COMPUTER STUDY OF STAGE 2 REACTIONS IN THE BCR TWO-STAGE SUPER-PRESSURE COAL GASIFICATION PROCESS

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INTRODUCTION

In the BCR two-stage gasification process, recycle char is used in Stage 1 to produce hot synthesis gas by reaction with oxygen and steam. The hot products from Stage 1 heat the fresh coal and steam entering Stage 2 and react with them to produce methane and additional synthesis gas.(1,2)* A schematic flow diagram of the process is given as Figure 1.

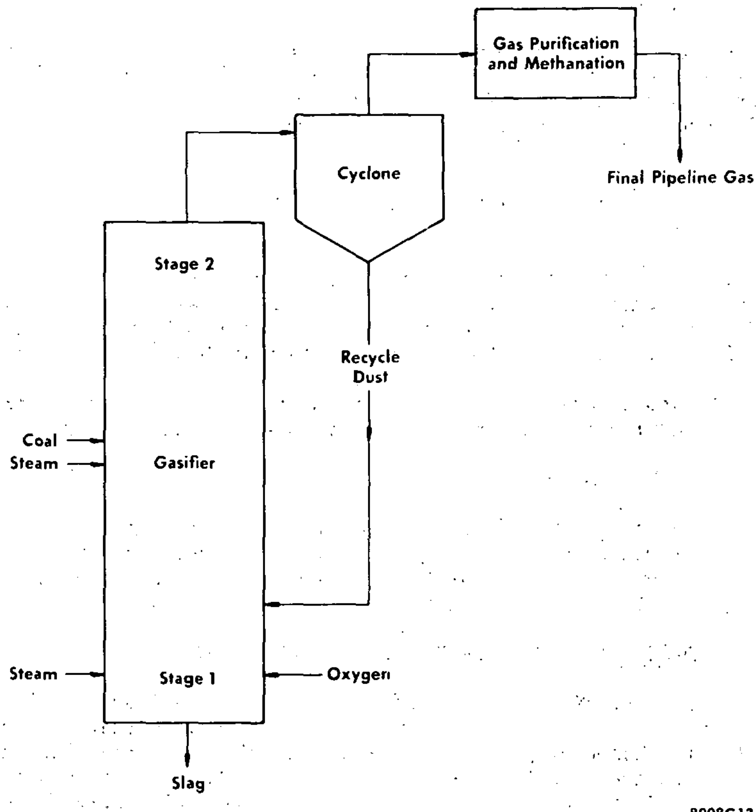

Figure 1. Simplified Flow Diagram for Two-stage Super-pressure Gasifier

* Numbers in parenthesis refer to list of References at end of paper.

For the past two years, laboratory research has been under way to establish the optimum conditions for operation of Stage 2 of this conceptual process. Results of some of these experimental studies have already been reported.(3,4) This paper reports the results of a computer study of the thermochemistry of the two-stage process with emphasis on the effects of variations in the operating conditions. These data were needed: (a) to guide the experimental studies; and, (b) to indicate the corresponding effects of these variables on the final cost of pipeline gas as derived in the initial economic evaluation of the process.(1,2)

According to the initial economic evaluation of the overall process (1), the yield of methane produced directly from coal is of major importance for the economics of the process. In a study of the thermochemistry involved, consideration must be given to this reaction and means must be available for determining the extent it occurs.

At the time the study was begun, kinetic data for the rate of methane formation were not available; however, it was known that methane formation at the temperatures visualized for Stage 2 is a very rapid reaction (5), and that observed methane yields correspond to the thermodynamic equilibrium of the reaction

$$C + 2H_2 = CH_4 \quad (1)$$

if an activity that varies from 1 to 3.4 is assumed for the carbon.(6)

Therefore, it was arbitrarily assumed for the present study that methane yields computed on this basis would be apt to respond to changes in Stage 2 temperature and pressure, and thus, they would be more realistic than selection of fixed methane yields. In addition, it was assumed that the rest of the carbon would be converted to $CO + H_2$ by reaction with steam and oxygen.

For the well known water-gas shift reaction, it was assumed that the reaction came to equilibrium at reaction temperature according to the equation:

$$CO + H_2O = CO + H_2 \quad (2)$$

For the evaluation of the effects of the various operating parameters, such as oxygen/coal ratio, steam/coal ratio, operating pressure, preheat temperatures, etc., one further assumption is necessary--namely, thermal equilibrium in each stage of the gasifier is achieved.

BASIS AND PROCEDURE FOR COMPUTER PROGRAM

In making the computer calculations, values for the various operating conditions prevailing in Stage 1 and Stage 2 are first designated, together with an arbitrarily chosen Stage 1 product gas composition. Then, the heat of reaction is calculated for the reaction of recycle char with oxygen and steam in Stage 1 to form the Stage 1 product gas of the arbitrarily chosen composition. The heat of reaction is calculated from the heating value of the recycle char and of the Stage 1 product gas, and then used to calculate the Stage 1 gas exit temperature.

Assuming that the water-gas shift equilibrium is established at this temperature of Stage 1, a new gas composition is calculated next and then used to correct the gas temperature. This process is repeated until a Stage 1 exit gas temperature is found that has a calculated accuracy of $\pm$ 5 C.

The Stage 1 product gas is then used in Stage 2 where coal and steam are added and reacted to form CH_4 in a concentration corresponding to the equilibrium of Equation 1 at a designated carbon activity and at an estimated temperature. The carbon in the coal which is not used in making methane is reacted with steam to form CO and H_2. Oxygen, nitrogen, and sulfur in the coal form H_2O, N_2, and H_2S; and the remaining hydrogen in the coal is liberated as gaseous hydrogen.

For this combination of gas from Stage 1 and Stage 2, again the temperature of the resultant gas mixture is calculated and the composition adjusted to reflect establishment of the shift reaction equilibrium. With the new composition, the equilibria for methane formation and the shift reaction are combined and the calculations reiterated until a Stage 2 temperature is obtained which is within $\pm$ 5 C of the actual temperature.

Computer Input

The nature of the input data required for the various individual computer calculations is shown in Table 1. The values for the different operating parameters were varied from one calculation to the next in accordance with the particular effect being evaluated.

TABLE 1. EXAMPLE OF COMPUTER INPUT DATA

Item	Stage 1	Stage 2	Total
Coal, daf, lb	--	100.0	100.0
Coal Preheat, C	--	204	--
Carbon Reacted,%	67	33	100.0
Carbon Activity, Equation 1	--	1.0	--
Oxygen, lb	71.0	--	71.0
Oxygen Preheat, C	327	--	--
Steam, lb	36.0	104.9	140.9
Steam Preheat, C	538	538	--
Pressure, atm	72.4	72.4	--
Heat Loss, Btu/lb Coal	250	--	250

Available data (7) for the heats of combustion, enthalpies, and thermodynamic equilibria were used in the computer program.

Computer Output

The type of information given in the printout for each computer run is shown in Table 2.

In addition to the results given in the computer output, some parameters indicative of the cost of the final gas, such as "total methane after methanation," "oxygen consumption lb/MM Btu in the final gas," or "the CO_2 production" have been manually calculated.

TABLE 2. EXAMPLE OF COMPUTER OUTPUT DATA

Item	Stage 1, Moles	Stage 2, Moles	Stage 2, Mole Fraction
Gas Composition			
CO	3.900	3.473	0.3138
H_2S	0.000	0.084	0.0076
CH_4	0.000	1.165	0.1052
H_2	1.036	3.900	0.3524
N_2	0.000	0.057	0.0052
CO_2	0.787	2.390	0.2159
Total	5.723	11.069	1.0001
H_2O	--	3.902	--
$(CO + H_2)$	--	7.373	--
Temperatures, C	1715	935	--
Oxygen/Steam Ratio	1.972	--	--
Oxygen/Coal Ratio	--	0.710	--
Preformed Methane,%	--	38.722	--
C as Methane,%	--	16.575	--

COALS USED

Three coals varying in rank from high volatile A bituminous to lignite were used in the study to obtain an indication of the effect of coal composition. The analyses used for these coals are given in Table 3.

TABLE 3. COAL ANALYSES USED FOR COMPUTER STUDY

	Seam		
	Pittsburgh	Illinois No. 6	Lignite
H_2O, lb per 100 lb daf Coal	1.3	1.3	1.3
Ash, lb per 100 lb daf Coal	7.7	9.1	15.5
Ultimate Analyses, Percent daf			
C	84.4	81.3	74.3
H	5.7	5.4	4.8
N	1.6	1.5	0.9
O	5.6	9.6	18.5
S	2.7	2.6	1.5
Net H per 100 C	5.3	4.6	3.0
Gross Heating Value, Btu/lb	15,270	14,480	12,270

RESULTS AND DISCUSSION

The data from the thirteen runs using Pittsburgh seam coal in normal operation of the gasifier are summarized in Tables 4 and 5. These were Runs 27 through 37, 42, and 43. The data from the four runs with char withdrawal are summarized in Table 6; these were Runs 48, 49, 50, and 53, using Pittsburgh seam coal. Runs 38 and 39 using Illinois No. 6 seam coal, and Runs 51 and 52 using North Dakota lignite are summarized in Table 7.

The computer data were used to calculate parameters that can be used directly in comparing the costs of gases obtained with different computer input data or different operating conditions. These parameters are referred to one million Btu in the final gas after methanation, and are based on costs derived from the initial economic evaluation (1) as follows:

Coal:	15¢/MM Btu
Oxygen:	\$5/ton = 0.25¢/lb
CO_2 Removal:	\$1/ton = 0.05¢/lb
Steam:	30¢/1000 lb

Oxygen/Coal Ratio and Temperature

For Pittsburgh seam coal, the influence of a change in the oxygen/coal ratio is shown in Figure 2, the oxygen/coal ratio is plotted versus Stage 2 temperature, oxygen consumption, CO_2 production, carbon as methane, and gasification efficiency. As expected, with increases in the oxygen/coal ratio, the Stage 2 temperature increases and all parameters connected with gasification cost indicate increased costs.

The data shown in Figure 2 are replotted in Figure 3 to show the effects of changes in Stage 2 temperature on these same parameters. Over the range studied, a Stage 2 temperature increase of 12 C causes a corresponding decrease in methane formation equal to about 1 percent of the carbon in the coal.

Carbon Activity

On the basis that experimental results may indicate a higher conversion to methane at a given temperature than indicated by Figures 2 and 3, adjustments were made in the computer calculations to reflect a higher activity for the carbon in Stage 2.

The results of computer runs using carbon activity 3.4 and 2, respectively, are compared in Table 8. The data show the influence of changes in methane yield from 14 to 24.6 percent on a carbon basis on the cost of the pipeline gas. A 1 percent unit increase in the conversion of the carbon in the coal into methane decreases the cost of raw materials and utilities for the pipeline gas by about 0.6¢/MM Btu.

In the initial evaluation of the processes (1), conversions of carbon into CH_4 in Stage 2 of 15, 20, and 24 percent were assumed; a 1 percent increase in the carbon conversion to methane decreased the pipeline gas cost by about 0.8¢/MM Btu.

Total Operating Pressure

In this study, the thermodynamic equilibrium is used to obtain the methane yield; therefore, the operating pressure exerts a major influence on the

TABLE 4. SUMMARY OF RESULTS OF COMPUTER RUNS 27-33

	Run Number 8014 BKC-						
	27	28	29	30	31	32	33
INPUT DATA							
Type of Coal	Pgh.	Pgh.	Pgh.	Pgh.	Pgh.	Pgh.	Pgh.
System Pressure, atm	72.4	72.4	72.4	72.4	72.4	72.4	102.4
Input Temperature, °C							
Coal	204	204	204	204	204	204	204
Steam	538	538	538	538	538	538	538
Oxygen	327	327	327	327	327	327	327
Stage 2							
Coal Feed Rate, lb daf	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Steam Feed Rate, lb	95.4	24.0	95.4	95.4	95.4	95.4	95.4
Carbon Activity	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Carbon Reacted, %	33.3	33.3	33.3	33.3	29.9	24.7	33.3
Stage 1							
Steam Feed Rate, lb	36.0	36.0	36.0	36.0	36.0	36.0	36.0
Oxygen Feed Rate, lb	71.0	71.0	71.0	71.0	74.5	80.0	71.0
Heat Loss, Btu/lb Coal	250	250	500	0	250	250	250
CALCULATIONS							
Stage 2							
Temperature (Exit) °C	935	945	905	955	955	985	955
Temperature (Exit) °F	1715	1733	1661	1751	1751	1805	1751
Gas Composition, Moles							
CO	3.473	4.990	3.180	3.662	3.616	3.796	3.374
H_2S	0.084	0.084	0.084	0.084	0.084	0.084	0.084
CH_4	1.165	0.958	1.303	1.077	1.046	0.882	1.254
H_2	3.900	3.209	3.639	4.064	4.013	4.147	3.643
N_2	0.057	0.057	0.057	0.057	0.057	0.057	0.057
CO_2	2.390	1.079	2.544	2.289	2.365	2.349	2.399
H_2O	3.902	1.043	3.886	3.915	4.027	4.222	3.981
Stage 1							
Temperature, °C	1715	1715	1575	1865	1735	1765	1715
Temperature, °F	3119	3119	2867	3389	3155	3209	3119
Gas, Moles							
CO	3.900	3.900	3.861	3.937	4.142	4.499	3.900
H_2	1.036	1.036	1.075	0.999	1.054	1.083	1.036
CO_2	0.787	0.787	0.826	0.749	0.784	0.792	0.787
H_2O	0.962	0.962	0.923	1.000	0.945	0.915	0.962
Stage 2							
Total Gas, Dry Moles	11.068	10.377	10.807	11.232	11.181	11.315	10.811
Total (CO + H_2) Moles	7.373	8.198	6.819	7.725	7.629	7.943	7.017
Preformed CH_4, %	38.7	31.9	43.3	35.8	35.4	30.7	41.7
Carbon as Methane, %	16.6	13.6	18.5	15.3	14.9	12.5	17.8
Total							
Thermal Efficiency	0.836	0.864	0.825	0.842	0.828	0.813	0.830
Steam Decomposition, %	47	69	47	47	45	42	45
Moles, Total Methane after Methanation	3.01	3.01	3.01	3.01	2.95	2.86	3.01
% Btu in Coal, Total Methane after Methanation	75.5	75.5	75.5	75.5	74.0	71.7	75.5
Oxygen Consumption, lb/MM Btu in CH_4	61.8	61.8	61.8	61.8	65.9	72.7	61.8
CO_2 Production, Mole per Mole CH_4	4.02	4.02	4.02	4.02	4.08	4.17	4.02
CO_2 Production, lb/MM Btu in Gas	154	154	154	154	159	167	154

TABLE 5. SUMMARY OF RESULTS OF COMPUTER RUNS 34-37, 42, AND 43

	Run Number 8014 BKC-					
	34	35	36	37	42	43
INPUT DATA						
Type of Coal	Pgh.	Pgh.	Pgh.	Pgh.	Pgh.	Pgh.
System Pressure, atm	51.0	72.4	72.4	72.4	72.4	72.4
Input Temperature, °C						
Coal	204	204	204	204	204	204
Steam	538	538	538	538	538	538
Oxygen	327	327	327	327	327	327
Stage 2						
Coal Feed Rate, lb daf	100.0	100.0	100.0	100.0	100.0	100.0
Steam Feed Rate, lb	95.4	104.9	95.4	95.4	95.4	60.0
Carbon Activity	1.0	1.0	3.4	2.0	1.0	1.0
Carbon Reacted, %	33.3	33.3	39.8	39.8	39.8	33.3
Stage 1						
Steam Feed Rate, lb	36.0	36.0	36.0	36.0	36.0	36.0
Oxygen Feed Rate, lb	71.0	71.0	63.9	63.9	63.9	71.0
Heat Loss, Btu/lb Coal	250	250	250	250	250	250
CALCULATIONS						
Stage 2						
Temperature (Exit) °C	905	925	965	935	885	945
Temperature (Exit) °F	1661	1697	1769	1715	1625	1733
Gas Composition, Moles						
CO	3.476	3.256	2.792	2.961	3.045	4.137
H_2S	0.084	0.084	0.084	0.084	0.084	0.084
CH_4	1.121	1.220	1.729	1.595	1.475	1.065
H_2	4.070	3.895	2.768	3.134	3.529	3.636
N_2	0.057	0.057	0.057	0.057	0.057	0.057
CO_2	2.430	2.551	2.506	2.471	2.506	1.825
H_2O	3.819	4.326	3.906	3.807	3.652	2.401
Stage 1						
Temperature, °C	1715	1715	1665	1665	1665	1715
Temperature, °F	3119	3119	3029	3029	3029	3119
Gas, Moles						
CO	3.900	3.900	3.458	3.458	3.458	3.900
H_2	1.036	1.036	1.009	1.009	1.009	1.036
CO_2	0.787	0.787	0.773	0.773	0.773	0.787
H_2O	0.962	0.962	0.990	0.990	0.990	0.962
Stage 2						
Total Gas, Dry Moles	11.238	11.063	9.936	10.302	10.697	10.804
Total ($CO + H_2$) Moles	7.546	7.152	5.560	6.095	6.575	[illegible]
Preformed CH_4, %	37.3	40.6	55.4	51.1	47.3	35.4
Carbon as Methane, %	16.0	17.4	24.6	22.7	21.0	15.2
Total						
Thermal Efficiency	0.838	0.830	0.832	0.840	0.847	0.848
Steam Decomposition, %	49	45	46	48	50	55
Moles, Total Methane after Methanation	3.01	3.01	3.12	3.12	3.12	3.01
% Btu in Coal, Total Methane after Methanation	75.5	75.5	78.3	78.3	78.3	75.5
Oxygen Consumption, lb/MM Btu in CH_4	61.8	61.8	53.5	53.5	53.5	61.8
CO_2 Production, Mole per Mole CH_4	4.02	4.02	3.91	3.91	3.91	4.02
CO_2 Production, lb/MM Btu in Gas	154	154	144	144	144	154

TABLE 6. SUMMARY OF RESULTS OF COMPUTER RUNS 48, 49, 50, AND 53

	Run Number 8014 BKC-			
	48	49	50	53
INPUT DATA				
Type of Coal	Pgh.	Pgh.	Pgh.	Pgh.
System Pressure, atm	72.4	72.4	72.4	72.4
Input Temperatures, °C				
Coal	204	204	204	204
Steam	538	538	538	538
Oxygen	327	327	327	327
Stage 2				
Coal Feed Rate, lb daf	100.0	100.0	100.0	100.0
Steam Feed Rate, lb	71.0	2.0	2.0	2.0
Carbon Activity	1.0	1.0	3.4	7.0
Stage 1				
Steam Feed Rate, lb	24.0	24.0	24.0	24.0
Oxygen Feed Rate, lb	65.0	28.0	20.0	20.0
Heat Loss, Btu/lb Coal	250	250	250	250
CALCULATIONS				
Stage 2				
Temperature (exit)°C	1035	945	915	945
Temperature (exit)°F	1895	1733	1679	1733
Gas Composition, Moles				
CO	3.178	0.954	0.526	0.452
H_2S	0.084	0.084	0.084	0.084
CH_4	0.583	0.548	0.933	0.001
H_2	3.567	1.668	0.971	0.774
N_2	0.057	0.057	0.057	0.057
CO_2	1.601	0.572	0.572	0.579
H_2O	3.378	1.518	1.445	1.506
Stage 1				
Temperature, °C	2355	995	725	725
Temperature, °F	4271	1823	1337	1337
Gas, Moles				
CO	1.737	1.551	1.129	1.129
H_2	0.244	0.845	0.981	0.981
CO_2	1.285	0.522	0.551	0.551
H_2O	1.088	0.488	0.351	0.351
Stage 2				
Total Gas, Dry Moles	9.070	3.882	3.143	2.946
Total (CO + H_2) Moles	6.745	2.621	1.497	1.225
Preformed CH_4, %	25.7	45.5	71.4	76.6
Carbon as Methane, %	8.3	7.8	13.3	14.2
Char Produced, lbs C	20.0	60.0	60.0	60.0
TOTAL				
Thermal Efficiency	0.651	0.325	0.331	0.327
Steam Decomposition, %	36.1	-5.1	0.0	-4.0
Total Methane after Methanation				
Moles	2.27	1.202	1.306	1.306
% Btu in Coal	57.5	30.5	32.9	32.9
% Btu in (Coal minus Char)	70.2	69.2	75.0	75.0
Btu in Char as % of Btu in Coal	18.6	55.7	55.7	55.7
Btu in Gas and Char as % of Btu in Coal	76.1	86.2	88.6	88.6
Oxygen Consumption, lb MM Btu in CH_4	75.5	60.5	40.0	40.0
CO_2 Production, Mole/Mole CH_4	1.36	0.73	0.56	0.56
CO_2 Production, lb MM/MM Btu in Gas	156	83	64	64

TABLE 7. SUMMARY OF RESULTS OF COMPUTER RUNS 38, 39, 51, AND 52

	Run Number 8014 BKC- 38	39	51	52
INPUT DATA				
Type of Coal	Illinois	Illinois	Lignite	Lignite
System Pressure, atm	72.4	72.4	72.4	72.4
Input Temperatures, °C				
Coal	204	204	204	204
Steam	538	538	538	538
Oxygen	327	327	327	327
Stage 2				
Coal Feed Rate, lb daf	100.0	100.0	100.0	100.0
Steam Feed Rate, lb	95.4	95.4	55.0	95.4
Carbon Activity	1.0	1.0	1.0	1.0
Carbon Reacted,%	30.6	41.4	22.6	22.6
Stage 1				
Steam Feed Rate, lb	36.0	36.0	36.0	36.0
Oxygen Feed Rate, lb	71.0	60.0	65.0	65.0
Heat Loss, Btu/lb Coal	250	250	250	250
CALCULATIONS				
Stage 2				
Temperature (exit) °C	955	885	915	895
Temperature (exit) °F	1751	1625	1679	1643
Gas Composition, Moles				
CO	3.388	2.855	3.055	2.357
H_2S	0.081	0.081	0.047	0.047
CH_4	0.975	1.391	0.910	1.038
H_2	3.837	3.395	2.853	3.039
N_2	0.054	0.054	0.032	0.032
CO_2	2.405	2.522	2.220	2.790
H_2O	4.180	3.791	2.839	4.640
Stage 1				
Temperature, °C	1705	1635	1405	1405
Temperature, °F	3101	2975	2561	2561
Gas, Moles				
CO	3.906	3.196	4.184	4.184
H_2	1.052	0.987	1.330	1.330
CO_2	0.792	0.771	0.604	0.604
H_2O	0.947	1.011	0.669	0.669
Stage 2				
Total Gas, Dry Moles	10.741	10.299	9.118	9.304
Total (CO + H_2) Moles	7.225	6.251	5.908	5.397
Preformed CH_4, %	35.1	47.1	38.1	43.5
Carbon as Methane, %	14.4	20.5	14.7	16.8
Total				
Thermal Efficiency	0.822	0.845	0.833	0.815
Steam Decomposition, %	43	48	44.0	36.6
Total Methane after Methanation, Moles	2.78	2.95	2.39	2.39
Total Methane after Methanation, % Btu in Coal	73.7	78.1	74.7	74.7
Oxygen Consumption, lb/MM Btu in CH_4	66.5	53.2	71.0	71.0
CO_2 Production, Mole per Mole CH_4	3.99	3.82	1.59	1.59
CO_2 Production, lb/MM Btu in Gas	165	148	183	183

TABLE 8. EFFECTS OF CHANGES IN CARBON ACTIVITY IN STAGE 2
(Basis: Pressure, 72.4 atm; Heat Loss, 250 Btu/lb Coal)

	Stage 2 Temperature, 935 C				Stage 2 Temperature, 965 C			
	Carbon Activity		Difference		Carbon Activity		Difference	
	2.0	1.0	Units	¢/MM Btu in Gas	3.4	1.0	Units	¢/MM Btu in Gas
Oxygen, lb/100 lb Coal	63.9	71.0	--	--	63.9	75.9	--	--
Carbon as CH_4, %	22.7	16.6	--	--	24.6	14.0	--	--
Gasification Efficiency, %	78.3	75.5	--	--	78.3	73.2	--	--
Oxygen, lb/MM Btu in Gas	53.5	61.8	8.3	2.07	53.5	68.1	14.6	3.65
CO_2, lb/MM Btu in Gas	144.0	154.0	10.0	0.50	144.0	163.0	19.0	0.95
Steam, lb/MM Btu in Gas	110.0	114.5	4.5	0.13	110.0	118.0	8.0	0.24
Coal, MM Btu/MM Btu in Gas	1.277	1.325	0.048	0.72	1.277	1.367	0.09	1.35
TOTAL				3.42				6.19

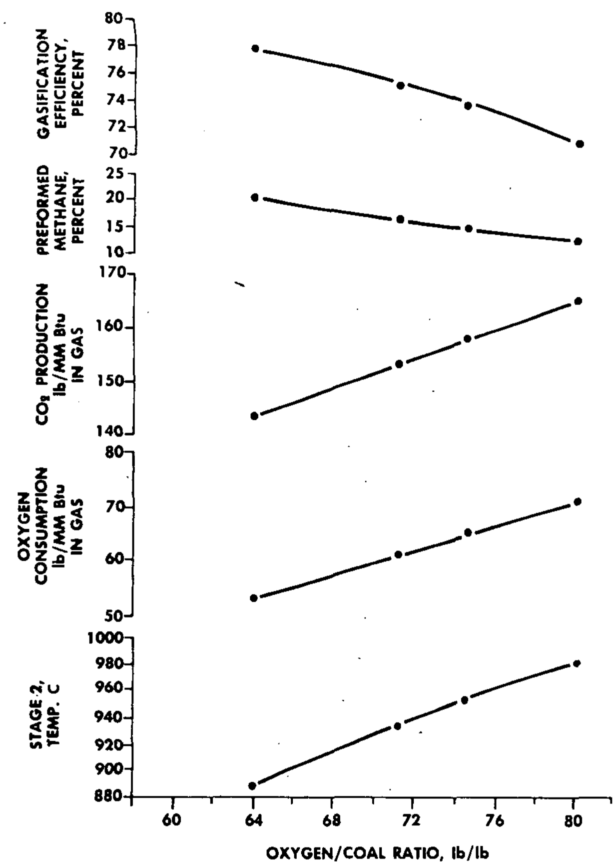

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Figure 2. Computer Program Results: Effects of Changes in Oxygen (Basis: Pressure, 72.4 atm, Heat Loss: 250 Btu/lb Coal)

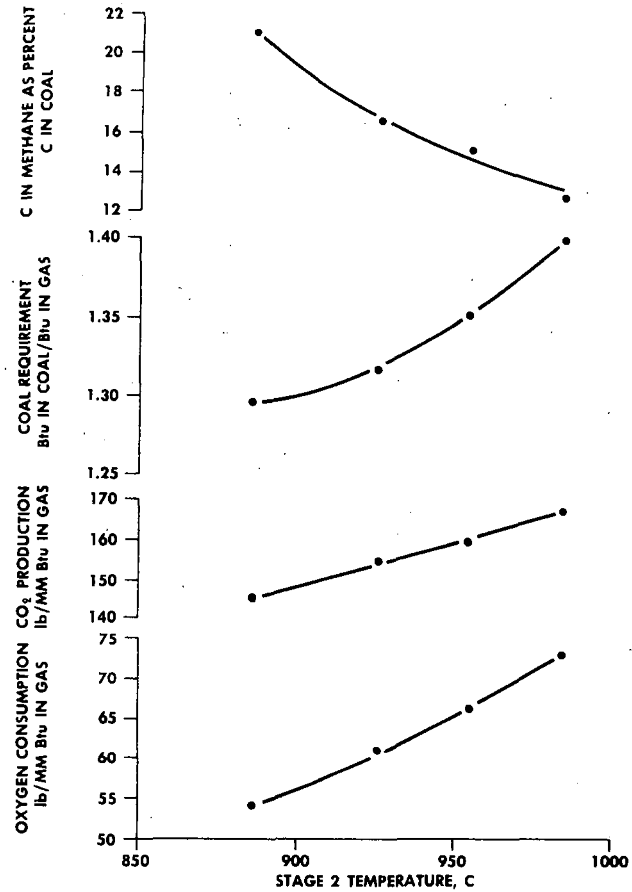

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Figure 3. Effects of Changes in Stage 2 Temperature (Basis: Pressure, 72.4 atm, Heat Loss: 250 Btu/lb Coal)

yield. By comparing the results from Run 33 and Run 34 with those from a run at the standard operating pressure, it is noted that a change in pressure, either from 72.5 to 51 atm, or from 72.5 to 102 atm, produces a change in raw material and utility costs equivalent to about 2¢/MM Btu pipeline gas; operation at the higher pressure gives the cheaper gas in each case. By comparison, the same change in gas cost of 2¢/MM Btu would be produced by a change of about $10 million in the investment costs for a 250 MM scfd plant. Further economic evaluations and experimental results will be needed to find the optimum pressure for the lowest cost of gas and/or capital investment.

Heat Loss and Preheat Temperature

Another factor influencing the gas yield is the heat loss in the gasifier. As reference value, a heat loss of 250 Btu/lb of coal, or 1.6 percent of the heating value of Pittsburgh seam coal, has been assumed. This is an arbitrarily chosen figure that is based on extrapolation of available data to pressure operation. Computer Runs 29 and 30 for heat losses of 500 and 0 Btu/lb of coal, respectively, were compared with results for 250 Btu heat loss at the same Stage 2 temperature. An increase in heat loss of 250 Btu/lb coal increases the gas cost by about 2¢/MM Btu pipeline gas. Again, experimental studies will be needed to determine whether the actual methane yield is influenced to the extent indicated here. Only experiments in a large pilot plant will establish reliable data for the heat loss in a commercial unit.

A study of different preheat temperatures of reactants did not appear necessary. Differences in the enthalpies of the various materials due to changes in preheat temperature, have the same influence as changes in heat loss.

Steam/Coal Ratio

Several computer runs were made using various steam/coal ratios:

In Computer Runs 28 and 35, data for 24.0 and 104.9 pound steam per 100 pound coal in Stage 2 were obtained for comparison to the "standard" quantity of 95.4 pound; no changes were made in the amount of steam entering Stage 1, 36.0 pound steam per pound coal being used in all instances.

In Computer Run 28 with 60 pound total steam per 100 pound coal, the Stage 2 temperature was 20 C above that in Run 35, being 945 C, as compared to 925 C.

Unless reaction kinetics demand a high steam/coal ratio, a ratio below 130 lb/100 lb coal should be selected for purely heat balance reasons. A further study of the utilization of the gasification steam in the shift reactor is indicated. Such a reactor would be part of an integrated pipeline gas plant.

Withdrawal of Recycle Char

On the premise that it may become desirable to withdraw recycle char for use as boiler fuel rather than fresh coal, Computer Runs 48, 49, 50, and 53 were made to indicate results which might be expected with such an operation. The partial gasification shows lower costs for pipeline gas in all cases: the lowest difference is 2.4 cents, the highest 13.3 cents per MM Btu based on raw material and utility costs only, assuming a char credit at the Btu price of the coal and only a minor char handling expense.

Additional experimental data are needed to better define the methane yield and operating temperature for char withdrawal in comparison to these same parameters for complete gasification.

Changes in Coal Feed Stock

To obtain data on the effect of coal rank on the cost of pipeline gas, several computer runs were made with coals differing in rank from Pittsburgh seam coal, namely, Runs 38 and 39 with Illinois No. 6 coal and Runs 51 and 52 with lignite. For Pittsburgh seam coal and Illinois No. 6 coal at the same price per MM Btu in the dried coal and the same Stage 2 temperature, the pipeline gas cost is similar. On the same basis, the greater thermal ballast in the lignite, mainly its high oxygen content, leads to a higher cost of gas made from lignite. However, if one assumes a 60 C lower Stage 2 temperature for lignite, the gas cost becomes the same.

Again, further experimentation will lead to a better definition of the best operating temperature for the various coals and a better comparison of cost will be possible.

Comparison of Experimental and Computer Results

Experimental Stage 2 gasification data for lignite (3) are compared with computer results in Table 9. The experimental results show a somewhat higher methane yield in spite of higher Stage 2 temperatures. This discrepancy is not surprising since the methane yield is determined by reaction kinetics and factors such as partial pressures of reactants and the ratios of Stage 1 gas, steam, and coal, rather than by the thermodynamic equilibria.

The higher experimental yield of ($CO + CO_2$) will lead to a smaller amount of char available for Stage 1 than used in the computer run. This will, at the same oxygen/coal ratio, lead to a higher Stage 1 temperature. To attain the higher temperature in Stage 2 indicated by the experiments, a higher oxygen/lignite ratio than the 0.65 lb/lb assumed in computer Run 51 will be needed. In the feed streams entering Stage 2 in the experimental runs, the partial pressure of ($CO + H_2$) is lower; and that of CO_2 is higher than in the computer run. This is in accord with a higher oxygen/lignite ratio as required to attain the higher temperature used in the experimental runs. It may be noted that the Stage 1 gas/lignite ratios and the steam/lignite ratios in the two experimental runs bracket these same parameters in the computer runs.

The computer data reported in this study have been useful in providing guidance for the selection of experimental parameters such as feed stream composition and reactant ratios for the externally-heated experimental 5 lb/hr flow reactor being used for the study of Stage 2 reactions. They will be equally useful in the operation of the internally-heated 100 lb/hr process and equipment development unit now being erected.

The computer program used in this study may also be useful as a basis in preparing an improved program in which the methane content of the Stage 2 gas is determined by kinetic data. It is expected that further operation of the 5 lb/hr unit, and later the 100 lb/hr unit, will supply such data.

TABLE 9. EXPERIMENTAL AND COMPUTER DATA FOR LIGNITE GASIFICATION IN STAGE 2

	Experimental Data		Computer Data
	Run 36	Run 38	Run 51
Temperature °C, Stage 1	--	--	1405
Stage 2	970	965	915
Pressure, atm	70	81.5	72.4
Lignite, g C/min	5.9	18.8	--
Stage 1 Gas, Nl/g C in Lignite	4.9	1.56	1.84
Steam, g/g C in Lignite	2.1	0.9	1.22
Partial Pressure of Gases Entering Stage 2, atm			
CO	25.5	26.5	30.8
H_2	8.4	8.7	9.8
CO_2	7.5	7.9	4.4
H_2O	24.5	34.0	27.4
Ar	4.1	4.4	--
Yields in Stage 2 alone as Percent of Lignite:			
C in CH_4	16.9	15.4	14.7
C in ($CO + CO_2$)	22.0	18.1	7.9
C Gasified in Stage 2	38.9	33.5	22.6
Btu in CH_4	33.8	29.5	28.2
Btu in ($CO + H_2$)	4.5	10.2	3.8

ACKNOWLEDGMENT

This paper reports results from a program of research being conducted by Bituminous Coal Research, Inc., with support from the Office of Coal Research, U.S. Department of the Interior, under Contract No. 14-01-0001-324. The authors wish to thank the Office of Coal Research for permission to publish this paper.

The authors also wish to express their thanks to Mr. E. J. Vidt and the Blaw-Knox Company for preparing the computer program and making the computations.

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