

AN ANALYSIS OF COAL HYDROGASIFICATION PROCESSES

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WAM/REA

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ABSTRACT

This monthly Technical Progress Report covers work performed during the period 1 February 1978 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.

During February, substantial progress was made on Tasks I, II, and III. Data from 11 recent Rocketdyne hydropyrolysis tests with subbituminous and bituminous coals and 16 recent Cities Service hydropyrolysis tests with subbituminous coal were entered into the computerized data base. The Cities Service data base was expanded to include values for carbon selectivity to BTX.

During February, semiempirical correlations for predicting overall carbon conversion and carbon conversion to gas, methane, CO, and CO₂ 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.

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Section 1

OBJECTIVES AND SCOPE

This report is the February 1978 Monthly 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

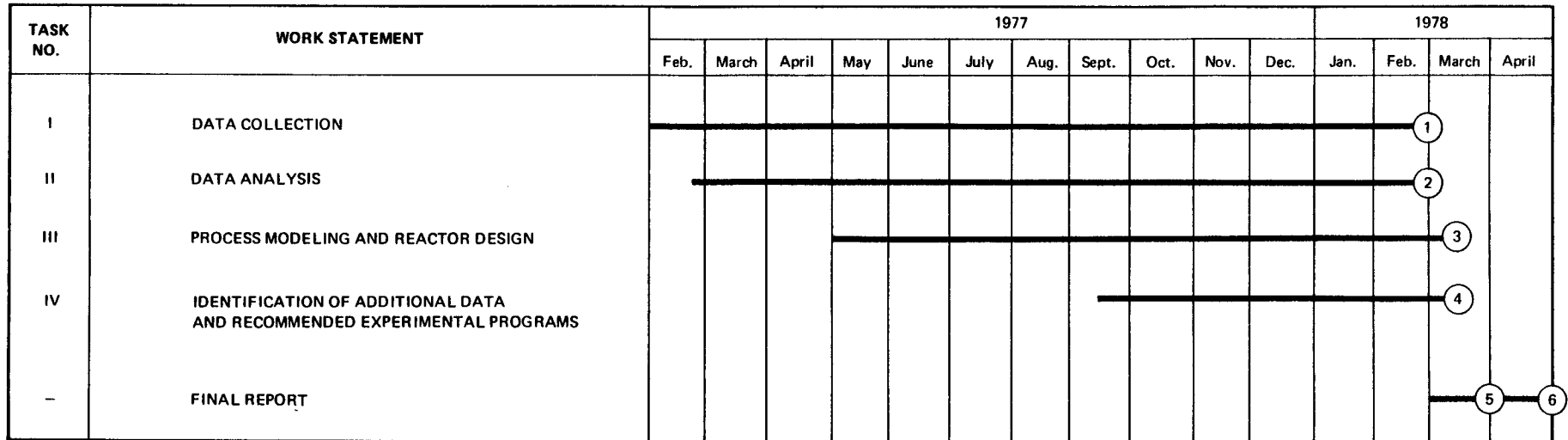
Figure 2-1 summarizes the program progress between February 1, 1977 (the program start date) and February 28, 1978. As shown in Figure 2-1, the contract period has been extended through April 30, 1978, to reflect contract modification A001.

During February, substantial progress was made on Tasks I, II, and III. Actual manhours expended in February were 675; budgeted manhours were 700. 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.

REPORT PERIOD: 1 Feb-31 December 77



LEGEND:

-  Schedule
 -  Planned Manhours and Progress
 -  Actual Manhours
 -  Actual Progress
- 1 Completion of Task I
 - 2 Completion of Task II
 - 3 Completion of Task III
 - 4 Completion of Task IV
 - 5 Submittal of Draft of Final Report
 - 6 Submittal of Final Report

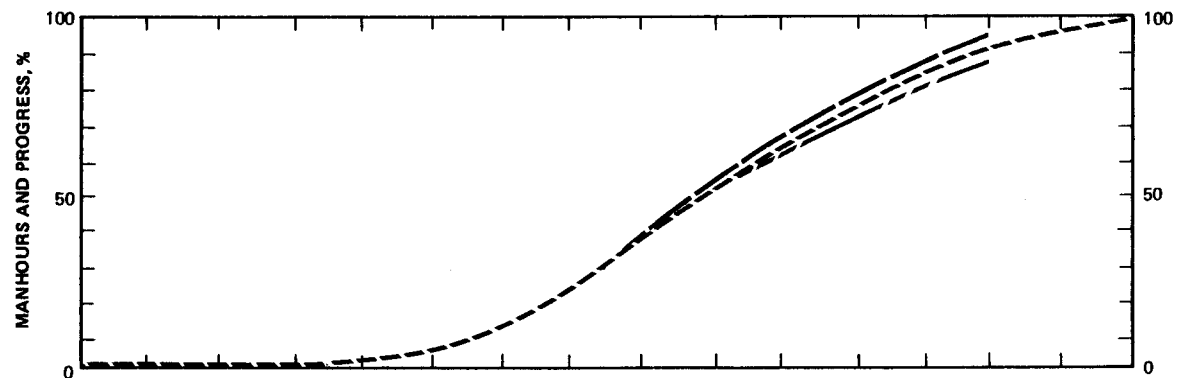


Figure 2-1. Progress and Performance Chart

Section 3

TECHNICAL PROGRESS

This section describes the technical progress for Tasks I, II, and III during the reporting period.

3.1 TASKS I AND II -- ROCKETDYNE DATA COLLECTION AND ANALYSIS

During this reporting period, Bechtel received additional hydrolysis data from Rocketdyne^{1,2} for 11 recently completed tests (Runs 011-22, 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 011-22 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.

The above hydrolysis data were entered into the computerized data base containing data from 49 earlier Rocketdyne hydrolysis and partial liquefaction tests. Table 3-1 gives a computer listing of all the available Rocketdyne data.

The recently acquired Rocketdyne data were obtained at reactor pressures of approximately 1,000 to 1,500 psig, outlet gas temperatures of approximately 1,420°F to 1,940°F (1,880°R to 2,400°R), and gas (or particle) residence times of approximately 980 to 3,420 milliseconds.

Overall carbon conversion for the Montana subbituminous coal ranged from 29 to 46 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

Table 3-1

ROCKETDYNE HYDROLYSIS DATA

RUN DESIG- NATION	DATE	COAL* TYPE	REACTOR	OVERALL FRACTION CONVERTED	CARBON	CARBON	CARBON	CARBON	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)
					SELEC- TIVITY TO GAS	SELEC- TIVITY TO METHANE	SELEC- TIVITY TO ETHANE	SELEC- TIVITY TO BTX							
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.

Table 3-1 (Cont'd)

RUN DESIG- NATION	DATE	COAL * TYPE	REACTOR	OVERALL FRACTION CARBON CONVERTED	CARBON	CARBON	CARBON	CARBON	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)
					SELEC- TIVITY TO GAS	SELEC- TIVITY TO METHANE	SELEC- TIVITY TO ETHANE	SELEC- TIVITY TO BTX							
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.

carbon conversion (71 percent) reported to date for 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^oF (2,440^oR), 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 78 percent was achieved; for the Illinois and Kentucky bituminous coals, maximum carbon selectivities to methane were 88 and 91 percent, respectively. Almost 100 percent carbon selectivity to gaseous products was obtained in Kentucky bituminous coal Run 300-12.

Insufficient information was available to calculate the carbon conversion and selectivity to BTX for the 11 recently acquired hyropyrolysis tests.

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

During this reporting period, Bechtel received additional hydrolysis data from Cities Service for 16 recently completed tests (Runs MR-9 through MR-48) using Montana Rosebud subbituminous coal.¹ A revised set of data was also received from Cities Service¹ for the 26 earlier hydrolysis tests that were previously reported by Bechtel.³

All the acquired hydrolysis data were entered into the computerized data base. Table 3-2 gives a computer listing of all the available Cities Service subbituminous data. The Cities Service data base has been expanded during this reporting period to include data for total reactor pressure and carbon selectivity to BTX.

The 16 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-19 gave the highest carbon conversion of 52 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 2,310 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.¹

Table 3-2

CITIES SERVICE HYDROLYSIS DATA

RUN DESIG- NATION	DATE	COAL TYPE	REACTOR	OVERALL FRACTION CARBON CONVERTED	CARBON	CARBON	CARBON	CARBON	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)
					SELEC- TIVITY TO GAS	SELEC- TIVITY TO METHANE	SELEC- TIVITY TO ETHANE	SELEC- TIVITY TO BTX							
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.

3.3 TASK III - CITIES SERVICE AND ROCKETDYNE REACTOR MODELING

During this reporting period, the Cities Service and Rocketdyne subbituminous data received to date have been fitted to semiempirical models proposed by Bechtel^{1,4} 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 Bechtel's January 1978 Monthly Progress Report¹), 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.¹

3.3.1 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:

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

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, °R

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

3.3.2 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:

$$X_G = 1 - \exp \left[- 0.277 \exp(-0.178 P_{H_2} / t_R) \exp(0.00358 P_{H_2}) \exp(-6.57 P_{H_2} / T_G) \right] \quad (2)$$

where X_G is the weight fraction carbon conversion to gas.

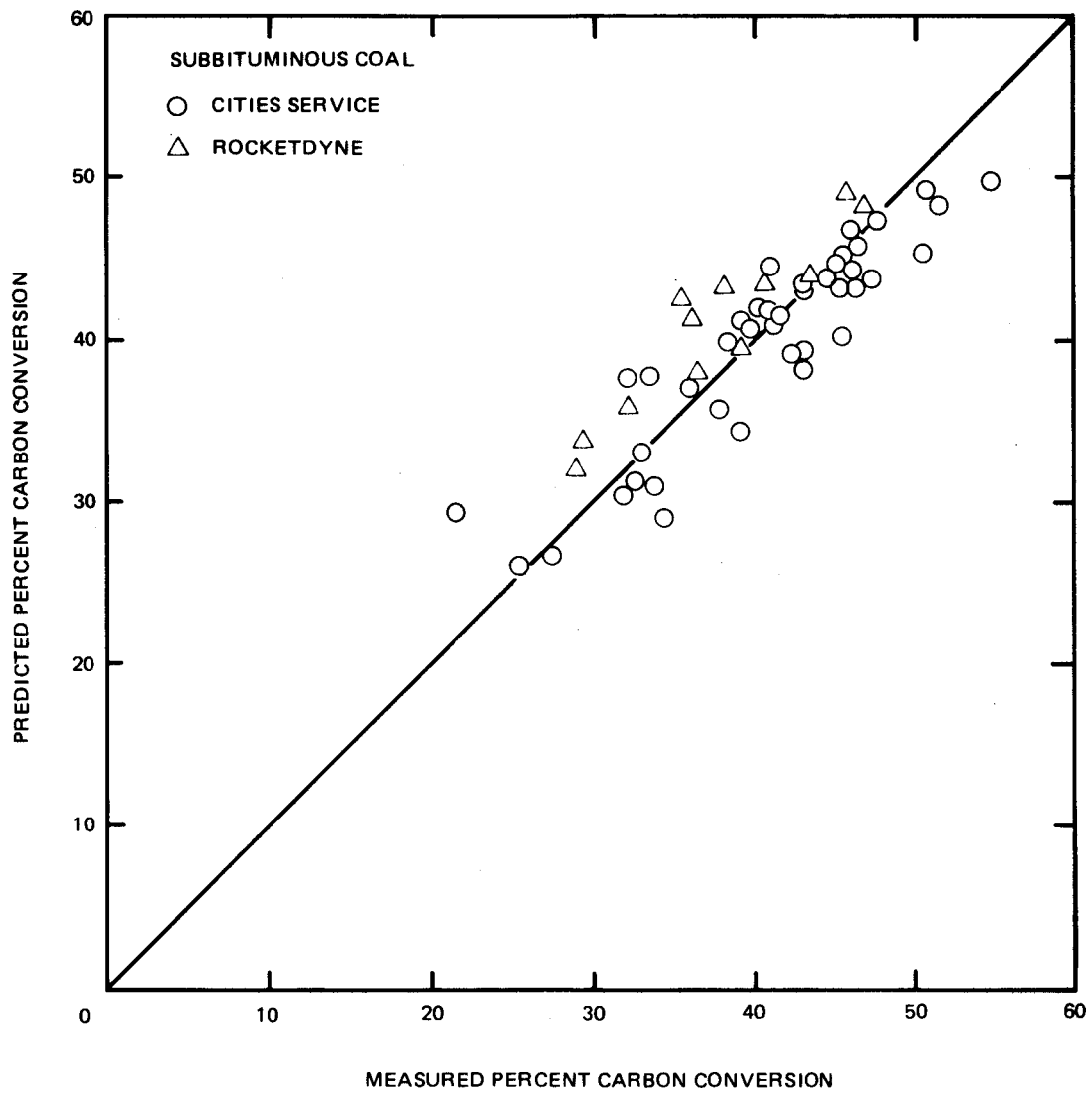


Figure 3-1. Comparison of Measured and Predicted Carbon Conversion for the Cities Service and Rocketdyne Reactors

As can be seen from Equation 2, 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 2 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 3-2. The statistics and Figure 3-2 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.

3.3.3 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:

$$X_M = 1 - \exp \left[-0.125 \exp(-0.286 P_{H_2} / t_R) \exp(0.00735 P_{H_2}) \exp(-13.9 P_{H_2} / T_G) \right] \quad (3)$$

where X_M is the weight fraction carbon conversion to methane.

As can be seen from Equation 3, 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.

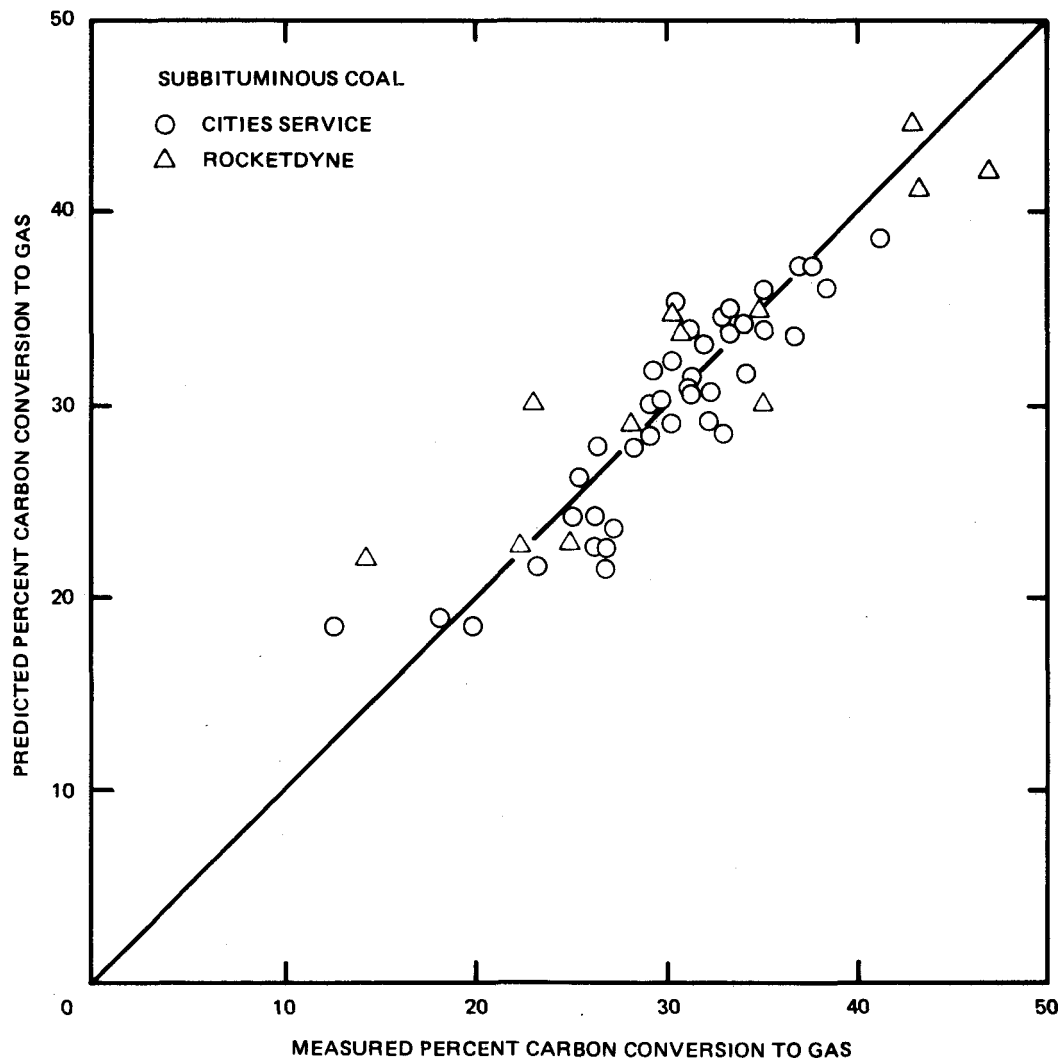


Figure 3-2. Comparison of Measured and Predicted Carbon Conversion to Gas for the Cities Service and Rocketdyne Reactors

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

3.3.4 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:

$$X_{CO} = 1 - \exp \left[-3.02 \exp(-0.248 P_{H_2} / t_R) \exp(0.677 H/C) \exp(-8,380/T_G) \right] \quad (4)$$

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 4, 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 4 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 3-4. The statistics and Figure 3-4 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.

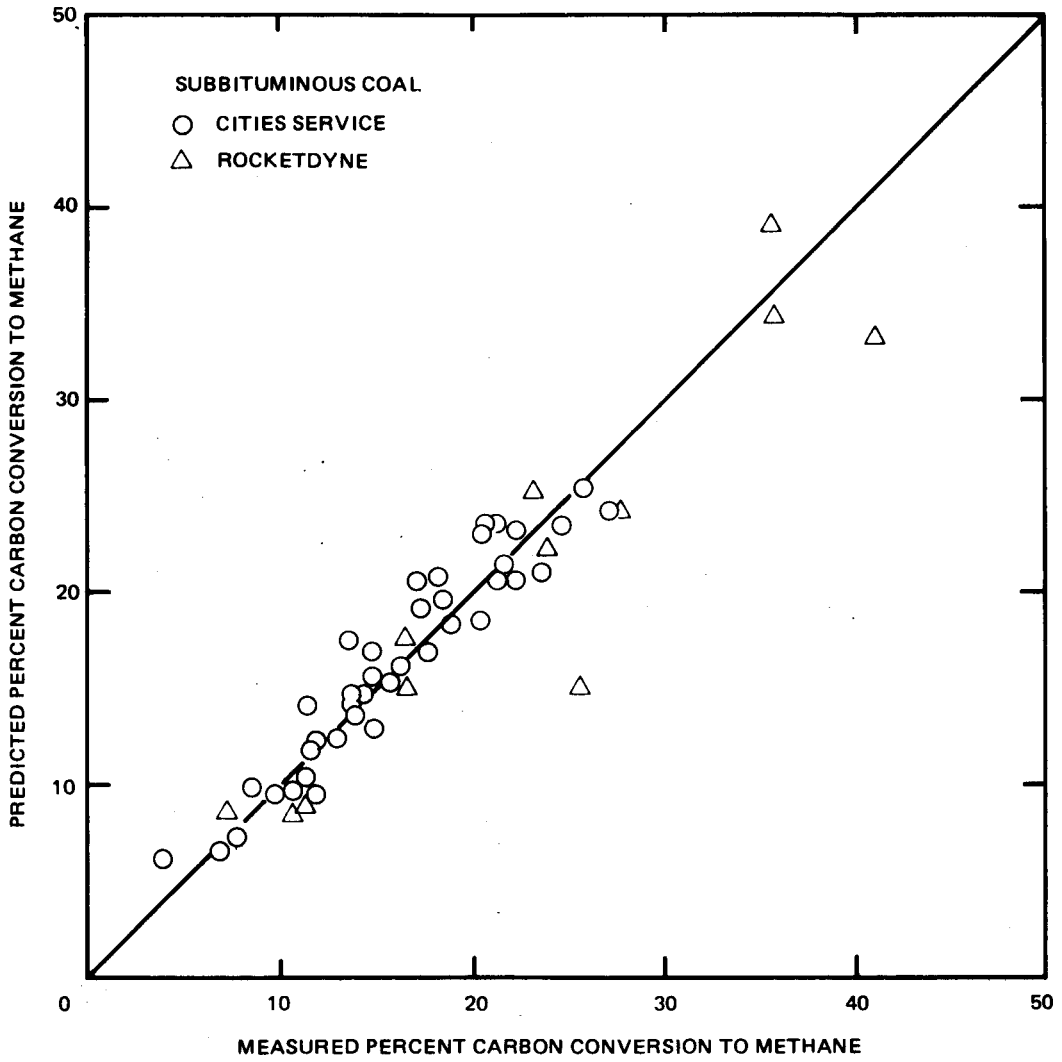


Figure 3-3. Comparison of Measured and Predicted Carbon Conversion to Methane for the Cities Service and Rocketdyne Reactors

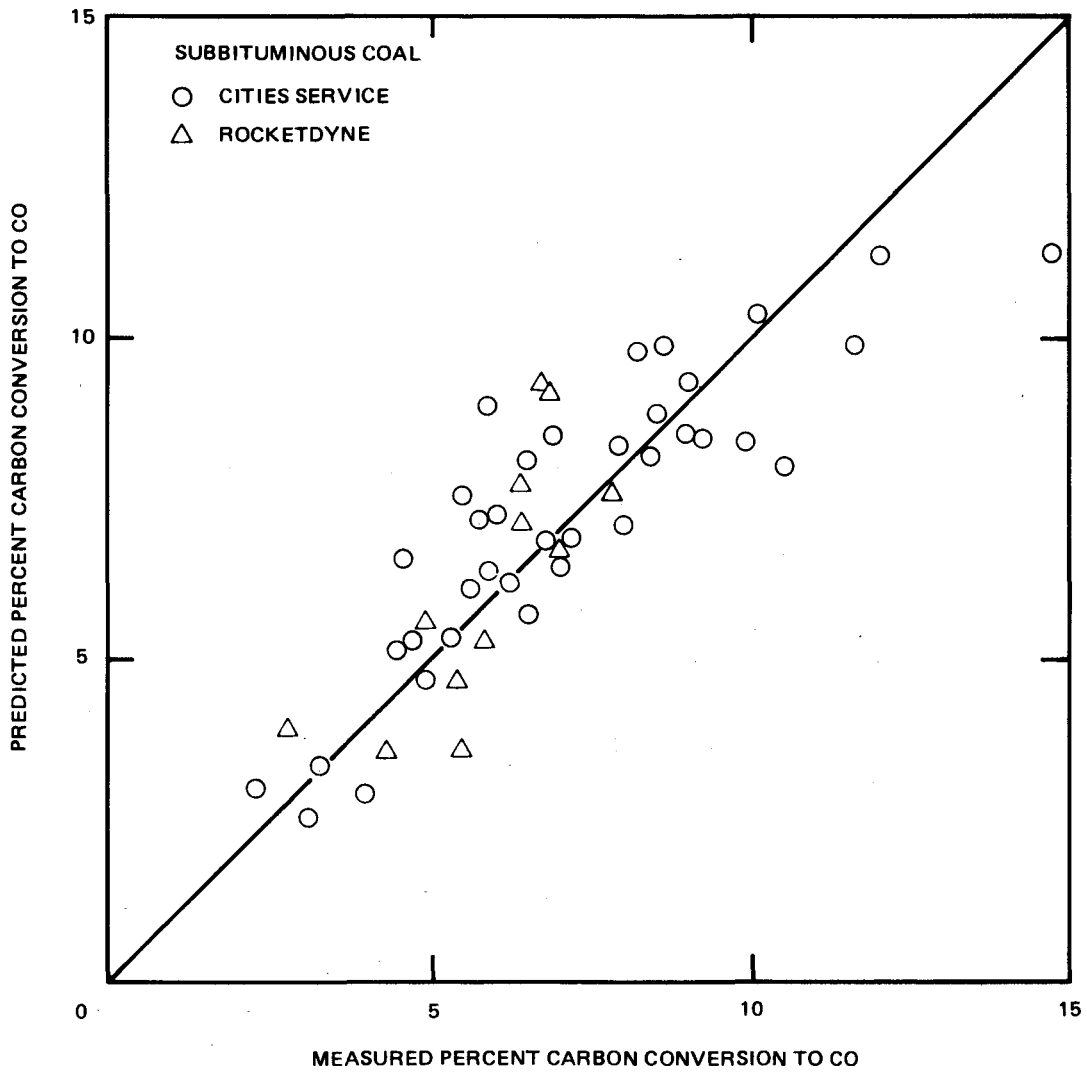


Figure 3-4. Comparison of Measured and Predicted Carbon Conversion to Carbon Monoxide for the Cities Service and Rocketdyne Reactors

3.3.5 Carbon Conversion to Carbon Dioxide

A statistical analysis of the fitted data indicated that carbon conversion to CO₂ 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:

$$X_{\text{CO}_2} = 1 - \exp \left[-0.0231 \exp(-0.000832 P_{\text{H}_2}) \exp(-1.36 \text{ H/C}) \exp(14,200/T_G) (t_R)^{-0.971} \right] \quad (5)$$

where X_{CO_2} is the weight fraction carbon conversion to CO₂.

As Equation 5 indicates, X_{CO_2} increases with decreasing residence time, gas temperature, hydrogen pressure, and hydrogen-to-coal ratio.

Equation 5 has a standard error of estimate of 0.2 percent in the predicted percent conversion. The measured and predicted conversions are shown in Figure 3-5. The statistics and Figure 3-5 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.

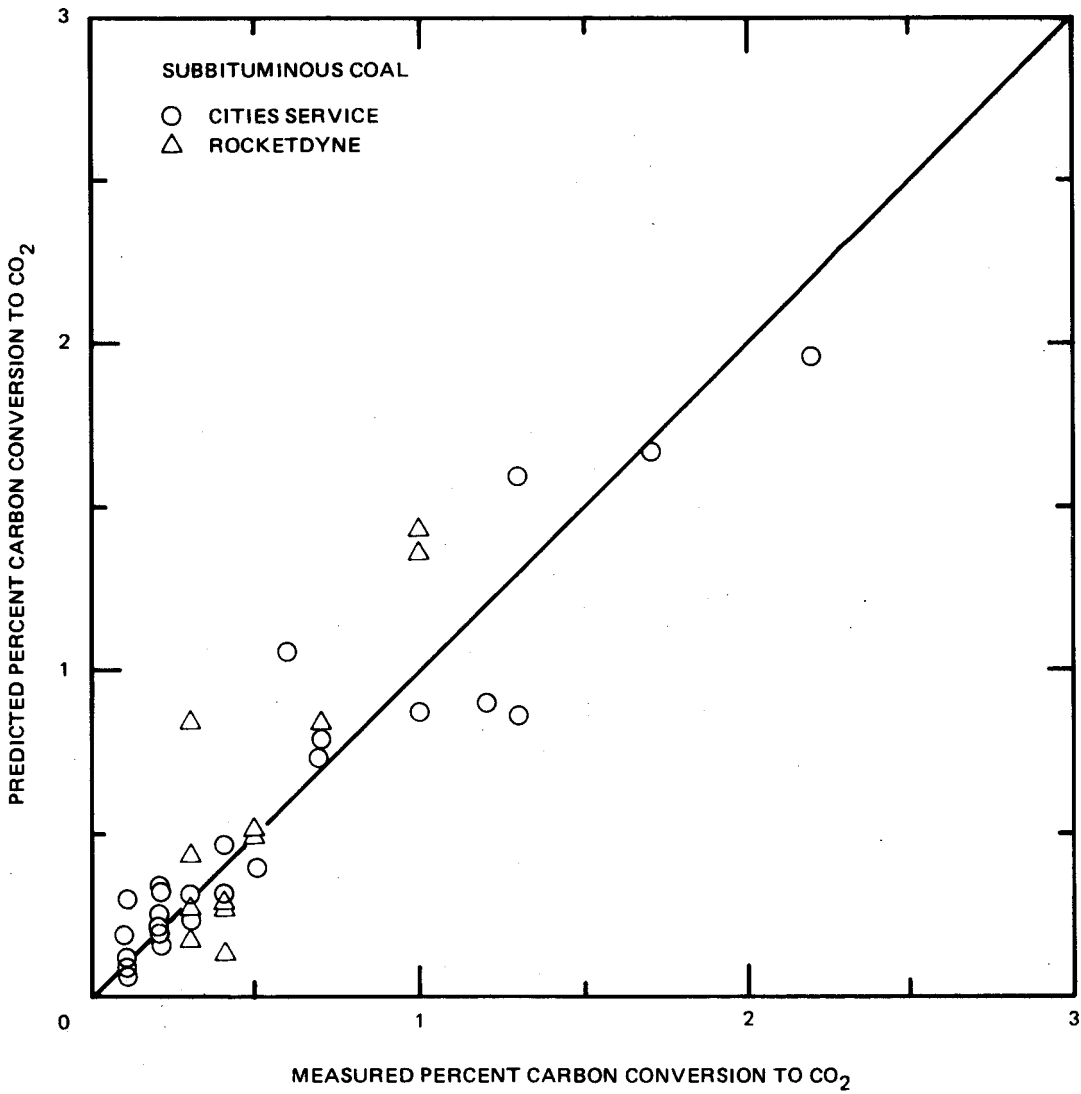


Figure 3-5. Comparison of Measured and Predicted Carbon Conversion to Carbon Dioxide for the Cities Service and Rocketdyne Reactors

3.4 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.

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

REFERENCES

1. Combs, L. P. and Greene, M. I. "Hydrogasifier Development for the Hydrane Process," Monthly Progress Report, January 1978, DOE Contract EX-77-C-01-2518 (February 1978).
2. Telephone Communication between T. P. Chen (Bechtel) and L. P. Combs (Rocketdyne) on March 3, 1978.
3. Bechtel Corporation, "An Analysis of Coal Hydrogasification Processes," Monthly Technical Progress Report for 1 December-31 December 1977, DOE Contract EF-77-A-01-2565 (January 1978).
4. Bechtel Corporation, "An Analysis of Coal Hydrogasification Processes," Quarterly Technical Progress Report for the Period 1 June-31 August 1977, DOE Contract EF-77-A-01-2565 (September 1977).