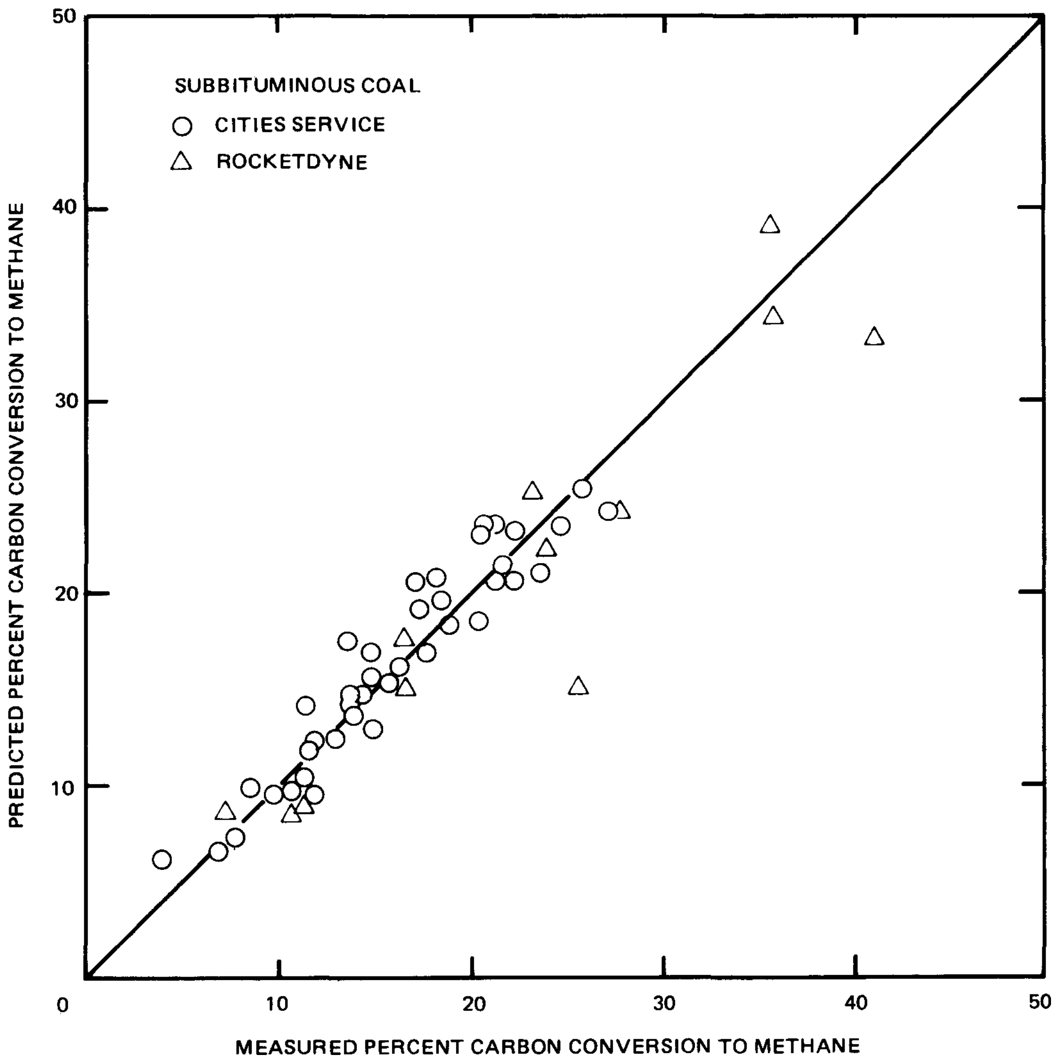

Figure 3-9. Comparison of Measured and Predicted Carbon Conversion to Methane for the Cities Service and Rocketdyne Reactors

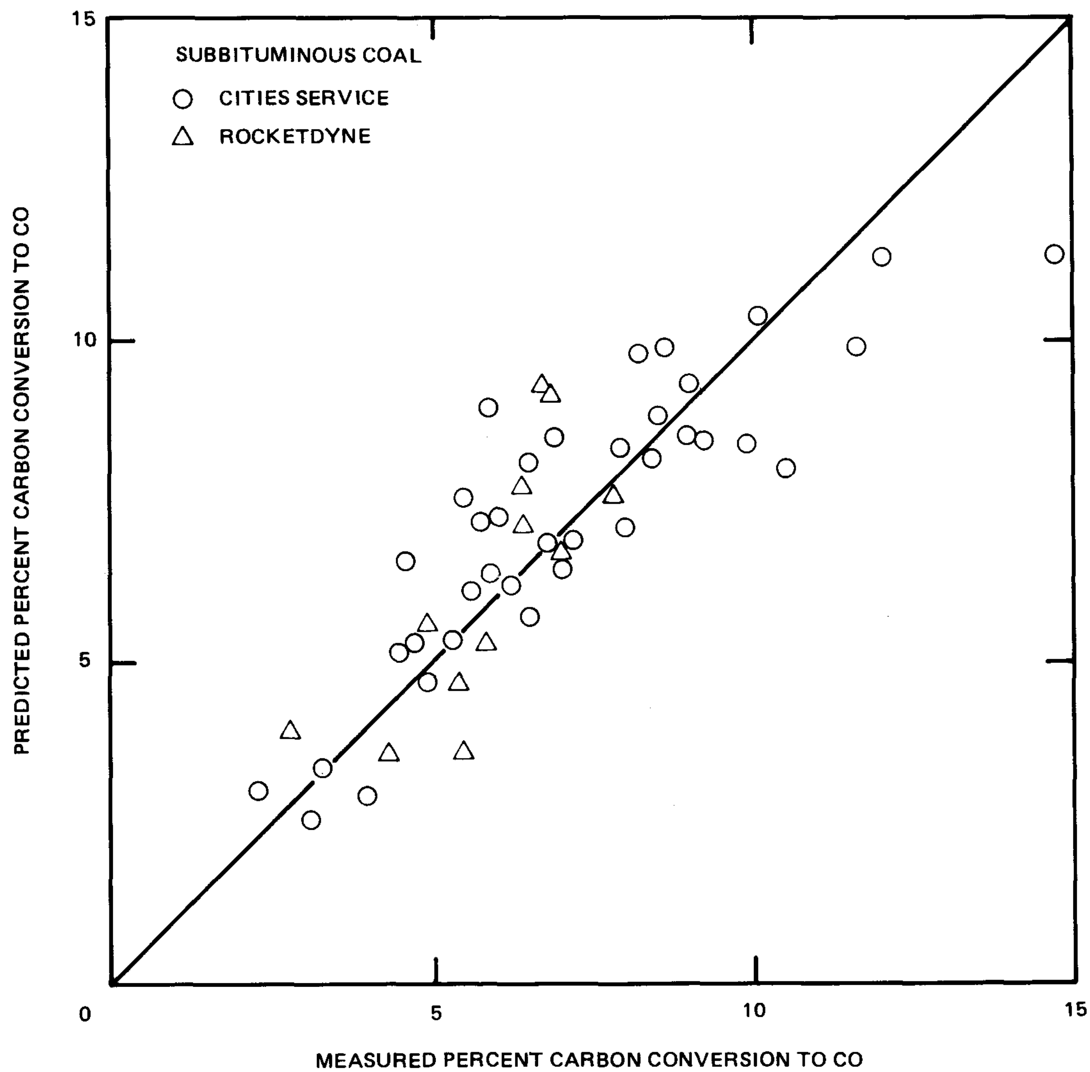

Figure 3-10. Comparison of Measured and Predicted Carbon Conversion to Carbon Monoxide for the Cities Service and Rocketdyne Reactors

3.5.5 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, gas velocity, or particle size within the region investigated. The correlation fitted to the Rocketdyne and Cities Service subbituminous data is:

$$X_{CO_2} = 1 - \exp\left[-0.0231 \exp(-0.000832 P_{H_2}) \exp(-1.36 H/C) \exp(14,200/T_G) (t_R)^{-0.971}\right] \qquad (9)$$

where X_{CO_2} is the weight fraction carbon conversion to CO_2.

As Equation 9 indicates, X_{CO_2} increases with decreasing residence time, gas temperature, hydrogen pressure, and hydrogen-to-coal ratio.

Equation 9 has a standard error of estimate of 0.2 percent in the predicted percent conversion. The measured and predicted conversions are shown in Figure 3-11. The statistics and Figure 3-11 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.

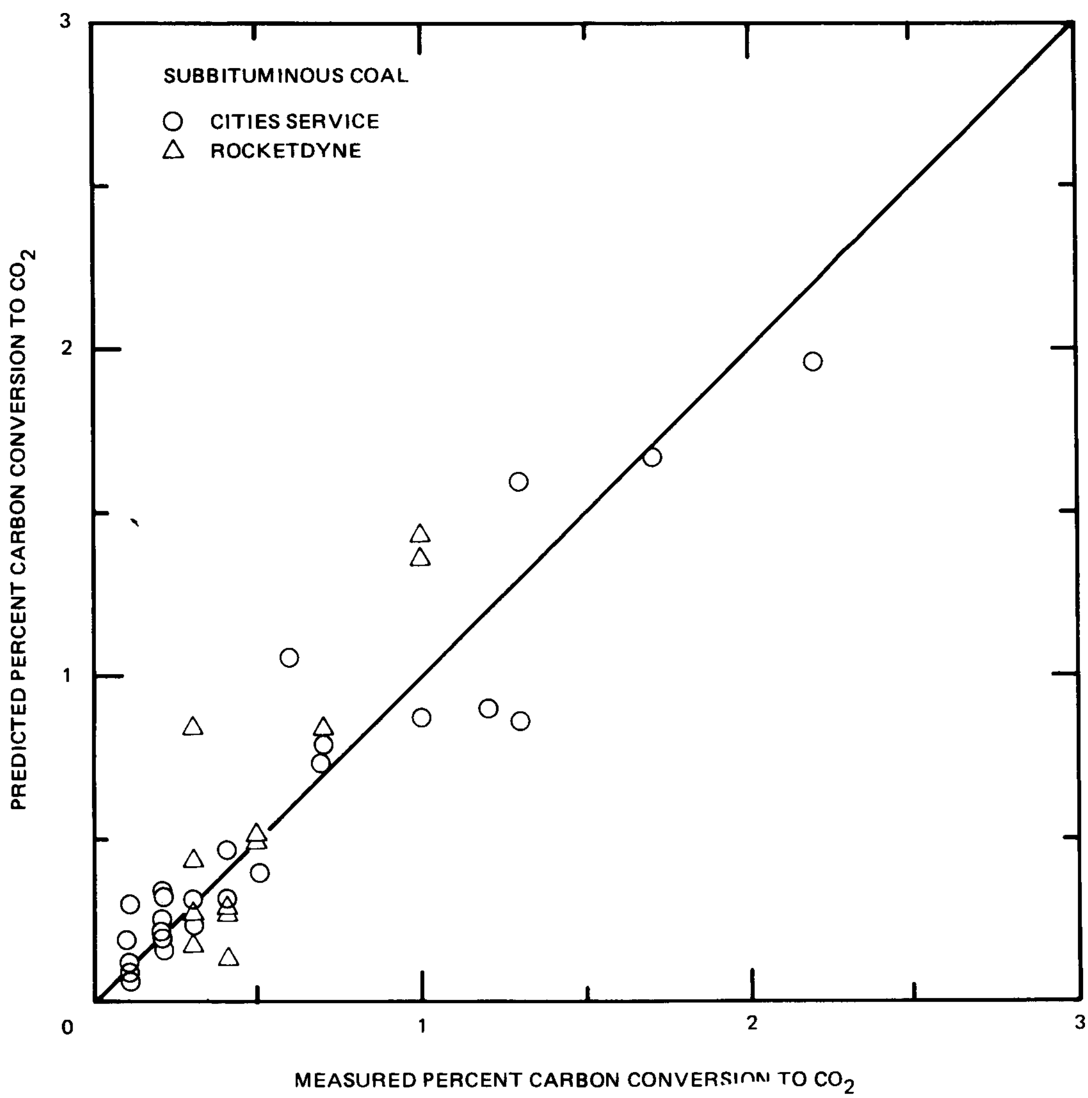

Figure 3-11. Comparison of Measured and Predicted Carbon Conversion to Carbon Dioxide for the Cities Service and Rocketdyne Reactors

3.6 TASK III — BROOKHAVEN REACTOR MODELING

Data from 48 Brookhaven National Laboratory lignite hydropyrolysis tests were tabulated in Bechtel's Third Quarterly Progress Report,[4] and are presented in Table 3-4 of this report. In Bechtel's Third Quarterly Report, overall carbon conversion data from the 48 tests were fitted to the semiempirical carbon conversion model proposed earlier.[8] A poor fit resulted, which was attributed to apparent inconsistencies in results from several tests conducted under comparable operating conditions. In addition, several anomalously high values of carbon conversion have been reported by Brookhaven (see Runs 18A, B, and C in Table 3-4).

During this reporting period, the Brookhaven lignite carbon conversion data were refitted to the proposed model, with the suspect data points removed. The eliminated tests were Runs 16A, 16B, 16C, 17, 18A, 18B, 18C, 48, 49, 56, and 62. A statistical analysis of the 37 remaining tests revealed that carbon conversion was a function of reactor wall temperature and hydrogen partial pressure. Carbon conversion was not significantly affected by gas or particle residence time, hydrogen-to-coal ratio, or gas velocity within the region investigated. The correlation fitted to the Brookhaven lignite carbon conversion data is:

$$X = 1 - \exp\left[-27.7 \exp(0.000254\ P_{H_2}) \exp(-7{,}980/T_W)\right] \qquad (10)$$

where,

X = overall carbon conversion, weight fraction

P_{H_2} = hydrogen partial pressure, psig

T_W = reactor wall temperature, ^oR

Table 3-4

BROOKHAVEN HYDROPYROLYSIS DATA

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 R)	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	1750.	1500.	3.38	.226	35.3	
7	1976	LIG	.301	.781	.312	.146	1750.	1500.	1.39	.239	33.4	
8	1976	LIG	.398	.721	.339	.0	1750.	1500.	5.80	.462	17.3	
9	1976	LIG	.215	.879	.265	.148	1660.	1500.	2.20	.439	18.2	
10	1976	LIG	.459	.649	.259	.137	1750.	2000.	1.48	.177	45.2	
11	1976	LIG	.171	.760	.158	.094	1570.	1500.	3.62	.415	19.3	
12	1976	LIG	.129	.977	.155	.085	1350.	1500.	4.85	.309	25.9	
13A	1976	LIG	.330	.867	.258	.139	1660.	1500.	5.63	.408	19.6	
13B	1976	LIG	.234	.855	.299	.167	1660.	1500.	0.90	.378	21.2	
14	1976	LIG	.566	.716	.387	.143	1890.	1500.	2.33	.481	16.6	
15	1976	LIG	.586	.759	.449	.089	1960.	1500.	2.80	.500	16.0	
16A	1976	LIG	.444	.722	.399	.131	1890.	1500.	0.98	.447	17.9	
16B	1976	LIG	.396	.714	.394	.134	1890.	1500.	1.40	.447	17.9	
16C	1976	LIG	.580	.705	.409	.133	1890.	1500.	1.53	.447	17.9	
17	1976	LIG	.692	.711	.397	.133	1870.	1500.	0.95	.426	18.8	
18A	1976	LIG	.860	.693	.367	.165	1830.	2100.	1.28	.286	28.0	
18B	1976	LIG	.822	.695	.354	.167	1830.	2100.	0.98	.286	28.0	
18C	1976	LIG	.888	.703	.359	.164	1830.	2100.	0.94	.286	28.0	
21	11/ 5/76	LIG	.428	.717	.348	.178	1800.	2000.	1.24	.213	37.5	8.6
22	1/13/77	LIG	.475	.680	.356	.168	1840.	2000.	1.32	.272	29.5	11.4
23	1/25/77	LIG	.448	.596	.368	.109	1910.	2000.	1.46	.240	33.4	12.2
24	1/27/77	LIG	.595	.655	.469	.094	1940.	2000.	3.62	.278	28.7	11.5
25	1/28/77	LIG	.381	.714	.336	.171	1800.	2000.	2.24	.270	29.6	11.1
26	1/31/77	LIG	.360	.647	.275	.150	1750.	2000.	2.20	.263	30.4	11.3
27	2/ 2/77	LIG	.388	.696	.317	.165	1820.	2000.	1.86	.273	29.3	11.2
28	2/ 3/77	LIG	.438	.710	.388	.148	1880.	2000.	2.29	.282	28.3	11.2
29	2/ 3/77	LIG	.358	.771	.377	.156	1880.	1500.	1.92	.342	23.4	10.5
46	4/26/77	LIG	.511	.818	.538	.115	1890.	2000.	0.42	.284	28.2	9.9
47	4/27/77	LIG	.467	.722	.358	.212	1910.	2000.	1.13	.273	29.3	8.3
48	5/ 6/77	LIG	.325	.800	.422	.178	1890.	1500.	0.66	.396	20.2	6.5

Table 3-4 (Cont'd)

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 R)	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	1900.	1500.	0.97	.345	23.2	6.8
50A	5/12/77	LIG	.407	.779	.474	.135	1930.	1500.	0.91	.380	21.1	6.8
50B	5/12/77	LIG	.591	.934	.766	.076	1930.	2500.	1.04	.224	35.8	8.8
51A	5/13/77	LIG	.503	.847	.630	.093	1930.	2000.	1.08	.264	30.3	8.1
51B	5/13/77	LIG	.634	.964	.801	.091	1930.	3000.	1.26	.171	46.9	9.5
52	5/16/77	LIG	.587	.818	.555	.164	1840.	3000.	0.89	.181	44.2	9.5
53	5/17/77	LIG	.482	.869	.643	.180	1890.	3000.	1.32	.176	45.5	9.5
55	6/ 7/77	LIG	.611	.975	.881	.074	1930.	3000.	0.51	.160	50.0	9.5
56	6/15/77	LIG	.384	.792	.477	.190	1840.	3000.	0.89	.143	56.1	10.0
57	6/16/77	LIG	.492	.758	.429	.207	1830.	3000.	1.23	.150	53.5	9.9
58	6/20/77	LIG	.497	.831	.551	.111	1840.	2000.	0.53	.201	39.8	8.7
59	6/21/77	LIG	.478	.799	.502	.142	1840.	1500.	0.61	.295	27.1	7.4
60A	6/23/77	LIG	.627	.986	.871	.030	1930.	2500.	0.63	.179	44.6	9.2
60B	6/23/77	LIG	.601	.938	.837	.035	1930.	2500.	0.63	.179	11.1	2.3
61A	6/27/77	LIG	.518	.809	.519	.158	1840.	2500.	0.62	.165	48.5	9.6
61B	6/27/77	LIG	.454	.722	.445	.156	1840.	2500.	0.62	.165	12.1	2.4
62	6/28/77	LIG	.663	.807	.572	.139	1840.	3000.	0.58	.134	59.6	2.5
63	6/29/77	LIG	.353	.824	.405	.167	1840.	1000.	0.60	.438	18.3	6.4

As can be seen from Equation 10, carbon conversion increases with increasing hydrogen partial pressure and reactor temperature. Equation 10 has a standard error of estimate of 5 percent in the predicted percent carbon conversion. The measured and predicted carbon conversions are illustrated in Figure 3-12. Both the statistics and Figure 3-12 indicate a good fit to the Brookhaven lignite data, with the 12 suspect data points removed.

An apparent discrepancy exists between the correlation fitted to the Brookhaven lignite data (Equation 10) and the correlation fitted to the Cities Service and Rocketdyne subbituminous data (Equation 5). The subbituminous correlation predicts an effect of particle (or gas) residence time on overall carbon conversion; the lignite correlation, on the other hand, does not predict such an effect. This discrepancy may be explained by the fact that most Brookhaven particle residence times are between 6 and 12 seconds, whereas most Cities Service and Rocketdyne particle residence times are between 0.5 and 3 seconds. Note that the effect of particle residence time on conversion, as predicted by Equation 5, becomes negligibly small for residence times greater than about 5 seconds.

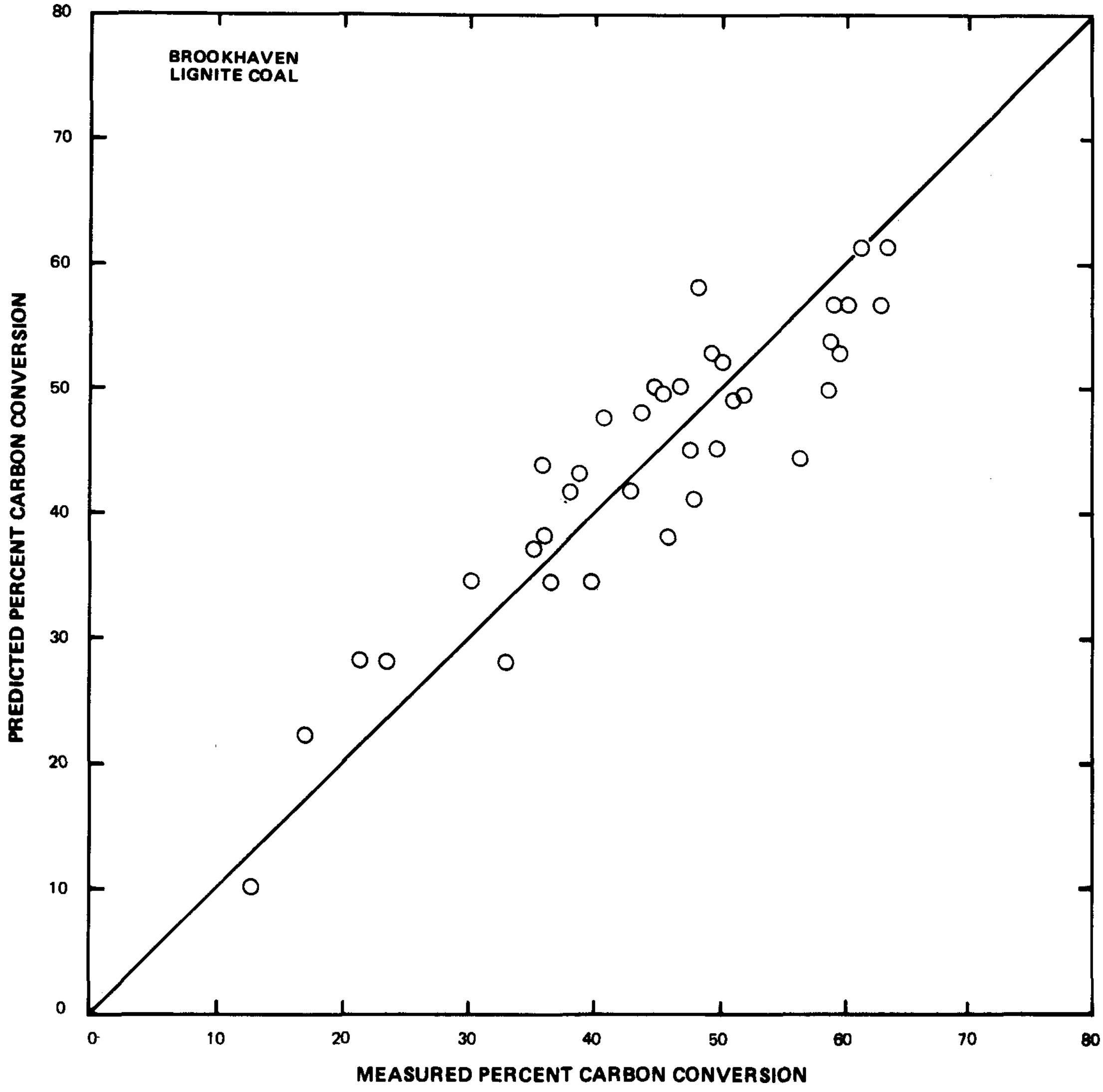

Figure 3-12. Comparison of Measured and Predicted Carbon Conversion for the Brookhaven Reactor

3.7 FUTURE WORK

During the next reporting period, work will be conducted in the areas discussed below.

Models developed for correlating the Rocketdyne, Cities Service, PERC, and Brookhaven carbon conversion and carbon selectivity data will be updated and improved upon.

The conceptual design of a reference, full-size hydrogasification reactor will be continued.

Additional data that may be required for reliable pilot plant design will be identified, and experimental programs necessary for the generation of the additional data will be recommended.

The draft of the Final Report will be prepared for submittal to DOE.

Section 4

CONCLUSIONS

Semiempirical correlations, based on presently available subbituminous coal data from Rocketdyne and Cities Service, can be developed to predict carbon conversion efficiency and carbon conversion to gas, methane, CO, and CO_2 for the reactor systems. The fitted models 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 conversion to gaseous products under comparable operating conditions. A semiempirical correlation, based on the Brookhaven lignite data, can also be developed for predicting carbon conversion efficiency as a function of the independent variables.

Results from a thermodynamic equilibrium computer model indicate that for bituminous and subbituminous coals methane is the major hydrocarbon product present at equilibrium. Higher hydrocarbon products, such as ethane and ethylene, are present only in trace amounts. The thermodynamic model also predicts the presence of significant quantities of CO and CO_2 in the gas phase. For the bituminous coal, the predicted amount of CO and CO_2 present is small relative to methane. For the subbituminous coal, which contains higher fractions of oxygen and moisture, the predicted quantities of CO and CO_2 can be significant relative to the methane.

The thermodynamic equilibrium computer model predicts a conversion of carbon to products at equilibrium of unity (100 percent) for all of the Rocketdyne, Cities Service, and Brookhaven tests, i.e., 100 percent of the carbon in the coal can be converted to methane at infinite particle residence time. This is due to the fact that these tests were conducted at large hydrogen-to-coal ratios, in excess of 0.5 lb/lb. The PERC tests, however, have been conducted at lower hydrogen-to-coal ratios, between 0.03 and 0.1 lb/lb. The predicted fraction carbon conversion at equilibrium for most of the PERC tests is, therefore, much less than unity.

Section 5

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Appendix

COMPUTER LISTING OF HYDROPYROLYSIS DATA

This appendix presents a computer listing of the Rocketdyne and Cities Service subbituminous coal 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 used 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, ^{o}F
TGMAX	Maximum gas temperature, ^{o}F
TPRES	Total pressure, psig
TWALL	Reactor wall temperature, ^{o}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

Table A-1

ROCKETDYNE SUBBITUMINOUS COAL DATA

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-1 (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-1 (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-1 (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-2

CITIES SERVICE SUBBITUMINOUS COAL DATA

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	0.268	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-2 (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-2 (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-2 (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	1.000	.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	.'97	.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	.088	.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

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