BITUMINOUS COAL RESEARCH, INC.
SPONSORED RESEARCH PROGRAM

GAS GENERATOR RESEARCH AND DEVELOPMENT

Progress Report No. 5

(BCR Report L-452)

I. INTRODUCTION

This report summarizes progress achieved during the ninety-seventh month of work on the general program, "Gas Generator Research and Development," being conducted by Bituminous Coal Research, Inc., for the Office of Coal Research. The program which was initiated under Contract No. 14-01-0001-324 December 20, 1963, was transferred to Contract No. 14-32-0001-1207 on August 19, 1971. Thus, this report represents the fifth report of progress under the new prime Contract.

The overall objective of the program continues to be to develop processes for gasifying coal to produce fuel gas and high-Btu pipeline gas.

Laboratory-scale coal gasification experimentation is to be continued together with process and equipment development. With the aid of engineering subcontractor(s), a multipurpose research pilot plant facility is to be designed, constructed, and test operated.

A. Work Schedule

Work on the project is being conducted according to a schedule reflecting the program outlined under the new prime contract. This schedule was shown in Figure 1, page 2, Progress Report No. 1.

B. Monthly Progress Charts

Monthly progress charts reflecting proposed rate of effort and expenditures are shown in Appendixes A-1 and A-2.

II. PHASE II PROGRESS ACHIEVED DURING MONTH ENDING JANUARY 25, 1972

A. Laboratory-scale Process Studies

1. Coal Composition and Beneficiation Studies, and Laboratory Pyrolysis of Coal (R. G. Moses, R. D. Saltsman, and J. E. Noll): Final editing of the summary report covering the work performed since September, 1970, continues. The report will be issued next month.

2. Fluidized-bed Gasification (E. K. Diehl and J. T. Stewart): Work on the two-phase project continued during the month of January, with some slight change in priorities established insofar as the fluidized-bed PEDU is concerned. Only a minor amount of work was done on the char reactivity studies due to equipment breakdown.

a. Fluidized-bed PEDU: A meeting with Koppers was held on January 11, 1972, to clarify the instructions they had received regarding additional design work for the PEDU. These instructions were to develop flow diagrams, general arrangements and specifications, and cost estimates for the following two modifications:

(1) Additional equipment and changes to the specifications required in order that the PEDU will be capable of processing coal as well as char;

(2) Additional equipment and changes to the specifications required to add a second-stage fluidized bed to operate in series with the single stage now designed.

The purpose of the design work was not to completely redesign the PEDU installation but to anticipate the above as future modifications. By anticipating the requirements for modification, initial space and equipment can be designed properly to accommodate the future changes.

On January 18, 1972, Koppers submitted preliminary specifications and drawings to support three alternate modifications to the design previously developed in September 1971:

(1) Alternate A - addition of a second fluidized-bed gasifier to operate in series with the original unit;

(2) Alternate B - addition of equipment for processing non-caking coals through the original single-stage unit;

(3) Alternate C - addition of equipment for processing caking coals through the original single-stage unit.

The above were discussed with OCR on January 20, 1972. At that time, OCR reviewed the objectives of the fluidized-bed gasification program, and set two commercial applications toward which the work should be aimed:

(1) Gasification of coal to produce clean fuel gas.

(2) Production of carbon monoxide from carbon dioxide in a closed MHD cycle.

OCR indicated that the clean fuel gas concept should get first priority. Further, OCR expressed the opinion that coal pretreatment, per se, should not be given much attention, since others have fairly well explored that area. CCR would rather BCR explore ways of introducing coal directly into the first-stage "gasification bed" and directing the off-gas into subsequent beds to destroy tar and volatiles.

BCR was asked to develop a design "package" that contains all vessels and equipment required, even though their inclusion into total operation may actually occur in several steps. OCR prefers to obtain blanket approval for the entire program.

b. Laboratory Investigations: No significant char reactivity data were collected during the month because of equipment failure. The x-y recorder from the TGA equipment has been sent out for repair and it is hoped it will be returned early in February.

While the TGA is out of service, various physical properties of chars are being investigated. The fluidization apparatus described in Progress Report No. 1, page 3, was used to determine the minimum fluidization velocity of FMC char (BCR Lot No. 2455). A plot of the experimental data is given in Figure 81. The observed minimum fluidization velocity, V_{mf}, was .083 ft/sec. This value of V_{mf}, along with the measured bulk density of 35 lb/cu ft, was used to determine the particle density.

A modified form of the Ergun equation may be used to predict V_{mf} for low Reynolds number systems.

$$V_{mf} = g \frac{(\rho_p - \rho_g)\, D_p^2 \, E^3}{150\mu\, (1 - E)}$$

where

V_{mf} = minimum fluidization velocity, ft/sec

g = gravitational acceleration, ft/sec^2

ρ_p = particle density, lb/cu ft

ρ_g = gas density, lb/cu ft

D_p = particle diameter, ft

E = porosity (dimensionless) = $\frac{\rho_p - \rho_B}{\rho_p}$

ρ_B = bulk density at minimum fluidization, lb/cu ft

μ = viscosity of fluidizing gas, lb/ft sec

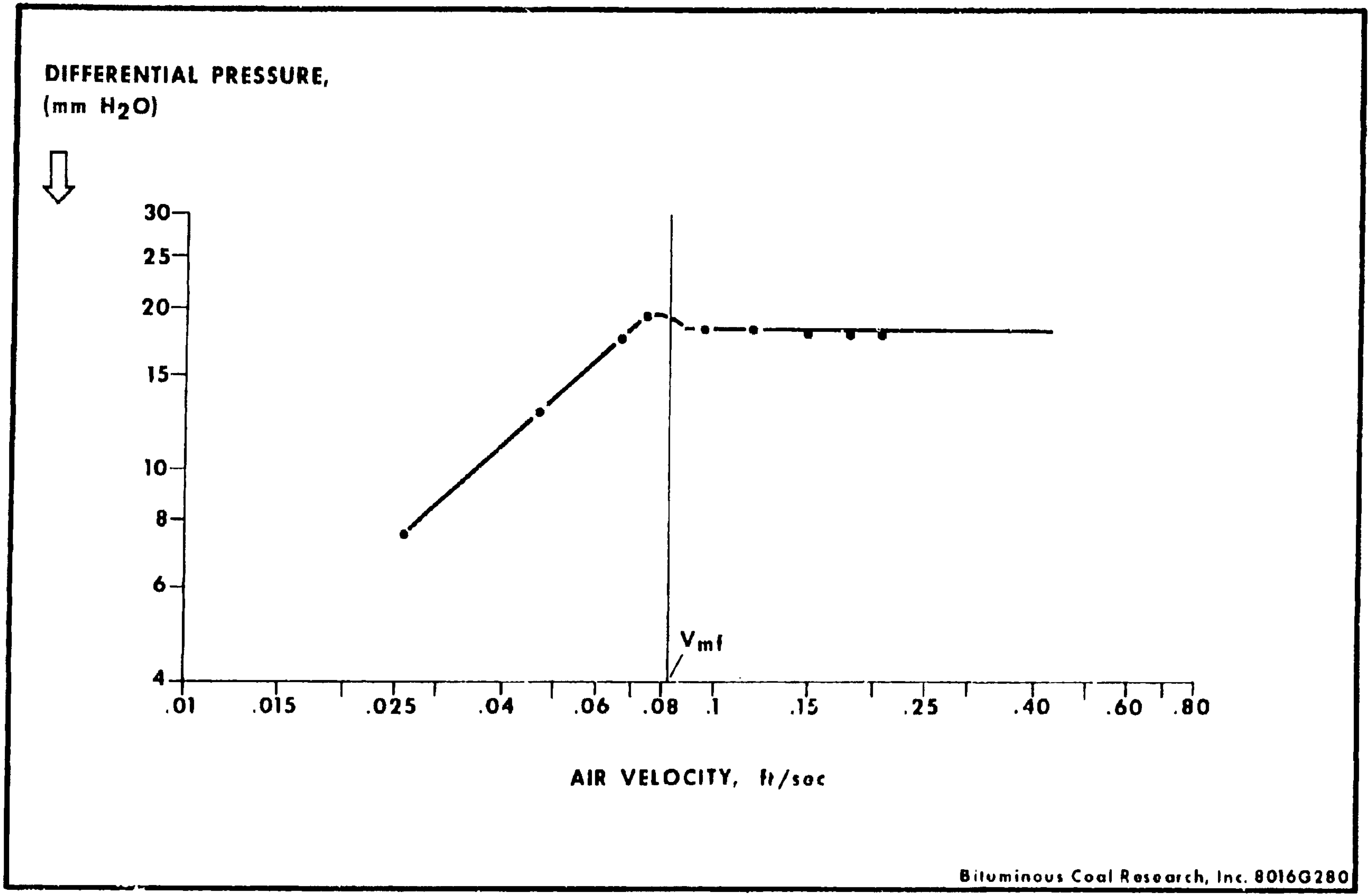

Figure 81. Minimum Fluidization Velocity of As Received (−60 Mesh) FMC Char

From the measured values of V_{mf}, ρ_B, D_p, and μ, the above equation may be solved by trial and error for ρ_p. A program was written for the Hewlett-Packard calculator which solves the Ergun equation for ρ_p by Newton's iterative method. This method gave a ρ_p of 64 lb/cu ft for FMC char.

This same char sample had been sent to American Instrument Company's testing laboratory for a density determination. The testing laboratory measures particle density by both a low pressure and a high pressure mercury intrusion method. Their measured values were 49.2 and 93.7 lb/cu ft, respectively. Thus, it can be seen that the "fluidization particle density" lies somewhere between the apparent particle density and the true particle density.

c. Future Work: Immediate future work will involve design revisions to conform with the priorities set at the January 20, 1972 meeting with OCR.

Char reactivity studies will continue as soon as equipment repairs are made.

3. Gas Processing (M. S. Graboski): Work continued in the area of gas processing during the month of January in accordance with the revised time schedule shown in Figure 82. A major modification has been made in this schedule from the previous one reported in Progress Report No. 1 (September 1971) with regard to the PEDU studies. Due to a delay in obtaining approval to detail and construct, latest estimates indicate that detail engineering will be completed by June 1, 1972; thus, subsequent operation of the PEDU will not take place until late in the first quarter of 1973.

Work covered in this report summarizes progress achieved in bench-scale and PEDU work for the month of January.

a. Bench-scale Studies: The purpose of the bench-scale program is to investigate methanation catalysts under conditions imposed by the BI-GAS process. These include high carbon monoxide concentrations, high pressure, and a 3/1 hydrogen to carbon monoxide ratio.

Three processing schemes are currently under investigation. These are summarized in Figure 83. Scheme A reflects current planning where methanation follows carbon monoxide shift and acid gas removal. Schemes B and C consider carbon dioxide removal and hydrogen sulfide and carbon dioxide removal, respectively, after methanation. The three schemes are further discussed in BCR Suggestion 194. Bench-scale tests are being conducted to determine which scheme is optimal for the BI-GAS process.

(1) BSM Tests: During the month, one successful BSM test, No. 49, was conducted. The catalyst used was a copper chromite powder from Harshaw Chemical Company identified as BCR Lot 2907. Two other tests, 50 and 51, were attempted using a modified system but in both cases there was a mechanical failure.

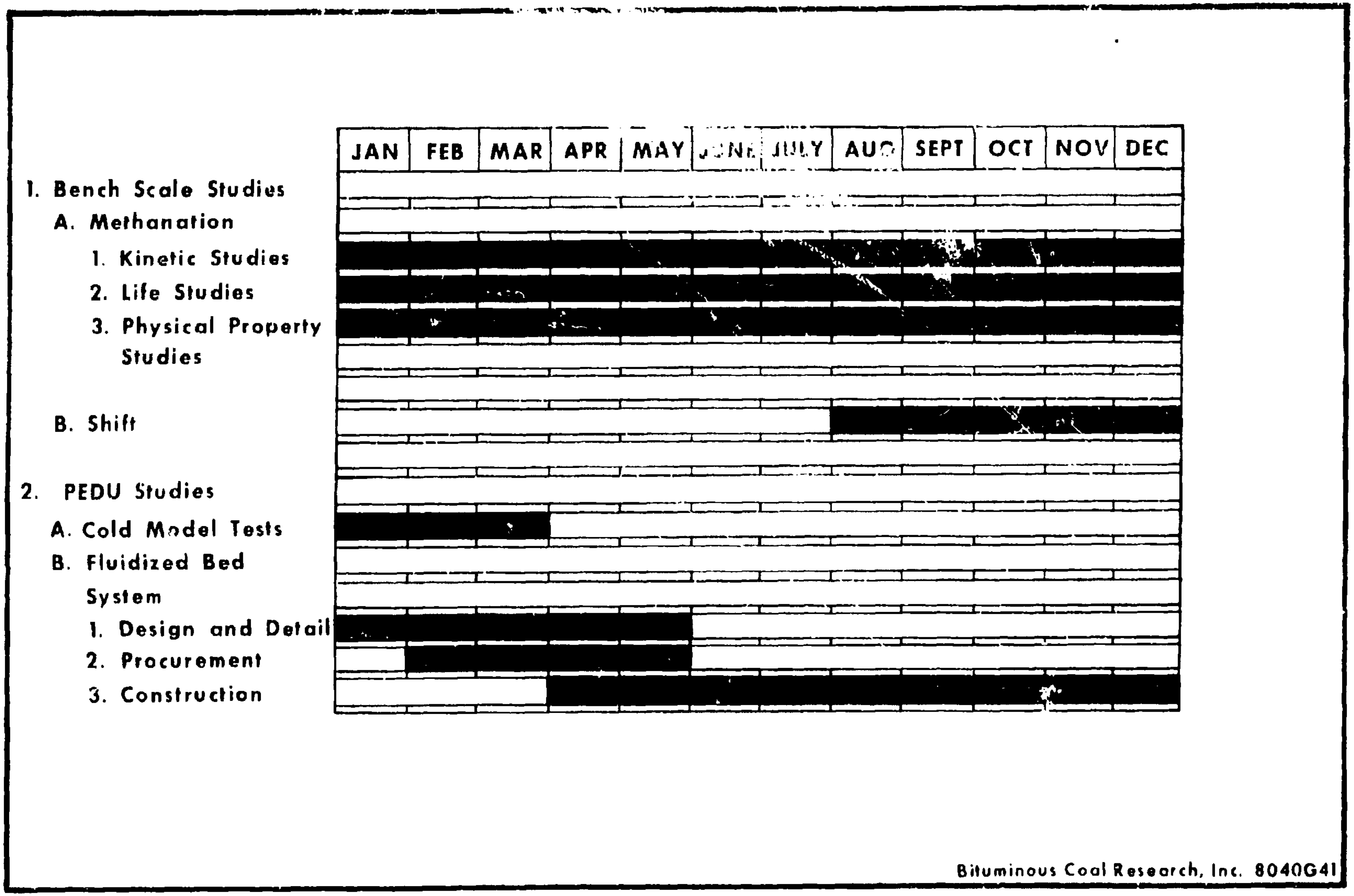

Figure 82. Gas Processing Work Schedule for Calendar 1972

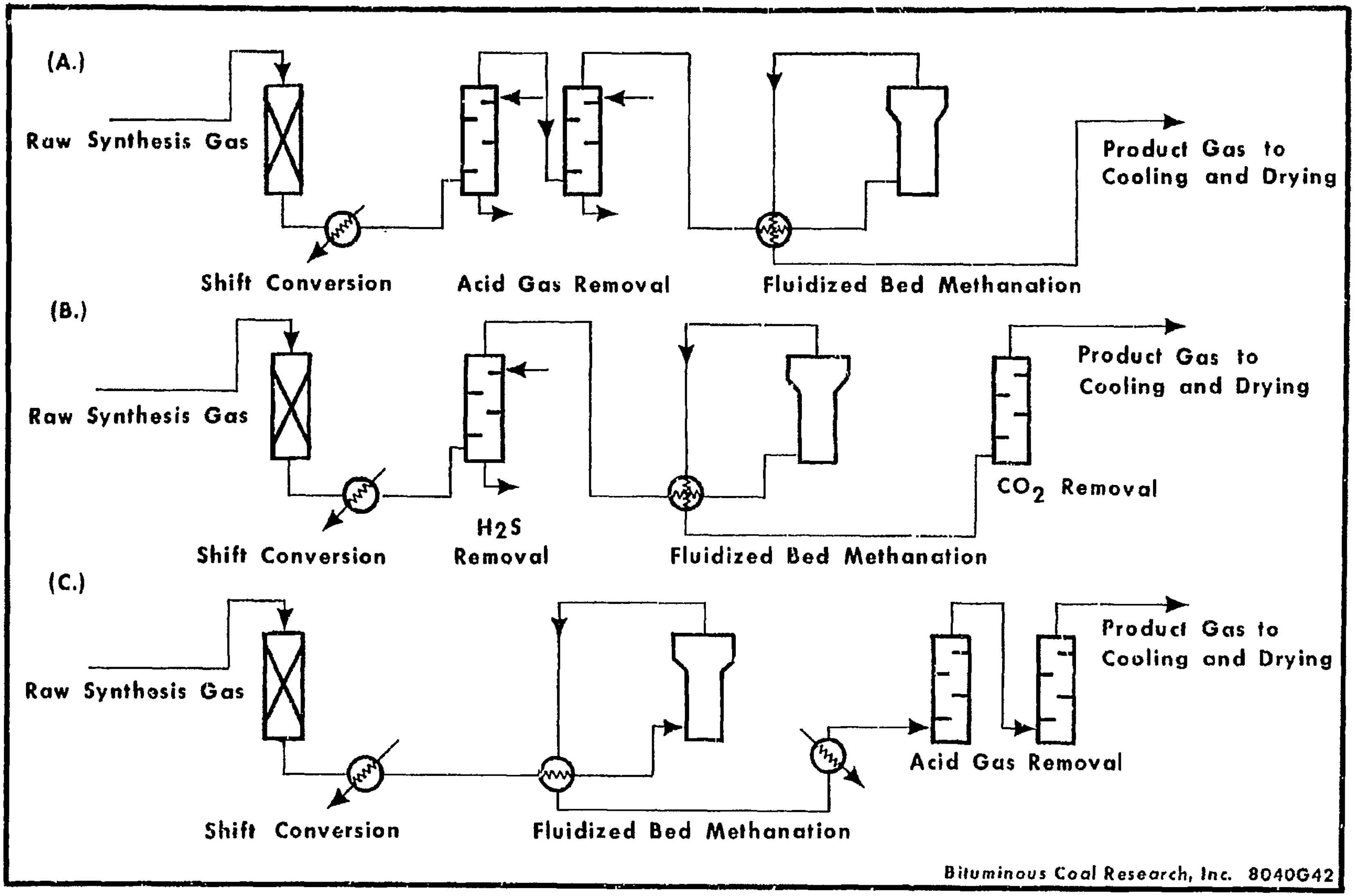

Figure 83. BI-GAS Gas Processing Systems

BSM Test 49 was conducted with 3.0 grams of copper chromite catalyst at 1150 psia and 655 and 755 F under high carbon monoxide partial pressure. At 655 F, little methanation occurred; while at 755 F, a larger portion of the reacted carbon monoxide went to methane. At the lower temperature, the product "water" analysis indicated a high grade crude methanol was being produced.

During Period 1, at 1150 psia and 655 F, on-line testing indicated little change in gas composition. Material balance calculations have been made based on flows and compositions with results indicating possibly a trace of methanation. Product water analysis, however, indicated the presence of at least six components with the primary one being methanol. Data for Period 1 are summarized in Table 65.

No attempt has been made to normalize the carbon balance in Table 65. Thus, the gas molar flow rates are slightly in error. Comparison of inlet and outlet methane rates shows no change. However, the carbon balance is 7 percent lower in the product than the feed and the liquid product contains water. Thus it can be stated that some methane was formed in synthesis. The crude methanol liquid product composition from Period 1 is subject to error in the ten percent range due to use of only a rough chromatograph calibration. It is evident from Period 49-1 that methanol is the prime product at moderate temperatures using copper chromite for a catalyst.

During Period 2, at 1150 psia and 755 F, methane was apparent in the product gas. Analysis of the liquid products showed a larger percentage of water with ten components present. The largest percentage of these was water followed by methanol, ethanol, and probably isopropanol. Acetone and methyl ethyl ketone were also identified as being present in trace amounts. The data from Period 49-2 are summarized in Table 66.

Data for 49-2 were normalized to the exit carbon content. Water and hydrogen balances from stoichiometric considerations are in some error due to the approximate nature of the liquid analysis. Period 49-2 results show a split between methane and methanol in about the ratio of 4/1. Such a result is interesting and suggests some further possibilities for gas processing which may have a significant effect on process economics.

(2) Catalyst Life Tests: During the past several months, continuing tests of BCR Lot 2903 catalyst have been carried out based on the test sequence outlined in Progress Report No. 2, page 118. Data reported through last month covered testing to 1700 hours of catalyst life based on a carbon dioxide-free feed gas representative of processing System A on Figure 83 as previously described.

During January, conditions were varied using two feed gases which represent Systems B and C of Figure 83. The gas compositions used were:

Component	Case B	Case C
Hydrogen	42.87	42.38
Nitrogen	1.35	1.58
Carbon Monoxide	14.35	14.38
Carbon Dioxide	30.12	29.94
Methane	11.31	10.91
Ethane	0.00	0.04
Hydrogen Sulfide	0.00	0.77
	100.00	100.00

TABLE 65. RESULTS FOR TEST PERIOD 49-1

Catalyst: 3.0 g 2907
Temperature: 655 F
Pressure: 1150 psia

Component	Feed Data Percent	Feed Data g moles/hr	Product Data Percent	Product Data g moles/hr
Gas				
H_2	61.3	17.1	61.1	15.7
N_2	2.2	0.6	2.2	0.6
CO	20.7	6.0	19.8	5.1
CO_2	-	-	0.1	0.0
CH_4	15.7	4.4	16.7	4.3
C_2H_6	0.1	0.0	0.1	0.0
	100.0	10.5 (C in gas)	100.0	9.5 (C in gas)
Liquid				
CH_3OH	-	-	79.2	0.23
C_2H_5OH	-	-	4.0	0.01
H_2O *	-	-	16.8	0.09
			100.0	0.25(C in liquid)
Total C		10.5		9.07

* Contains trace organics

TABLE 66. RESULTS FOR TEST PERIOD 49-2*

Catalyst: 3.09 g 2907
Temperature: 755 F
Pressure: 1150 psia

	Feed Data		Product Data	
Component	Percent	g moles/hr	Percent	g moles/hr
Gas				
H_2	61.3	17.6	57.3	14.5
N_2	2.2	0.6	2.5	0.6
CO	20.7	6.0	18.1	4.6
CO_2	-	-	0.3	0.1
CH_4	15.7	4.5	21.3	5.4
C_2H_6	0.1	0.0	0.4	0.1
	100.0	10.5 (C in gas)	100.0	10.3 (C in gas)
Liquid				
CH_3OH	-	-	29.9	0.26
C_2H_5OH*	-	-	3.9	0.02
H_2O **	-	-	66.2	1.02
			100.0	0.3 (C in liquid)
Total C	-	10.5		10.6

* Normalized to exit carbon content
** Contains trace organics

Data were analyzed for Cases B and C and compared with a representative Case A sample, 2903-40. Three parameters were used in the comparison. These were:

(a) Useful Conversion, α: This is defined as the total moles of $(CO+H_2)$ converted to hydrocarbons divided by the total moles of $(CO+H_2)$ in the feed gas. This parameter permits comparison of conversion for all feed gas compositions since the shift reaction is normalized out of the term.

$$\alpha = [(CO+H_2)\text{ used} / (CO+H_2)\text{ Fed}]\ 100$$

(b) Ethane Selectivity, β: This term defines the formation of ethane as a function of the total moles of hydrocarbon produced.

$$\beta = [C_2 / (C_1+C_2)]\ 100$$

where C_2 equals the moles of ethane and C_1 equals the moles of methane.

(c) Shift Equilibrium Constant, K_S: The apparent shift equilibrium constant is determined from a water material balance and the expression:

$$K_S = \frac{(CO_2)\ (H_2)}{(CO)\ (H_2O)}$$

Results for test samples 2903-54 through 2903-66 are given in Table 67 and compared to sample 2903-40.

The base case, A, showed a useful conversion of 59 percent with an ethane selectivity of 10 percent throughout the 1628 test hours previously reported.

The effect of carbon dioxide is clearly indicated when Case B results are compared with those of Case A. Deactivation was not effected by change in composition of the feed. However, the useful conversion of $(CO+H_2)$ was reduced to about 35 percent. Correspondingly, a higher selectivity to ethane occurred. In each case, A and B, shift equilibrium was maintained. The lower conversion in Case B is due to steam deactivation on the catalyst surface. In Case A, the shift reaction driving force is towards carbon dioxide. Hence, any water of hydrogenation is consumed immediately on the surface. In Case B, however, the driving force for water consumption is not present; and at low conversions shifting goes toward carbon monoxide, forming additional water. The water deactivation mechanism has been shown, in Progress Report No. 92, to occur. The higher ethane yield in Case B is a result of a lower

TABLE 67. COMPARISON OF DATA FROM LIFE TEST 2903

CASE A

	Temp, F	Life Test Time, hr	B	C	K_c
2903-40	820	1340	10.0	59.0	6.7

CASE B

	Temp, F	Life Test Time, hr	B	C	K_c
2903-54	820	1820	13.1	36.2	7.4
55	820	1844	13.7	34.7	7.1
56	820	1870	13.0	32.2	6.7
58	820	1966	13.5	38.4	6.9
59	820	1990	12.9	34.3	6.7
60	820	2014	13.3	40.2	6.3
61	820	2038	13.5	32.6	6.8

CASE C

	Temp, F	Life Test Time, hr	B	C	K_c
2903-62	820	2110	7.0	5.9	6.7
63	820	2134	9.5	5.9	7.0
64	920	2158	10.3	5.9	6.8
65	920	2182	6.4	11.3	5.2
66	980	2206	4.6	16.5	4.3

mean H_2/CO ratio in the reactor. Under Case A conditions, H_2/CO ratios of 10 can occur before reconsumption of carbon dioxide. In Case B, however, the ratio remains between 2 and 3. Gas composition changes did not alter the ability to shift.

Case C data indicate further deactivation from sulfiding, which also tends, apparently, to retard the formation of higher hydrocarbons. Periods 64 through 66 show the effect of increased temperature on the conversion over the sulfided catalyst. The shift equilibrium constant is decreased by increasing temperature while the useful conversion of $(CO+H_2)$ is increased. As the temperature is raised, the ethane selectivity decreases since ethane is less favored, thermodynamically, at high temperatures.

With Test Sample 66, life test work with catalyst 2903 has been terminated temporarily. Results have been very encouraging and further work on catalyst 2903 has been planned.

Life Test 2904 has been initiated on a chromic oxide catalyst. Data will begin to be reported next month.

b. PEDU Program: Work continued on the methanation PEDU during the month of January.

(1) PEDU Status: Important items concerning the program are summarized below.

(a) Official approval to procure and construct the methanator was received on January 26, 1972, from the Office of Coal Research.

(b) Negotiations with Koppers were held to finalize the PEDU detail engineering program. A summary of the items requested of Koppers is found in BCR's letter of January 13, 1972, to J. F. Farnsworth. In early February, Koppers will be providing an engineering time schedule and cost breakdown for the detail engineering work.

(c) PEDU equipment specifications were reviewed and bid requests were mailed to vendors in January on a number of items.

(d) Specifications for the fluid-bed reactor were reviewed and finalized.

(e) The methanator instrumentation panel board sketch, as prepared by Koppers, was reviewed. Final changes in the drawing and of the bid specifications are currently being completed.

(f) Revised material balance and flow sheets are being prepared.

(g) The critical major items to be cleared during February are the following.

(i) Application for the necessary building and air pollution permits.

(ii) Completion of bid mailings. Koppers is currently developing the necessary sketches required to obtain bids on the remaining equipment items so that these can be solicited in February.

(iii) The transformer requirements for both PEDUs must be finalized, based on the gasification electrical needs.

(2) Cold Model Program: During the month, data collection in the cold model program began. The general concept of the program was outlined in Progress Report No. 3, pp. 177 to 180. Figure 84 shows the modeling apparatus.

(a) Catalyst Minimum Fluidization: The minimum fluidization velocities of two methanation catalysts were determined using bench-scale apparatus. The data were analyzed with the ERGUN[1] equation to determine consistency.

The apparatus used for the measurements consisted of a 1-inch ID by 2-foot pyrex tube. A porous plate gas distributor was used to contain the solids. Pressure drop measurements were obtained from a manometer, and the air flow rate was measured by a 100 cc bubble flow meter.

In the tests, known charges of catalyst were put in the tube and gas flow was adjusted. The pressure drop across the bed was determined along with the gas rate, and the data were analyzed.

Catalyst 2904: The minimum fluidization velocity data and bulk density at minimum fluidization for Catalyst 2904 are shown in Figure 85. Extrapolation of the fixed and fluidized regions resulted in a minimum fluidizing rate of 125 cc/min or, equivalently, 0.0135 ft per sec. The bulk density was determined as 56 lb per cu ft.

The ERGUN equation in the low Reynolds number region is given as the following:

$$U_{mf} = \frac{\rho_B g \, d_p^2}{100\mu} \frac{\varepsilon^3}{(1-\varepsilon)^2} \qquad (1)$$

where

U_{mf} = minimum fluidization velocity

ρ_B = bulk density = $\rho_S (1-\varepsilon)$

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[1] Ergun, S. CEP 48 p. 89, 1952

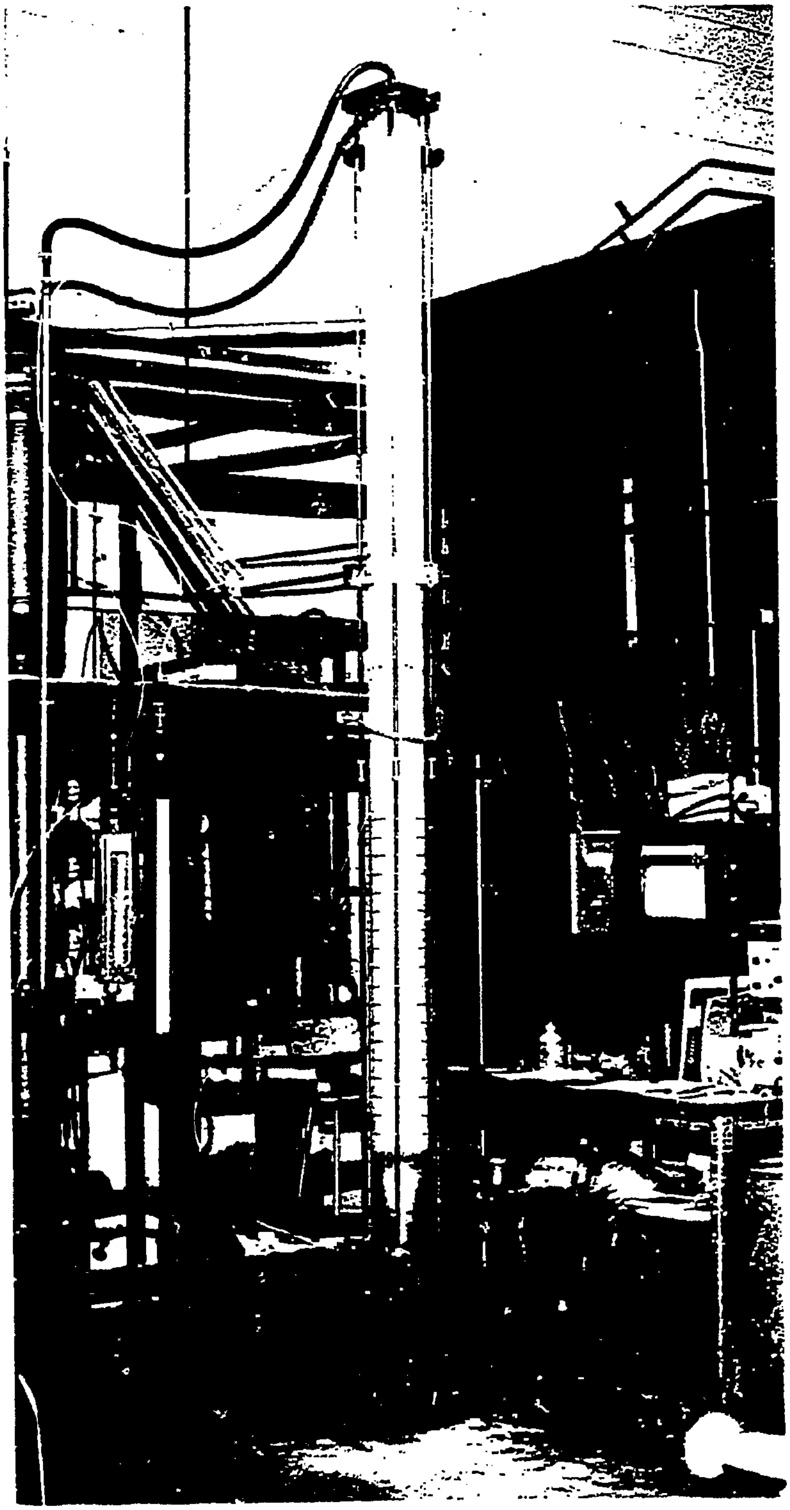

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Figure 84. Plastic Pipe Apparatus for Cold Model Program

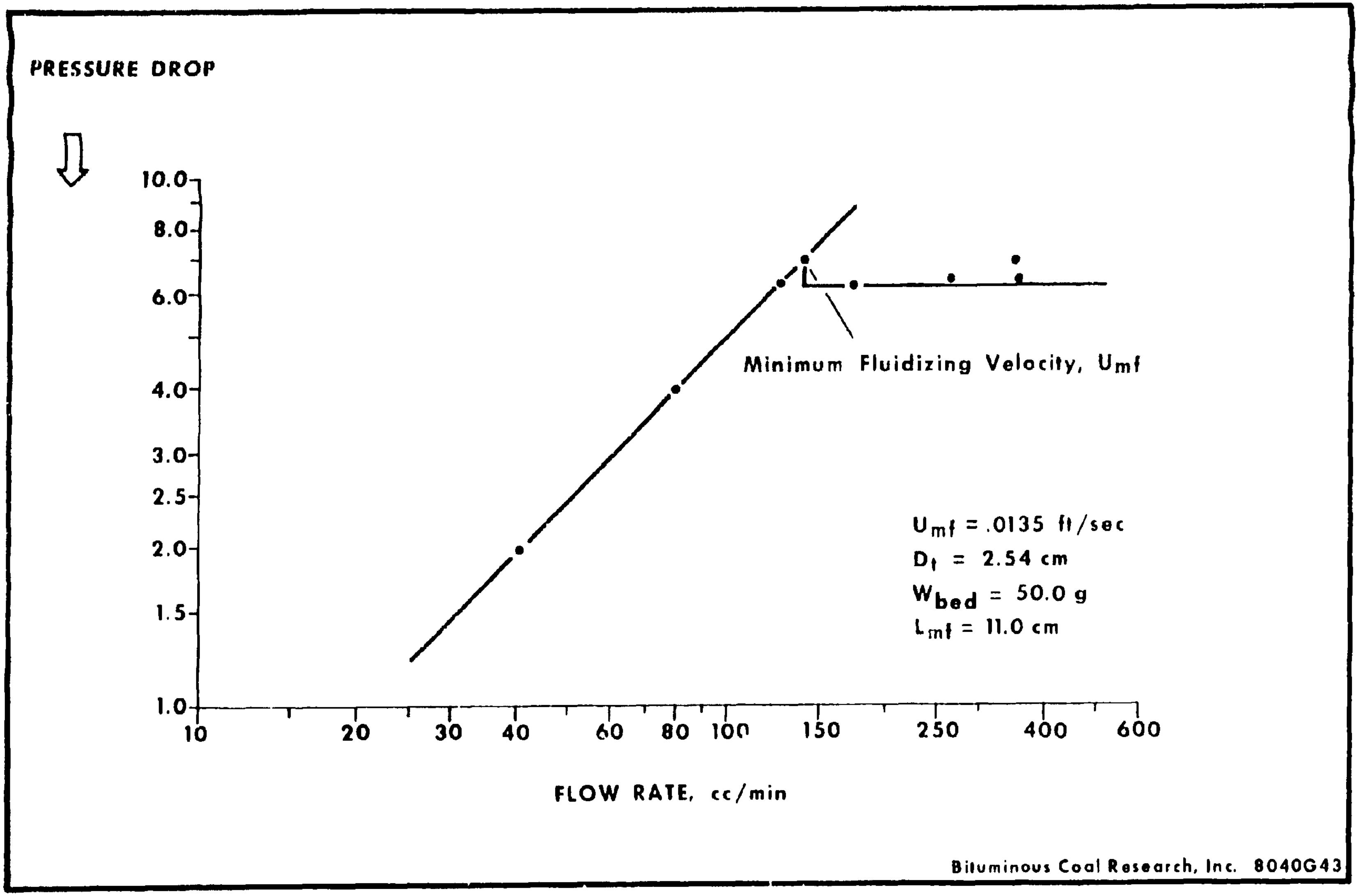

Figure 85. Minimum Fluidization Velocity for Chromic Oxide on Alumina Catalyst (BCR Lot 2904)

ρ_s = apparent particle density

g = gravitational constant

d_p = particle diameter

μ = viscosity

ϵ = voidage

It was assumed that the gas density was small compared to the solids density. The mean particle size was calculated from the expression:

$$\bar{d}_p = \frac{100}{\Sigma \text{ wt\%}/d_p}$$

Size data for catalyst 2904 are shown below along with the mean particle calculation. An average size for minus 325 mesh particles of 20 microns was used.

x, Wt %	d_p, microns	x/d_p
13.5	163	0.083
10.0	137	0.073
13.8	115	0.120
13.3	97	0.137
9.8	81	0.121
6.9	68	0.102
8.9	58	0.153
8.6	48	0.179
15.2	20	0.760
100.0		Σ 1.726

$$\bar{d}_p = \frac{100}{1.726} = 58 \text{ microns}$$

Physical property input data needed for the ERGUN equation are summarized as:

$\mu = 0.018\text{cp} = 1.21 \times 10^{-5}$ lb per ft sec

$g = 32$ ft per sec

$U_{mf} = 0.0135$ ft per sec

$d_p = 58$ microns $= 1.9 \times 10^{-4}$ ft

$\rho_B = 56$ lb per cu ft

Rearranging the ERGUN equation yields:

$$\frac{\epsilon^3}{(1-\epsilon)^2} = \frac{180 \mu \, U_o}{\rho_B g \, dp^2} \qquad (2)$$

or for the assigned values

$$\frac{\epsilon^3}{(1-\epsilon)^2} = 0.455 \qquad \epsilon = 0.49$$

This results in a solids density of

$$\rho_s = \frac{56}{0.51} = \underline{\underline{110 \text{ lb}}} \text{ per cu ft}$$

The reasonable voidage and solids density indicate that the ERGUN equation can be extrapolated to PEDU conditions. In the PEDU, one can expect a gas viscosity of 0.023 cp. Taking a ratio of Equation 1 from model to PEDU conditions yields a minimum fluidization velocity of

$$U_{PEDU} = U_{model} \frac{\mu_{model}}{\mu_{PEDU}} = 0.0135 \times \frac{0.018}{0.023}$$

$$U_{PEDU} = 0.0105 \text{ ft per sec}$$

Catalyst 2903: The same procedure was applied to the molybdenum catalyst 2903. Data are shown in Figure 86 and are summarized as follows:

$\mu = 1.21 \times 10^{-5}$ lb per ft sec

$g = 32$ ft per sec^2

$U_{mf} = 0.0065$ ft per sec

$d_p = 43$ microns

$\rho_B = 38$ lb per cu ft

x, Wt %	d_p	x/d_p
3.2	149	0.021
3.0	115	0.026
10.5	97	0.108
10.3	81	0.127
12.9	68	0.190
16.9	58	0.292
19.9	48	0.415
23.3	20	1.160
		2.339

$\bar{d}_p = 43$ microns

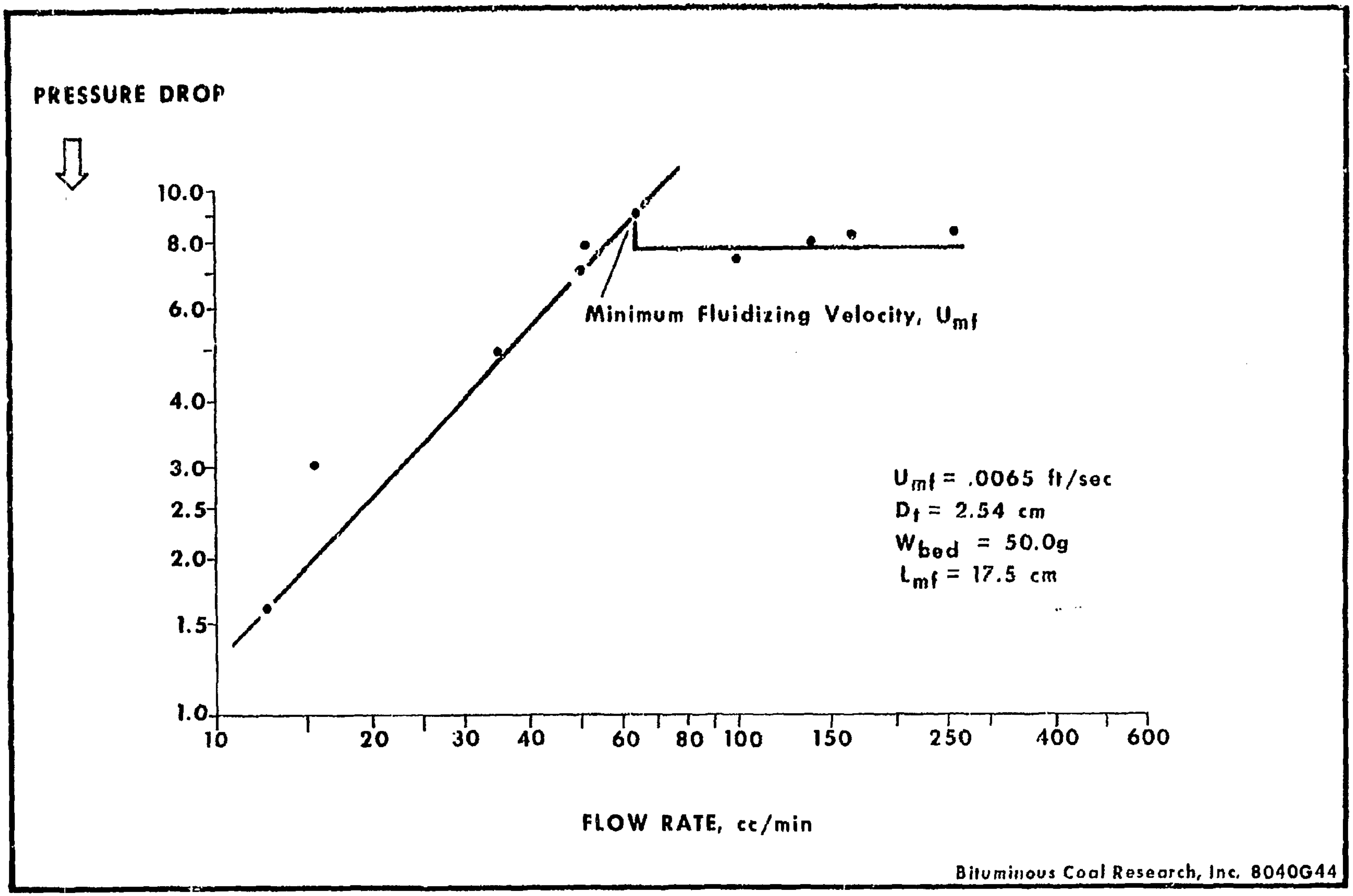

Figure 86. Minimum Fluidization Velocity for Molybdenum Oxide on Alumina Catalyst (BCR Lot 2903)

for these values:

$$\frac{\varepsilon^3}{(1-\varepsilon)^2} = 0.636 \qquad \cong 0.53$$

This results in an apparent solids density of

$$\rho_s = 81 \text{ lb per cu ft}$$

(b) Fluidization of Sand with Freon: The minimum fluidizing velocity of a sand mixture was determined using air. The gas distribution plate consisted of three 0.050 orifices drilled on a 0.5-inch radius at 120 degree intervals. Calculations had suggested this design for the air-sand system. Data for the fixed and fluidized regions are shown in Figure 87. Extrapolation of these regions yields a minimum fluidization velocity of 0.02 ft per sec for sand.

For the Freon-sand system, a gas distributor was designed which would permit operation in the range of 2 to 6 times minimum fluidization. This distributor was based on the criteria set forth by Kuni and Levenspeil. Basically this states that:

$$U_{OR} = (0.33 - 0.85) \frac{(2\, g_c\, \Delta P_{BED})}{\rho_g}$$

where

U_{OR} = orifice hole velocity

ΔP_{BED} = bed pressure drop

ρ_g = gas density

g_c = gravitational constant

For the 0.125 inch orifice specified by this relation, the following data were calculated:

Freon Pressure, psig	U/U_{mf}	Jet Penetration, Inches
45	2.3 - 5.9	0.4 - 7.5
55	2.1 - 5.5	1.1 - 8.0
65	2.0 - 5.1	1.6 - 8.9

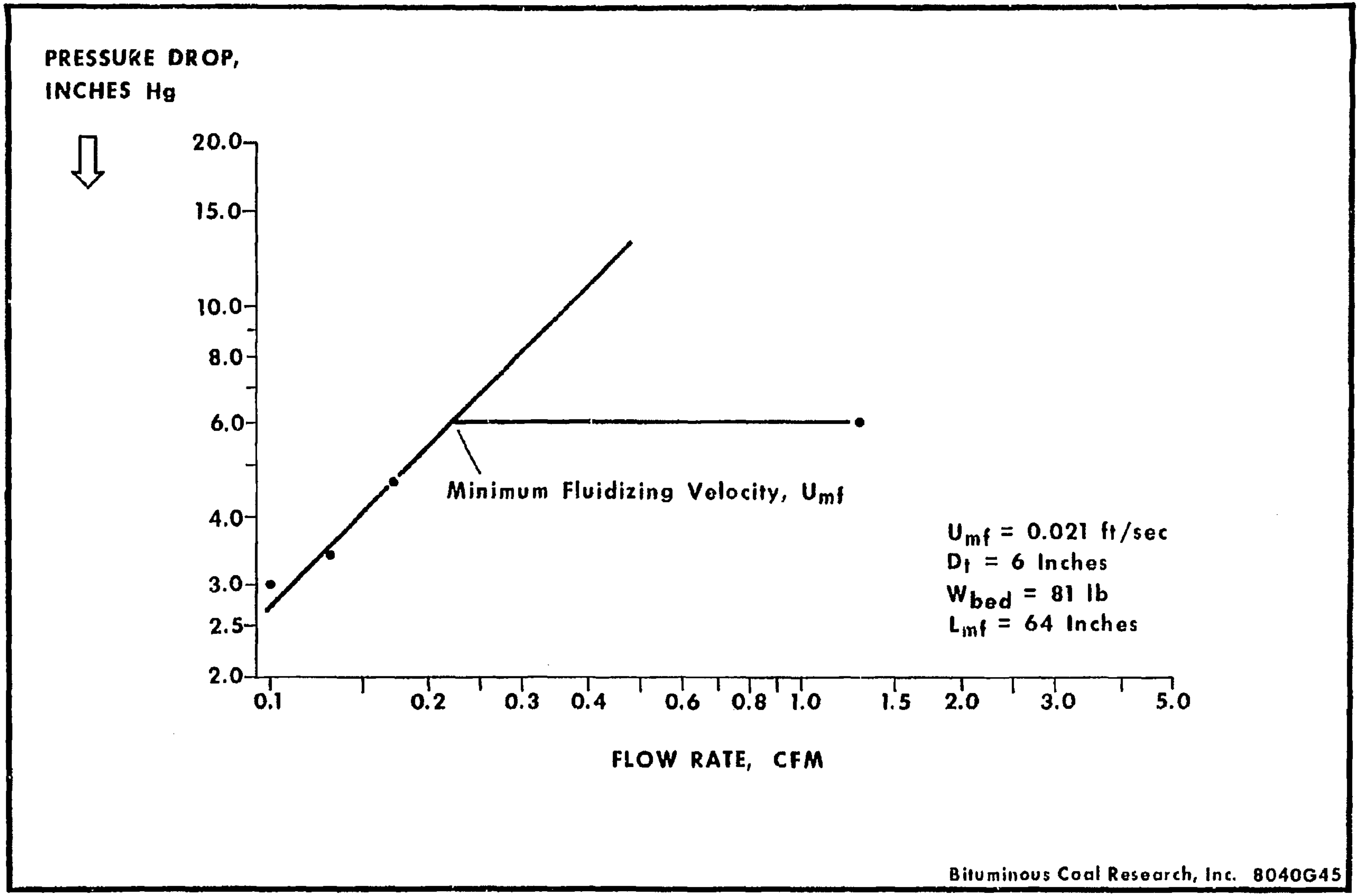

Figure 87. Minimum Fluidization Velocity of Air-Sand System for Methanation Cold Model Studies

Several test runs were conducted with air at atmospheric pressure and with compressed freon. From visual observations, the quality of the fluidization with compressed freon was much better than with air at similar conditions. Bed height fluctuation was considerably less at non-slugging conditions in the case of dense freon. The data for the tests conducted to date are given in Table 68.

TABLE 68. RESULTS OF COLD MODEL FLUIDIZATION STUDIES

Gas Pressure, psig	U/U_{mf}	ρ_s/ρ_g	Comments
	Air Studies		
0	4.6	2,200	
0	6.3	2,200	Slugged Violently
	Freon Studies		
45	1.33	120	
45	1.76	120	
38	2.48	133	
32	3.52	153	
21	5.10	200	
16	6.10	250	Onset of slugging

From Table 68 it is apparent that at a solids-to-gas density ratio of 200, and 5 times minimum fluidizing velocity, good fluidization is occurring. In the PEDU, that density ratio will be lowered to about 100. Thus, at these conditions slugging will not be a problem in the PEDU.

Further tests and more detailed data analysis will be presented in a following report.

c. Other Work

(1) Status of BCR Suggestion 193: A preliminary report has been submitted and a detailed literature search is underway.

(2) Status of BCR Suggestion 194: A formal report has been submitted.

d. Future Work. Work will continue according to the gas processing schedule during the coming month.

At the bench-scale level, fluidization tests of molybdenum and chrome catalysts will be conducted. Life testing of chrome oxide catalyst will continue.

PEDU work will continue. Bids on equipment will be solicited. Koppers will pursue the detail engineering and scheduling of the PEDU work. Necessary permits for construction will be applied for.

PEDU model studies will continue.

4. Analytical Services (J. E. Noll): During the past month, 27 samples were analyzed by gas chromatography and two samples by special procedures. The manner and type of analyses requested were as follows:

Type of Analysis Requested	No. of Samples Analyzed
Gas Chromatography	
Methanation Unit	
Gas Samples	25
Liquid Samples	2
Special Procedures	
Apparent particle density for fluidization	2
Total	29

5. Gas Chromatographic Procedures (J. E. Noll): No work was required in this area during the past month.

Future Work: Performing sample analyses is the only work planned.

B. Stage 2 Process and Equipment Development Unit--100 lb/hr (R. J. Grace, E. E. Donath, and R. L. Zahradnik)

During the month, time was distributed between preparation and editing of the bid packages for the multipurpose research pilot plant facility (MPPF) for the bidder's conference on January 19, 1972; supervision of final dismantling operations of the Stage 2 PEDU; rechecking revised, alternate reactor design for 5 tph pilot plant submitted by Foster Wheeler Corporation: and preparation of the final summary report, Phase II, Process and Equipment Development.

1. Inspection of Stage 1 Cooling Coils and Refractories: Initial inspection of Stage 1 components was discussed and illustrated in Progress Report No. 4 for December 1971. Portions of Stage 1 refractories, (HBW Korundal) were removed along with a section of the Stage 1 cooling coils. These materials were delivered to Dr. J. Bialosky, Metallurgical Laboratory, Koppers Co., on January 10, 1972 for inspection and analysis. Figure 88, "Section of cooling coil from Stage 1, after Test 58" shows the area of Stage 1 from which the cooling coil section was removed.

Report of Koppers Co. findings will be given in next month's report.

2. Status of Phase 2 Summary Report: Review of the original rough draft of the Summary Report, with additions and suggestions by Dr. Zahradnik, was completed on January 18, 1972.

Concentrated effort will be made to complete the draft by early February.

3. Shipment of Surplus Items from 100 lb/hr PEDU: Several items of the 100 lb/hr PEDU were declared surplus and were requested by the University of Utah. These items, the star-wheel feeder and the Petrocarb coal feeder, and associated equipment are listed and identified by BCR and OCR numbers in Table 69. They were shipped on January 13, 1972.

TABLE 69. SURPLUS ITEMS SHIPPED TO UNIVERSITY OF UTAH FROM CONTRACT 14-32-0001-1207 100 LB/HR PEDU

January 18, 1972

Item	BCR No.	OCR No.
Star wheel feeder	5545	28979
Emery weighing unit consisting of 1 Foxboro transmitter 3 weigh cells 1 totalizer 1 air regulator 1 dial reading 0 to 1200	5318	2566
Petrocarb coal feeder	5627	26850
Dollinger filter	5369	26610
Coal feed tank	5414	28919
Flowrator	5393	28921

8016P266

Figure 88. Section of Cooling Coil from Stage 1, after Test 58

4. Future Work: Future work will include:

a. Necessary work to expedite final dismantling of the 100 lb/hr FEDU.

b. Attendance at meeting for AGA Materials Evaluation Program and necessary associated work.

c. Report of Koppers Co. findings relative to inspection of Stage 1 coils and refractories.

d. Evaluation and design modification for components of 5 tph MFRF.

e. Completion of draft of Phase II Summary Report.

C. Cold Flow Model Experiments--5 ton/hr Two-stage Gasifier (R. J. Grace, J. E. Noll, R. D. Harris, R. L. Zahradnik, and E. E. Donath)

Work during the month proceeded mainly on the characterization of FEDU chars, and the work outlined in the schedule presented in Progress Report No. 92, page 3912, was consequently delayed.

The model studies to be carried out in the following months are expected to indicate both the location and size of nozzles and the shape of the reactor which will avoid excessive localizing of temperatures near the reactor walls. Stages 1 and 2 of the gasifier are to be studied independently at first, followed by tests of the two stages together.

The Stage 1 studies have been divided into three phases, now underway: (I) single-burner tests, (II) multiple-burner tests, and (III) multiple-burner tests plus simulated slag. The experimental requirements for the third phase are considered to be more difficult than those for the other phases. Provisional Phase III work is therefore being undertaken to solve some of the experimental problems so that Phase III data can be obtained immediately following Phase II tests.

The Phase II and III studies for Stage 1 of the two-stage gasifier were proceeding as planned and satisfactorily when it appeared expedient to review some of the assumptions on steam and char flow rates.

The Phase I model studies carried out so far were based on utilizing a 100 ft/sec velocity in the steam-char lines. Recent computer studies indicated that optimum pilot plant operation might well require a higher-than-anticipated burden of recycle char and hence a higher rate of char feed to Stage 1. These studies also indicated that optimum pilot plant operation might require a lower-than-anticipated steam rate to Stage 1. The results of these changes suggested that operation with a higher char packing of the steam-char lines could be expected.

In consequence, it was decided that it might be expedient to feed the steam-char mixture at 30 to 40 ft/sec instead of the planned 100 ft/sec. When considering these problems, it became evident that the FEDU chars, with apparent bulk densities as low as 10 lb/cu ft, were probably unusually cellular and might in fact be readily transportable even when tightly packed. It was also considered that the PEDU chars might be unusually reactive, thus reducing the need for high rates of recycle. (It was assumed that 60 percent of the char would be consumed as it passed through Stage 1).

It was therefore decided to analyze the physical properties of chars from three PEDU tests. Chars from PEDU Test 54 (lignite), PEDU Test 23 (Elkol sub-bituminous), and PEDU Test 27 (Pittsburgh seam high volatile bituminous) were selected for analysis.

1. Characterization of Selected PEDU Chars

a. Size Analysis: The size of the feed coals used in Tests 54, 23, and 27 were previously reported. These sizes are repeated in Table 70. The size of representative samples of the PEDU chars were also previously reported; additional samples were obtained for further study. The size distribution of these fractions is also given in Table 70. The cumulative size distributions were also plotted to obtain the "50 percent oversize size by weight" and the "size distribution coefficients"[1] shown in Table 70.

b. Bench-scale Fluidization Tests: Samples of PEDU char were fluidized in a 1-inch diameter laboratory unit. The fluidization tests were conducted to obtain graphically the velocity of minimum fluidization and to derive the bulk density at minimum fluidization and the particle density. The fluidization results for PEDU Test 27 scrubber char were shown in Figure 76 of Progress Report No. 4. Figure 89 gives results for the chars obtained in PEDU Tests 54 and 23.

The data derived from the fluidization tests are summarized in Table 71. The calculated particle densities were obtained by solving for ρ_p in the following equation:

$$V_{mf} = \frac{g(\rho_p-\rho_g)\left(\frac{(\rho_p-\rho_s)^2}{\rho_p}\right) D_p^2}{150\ \mu_g\ \frac{(1-\rho_p-\rho_s)}{\rho_p}}$$

Where V_{mf} = velocity at minimum fluidization, cm/sec
μ_g = gas viscosity, centipoise
ρ_p = particle density, g/cc
ρ_s = particle bulk density, g/cc
ρ_g = gas density, g/cc
D_p = particle mean diameter, cm

The expression given on page 233 of Progress Report No. 4 used an unjustified simplification.

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1 Landers, W. S. and Reid, W. T. "A Graphical Form for Applying the Rosin and Rammler Equation to Size Distribution of Broken Coal" U.S. Bureau of Mine I. C. 7346 1946.

TABLE 70. SIZE DATA ON FEED COALS AND CHARS FROM LISTED PEDU TESTS

Test No. / U.S. Sieve Size	PEDU FEED COALS, Percent		
	54(a)	23(b)	27(c)
+ 50	0.3	2.7	4.8
+ 100	25.1	26.2	36.3
+ 200	66.6	67.5	75.3
+ 325	81.1	85.7	92.3
50% Size, mm	0.098	0.105	0.125
Distribution Coefficient	1.56	1.58	1.64

Test No. / U.S. Sieve Size	PEDU CHARS, Percent		
	54(d)	23(d)	27(e)
+ 16	--	0.2	10.4
+ 30	0.3	3.0	41.6
+ 50	1.6	25.4	74.9
+ 100	17.4	67.0	93.6
+ 200	53.9	87.2	97.8
50% Size, mm	0.076	0.215	0.56
Distribution Coefficient	1.36	1.57	1.70

(a) Progress Report 92, Table 1048, p 3834 (b) Progress Report 79, Table 784, p 3044 (c) Progress Report 82, Table 804, p 3132 (d) Settling Tank product (e) Scrubber product

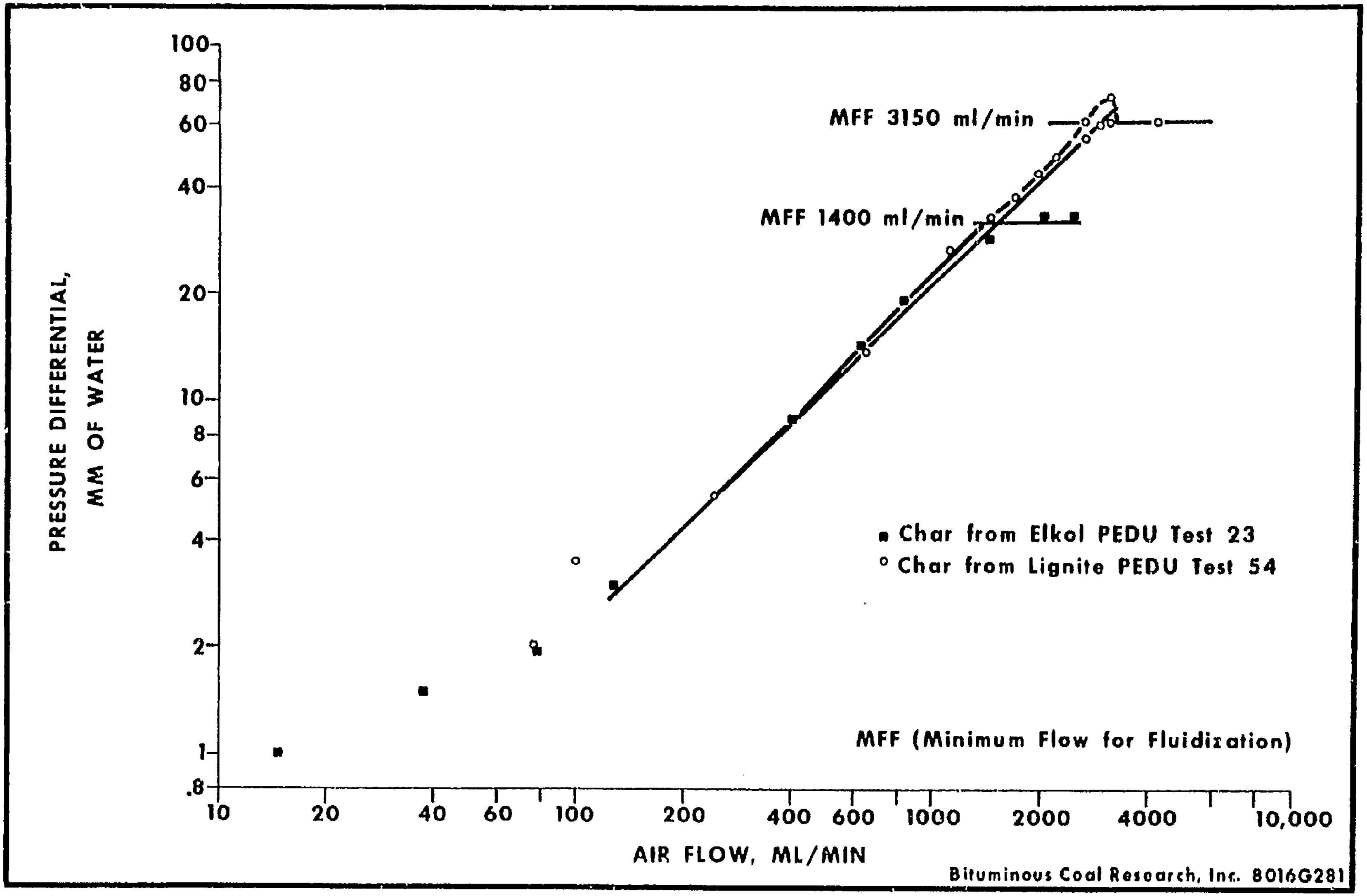


Figure 89. Pressure Differential across Fluidizing Bed as a Function of Air Flow for Chars from PEDU Test 23 (Elkol) and PEDU Test 54 (Lignite)

TABLE 71. PROPERTIES OF CHAR SAMPLES OBTAINED FROM TESTS IN 1-INCH FLUIDIZER

PEDU Test No.	Av. Particle Size, mm	Bulk Density At Rest lb/cu ft	Minimum Fluidization Bulk Density lb/cu ft	Minimum Fluidization Velocity ft/sec	Calculated Density lb/cu ft
54	0.076	28.3	11.3	0.33	73.5
23	0.215	6.0	6.4	0.14	19.3
27	0.56	9.4	7.7	0.38	34.6

c. Elutriation Tests: Calculated densities of the order of 20 to 35 lb/cu ft are hard to substantiate using liquid or air pycnometers. To substantiate the density data given in Table 71 samples were run in a 3-inch diameter air elutriator. A photograph of the laboratory elutriator is shown in Figure 90.

The elutriator consists of a 3 inch diameter, 4 ft long air-blown column. A weighed charge is placed in the unit and a metered air flow is admitted through the base. The air flow is adjusted until a desired fraction of the feed is elutriated and collected in the bag attached to the elbow at the top of the elutriator. The sample elutriated at the given flow rate is collected, weighed, and screened. The procedure is repeated at a number of higher air rates.

The results of the elutriation tests with the three test chars are plotted in Figure 91. These data substantiate the low density data given in Table 71. For example, 87 percent of the 2.66 to 3.10 cfm cut of Elkol char (PEDU Test 23) was coarser than 100 mesh (0.0149 cm) and finer than 50 mesh (0.0297 cm). Assuming a 0.022 cm mean size, a 19.3 lb/cu ft density (0.390 g/cc) at a 30.8 cm/sec lifting velocity was calculated using the Stokes law formula below:

$$v = 35.0 \frac{(\rho_p - \rho_a)}{\rho_a} d^2 (v^{-1})$$

where ρ_p = particle density
ρ_a = air density
d = particle diameter
v = kinematic viscosity

The average air flow of 2.88 cfm for the above cut corresponds to a 30.0 cm/sec lifting velocity.

d. Reactivity Tests: Reactivity studies were started with PEDU Test 27 char in the BCR thermo-gravimetric balance (TGA) using steam as the reacting gas or carbon dioxide at 900, 1000, and 1100 C. The data will be reported in later reports under "Laboratory-scale Process Studies." These studies will be delayed approximately one month while the recording unit is being rebuilt or replaced.

However, on the basis of the tests run to date, it has been tentatively concluded that the PEDU char is comparable in reactivity to FMC chars previously studied. Under laboratory conditions, the rate of reaction was found to be

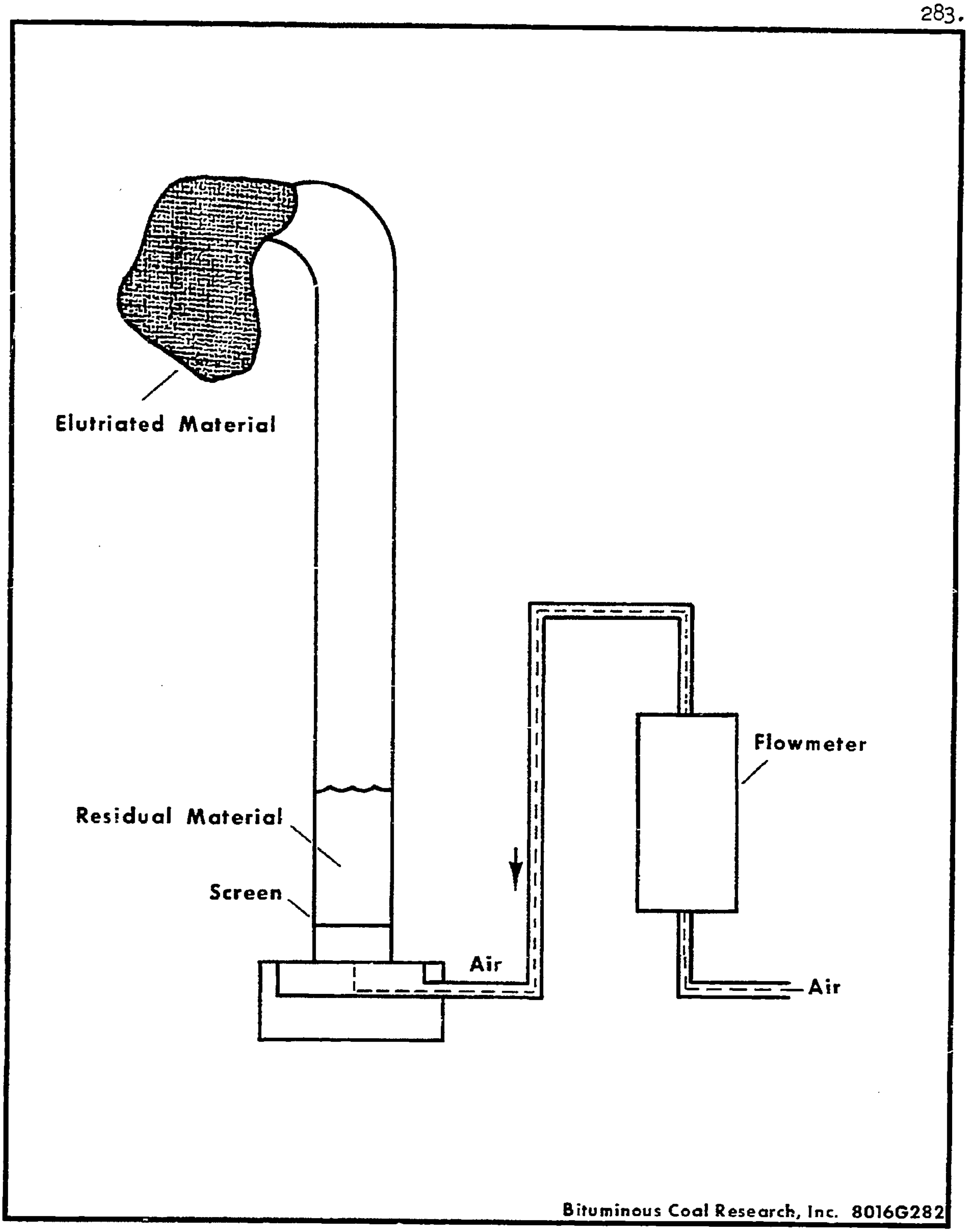


Figure 90. Three-inch Diameter Laboratory Air Elutriator

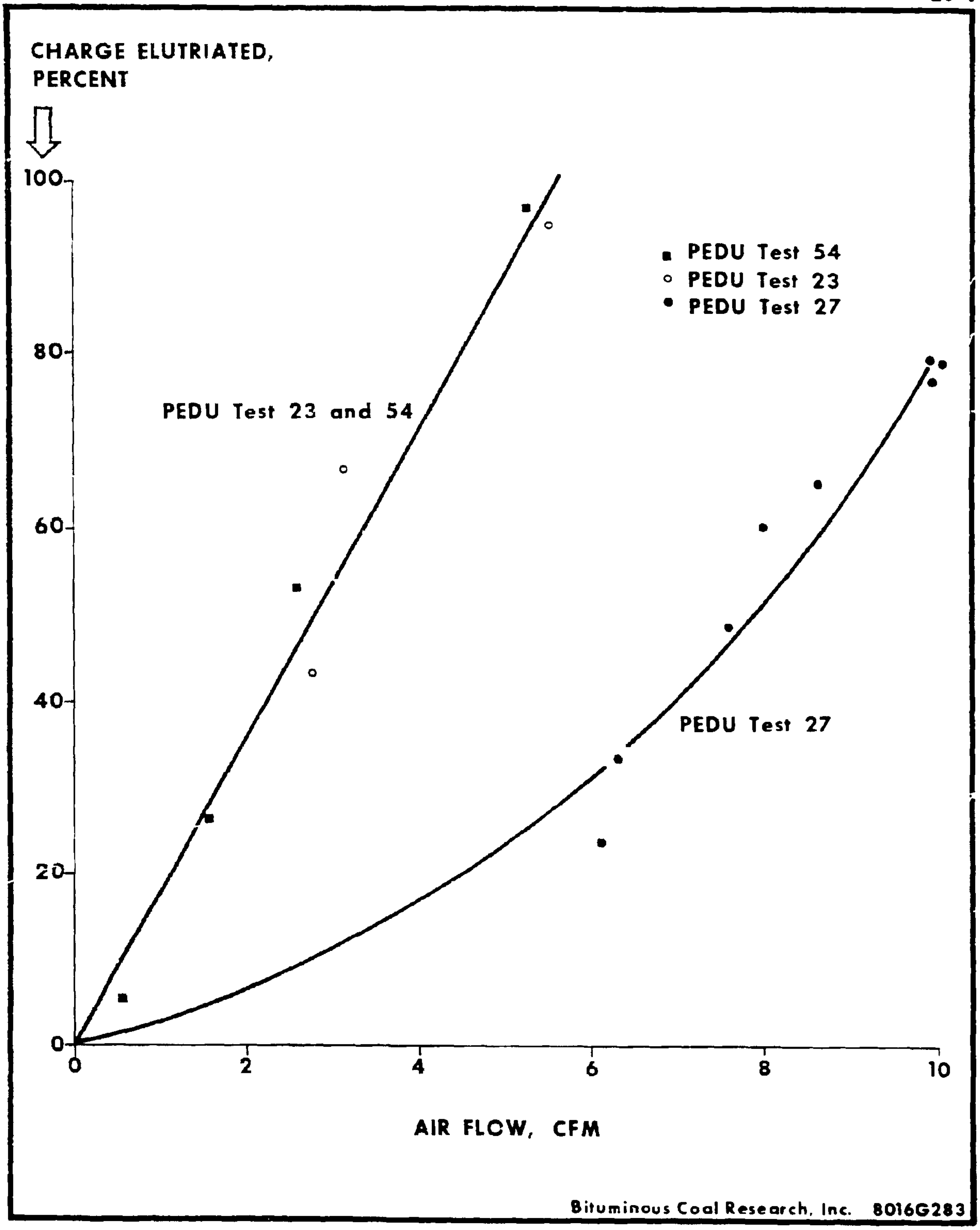


Figure 91. Air Elutriation Tests with Three PEDU Chars

independent of particle size. The laboratory data extrapolated to the expected Stage 1 operating temperature and pressure suggest that the Boudouard Reaction, $C + CO_2 \rightarrow 2CO$, may be more rapid that the steam-carbon reaction, $C + H_2O \rightarrow CO + H_2$.

e. Discussion of Results: The char produced in the PEDU tests with Pittsburgh seam coal was coarser than expected. It would appear, however, that this size will not be a deterrent to operation so long as the larger char particles are significantly smaller than the feed lines. Larger char particles should be more readily removed from the gas stream and should be more readily de-entrained from the gas stream in Stage 1. However, the reaction time in Stage 1 should be relatively independent of particle size. Therefore, larger particles in the char recycle should reduce the amount of char in the gas fed to Stage 2.

2. Future Work: Early in February, work will start again on Phases II and III of the cold flow model study. The equipment will be modified to run at various outlet gas rates.

D. Data Processing (R. K. Young and D. R. Hauck)

1. Commercial Gasifier Modeling: A calculational scheme for determining the Stage 1 gasifier temperature was described in Progress Report No. 4. This scheme included the determination of the oxygen rate by graphic relationship between methane yield and oxygen requirements for 0 percent and 25 percent char withdrawl. The information contained in this graph has been defined in equation form to allow easier determination of oxygen requirements at any desired char withdrawl rate. The expressions for West Kentucky No. 11, Pittsburgh seam, lignite, and Elkol coal are as follows:

West Kentucky No. 11 (1700 F exit temperature)

$$\frac{\text{lb } O_2}{\text{100 lb daf coal}} = 74 - 111\, Y_{CH_4} - 90.2\, WD(1 - Y_{CH_4} - Y_{CO})$$

Pittsburgh Seam (1700 F exit temperature)

$$\frac{\text{lb } O_2}{\text{100 lb daf coal}} = 81.5 - 115\, Y_{CH_4} - 94\, WD(1 - Y_{CH_4} - Y_{CO})$$

Lignite (1600 F exit temperature

$$\frac{\text{lb } O_2}{\text{100 lb daf coal}} = 68.3 - 97\, Y_{CH_4} - 78.7\, WD(1 - Y_{CH_4} - Y_{CO})$$

Elkol (1700 exit temperature)

$$\frac{\text{lb } O_2}{\text{100 lb daf coal}} = 67 - 103\, Y_{CH_4} - 82\, WD(1 - Y_{CH_4} - Y_{CO})$$

where:

$WD < 1$ (char withdrawl factor)

$Y_{CH_4} < 1$ (methane yield)

$Y_{CO} <$ (Stage 2 carbon-oxides yield)

Note: Equations are accurate to $\pm$ 1 lb of O_2

As indicated in Progress Report No. 4, the write-up of the calculational scheme presently utilized in computer program GASIFY was completed, and is included in this report as Appendix B.

2. Automated Data Acquisition: Delivery of the PDP8/E computer and peripherals is expected in e[illegible]ly February 1972.

3. Particle Density Calculation: A program was written for the Hewlett-Packard calculator to solve the Ergun Equation (see Section II. A. 2) for particle density. The solution is found by an iterative procedure known as the Newton Method.

4. Future Work: Plans for the next report period include:

a. Set up PDP8/E computer and peripherals

b. Generate simulation runs with subroutine GASIFY as required

E. Engineering Design and Evaluation

1. BI-GAS Process: The graphical methods described in Progress Report No. 4 for determining Stage 1 oxygen were defined in equation form to allow easier determination of oxygen requirement at any desired char withdrawal rate. These equations were described in Section II. D. 1. of this report.

A complete description of the commercial gasifier simulation program (Subroutine GASIFY) has been included as Appendix B of this report.

2. OCR/BCR Gasification--Power Generation: No discussions or inquiries were received during the month concerning this application of the two-stage gasifier.

F. Multipurpose Research Pilot Plant Facility (MPRF)

As mentioned last month, the Engineering Bid Package for the 5 ton/hr oxygen-blown system (BI-GAS Process) and the MPRF general facilities, was mailed to prospective bidders on December 29, 1971, after having been revised on December 17, 1971. A Bidders' Conference was held at the BCR laboratory on January 19, 1972, to answer any questions each company might have. A transcript of the meeting will be mailed to each of the prospective bidders.

Volume VI, Bid Package Cost Estimate, of the Process Engineering Bid Package, dated January 14, 1972, was received from Koppers. By letter dated January 18, 1972, a copy of Volume VI was transmitted to OCR. Submission of Volume VI of the bid package completes the assignment of Koppers under Part A, Step (a) of their current contract.

1. AGA Materials Evaluation Program: A report was written by the Subcommittee Work Group for the AGA Materials Evaluation Program based on areas common to each of the three coal gasification processes sponsored by OCR. Ten copies were sent to Mr. W. R. Hulsizer of International Nickel Company, Inc., New York, N. Y., for distribution to various members of the Task Group on Materials Design Data for Coal Gasification Process Equipment. The report prepared by the subcommittee will be reviewed by each Task Group member; it will be the basis for formulating the programs which are the main objective of the Task Group meeting set for January 26, 1972, at the Pittsburgh Airport Hotel, Pittsburgh, Pennsylvania.

2. Model Status. The process pilot plant model (1/4 inch = 1 foot) and the overall site model (1 inch = 20 feet) were completed and delivered to BCR on January 17, 1972. Photographs of the process pilot plant model will be sent to each prospective bidder.

3. Desk Top Model: At the request of OCR, BCR is proceeding to obtain quotations for a desk top scale-model of a 250 MM scf/day SNG plant, 1/32 inch = 1 foot, maximum size of 4 x 6 feet, based on process design as given in the Air Products report entitled "Engineering Study and Technical Evaluation of the Bituminous Coal Research, Inc. Two-stage Super Pressure Gasification Process," (OCR R & D Report No. 60). Authorization to request purchase of this model was given in OCR letter dated January 24, 1972.

G. Literature Search (V. E. Gleason)

Annotated literature references completed during the month are listed in Appendix C.

H. Other

1. Prime Contract Matters: Additional surplus equipment lists are being compiled and will be submitted in February. Early action is requested for the list submitted in September, as well as the lists to be submitted, because of limited storage facilities.

By letter dated January 12, 1972, Mr. Howard E. Thunberg requested BCR to submit details regarding estimated costs for fiscal years 1972 and 1973 under Contract 14-32-0001-1207 for his use in submitting a statistical report to the National Science Foundation. This information was transmitted to OCR on January 24, 1972.

2. Outside Engineering and Services: Koppers continues to provide engineering assistance as required and as reported in their Progress Report No. 30 in Appendix D.

Action by OCR on the request for approval of proposed Amendment No. 7 to Subcontract No. 2, signed by Koppers and submitted to OCR on October 20, 1971, has not been received.

3. Brigham Young University: The project entitled "Study of High Rate, High Temperature Pyrolysis of Coal" with joint funding by Brigham Young University and BCR is now in its tenth month. Figure 92, Monthly Progress Chart, Expenditures, shows the current budget status. The letter report of progress by BYU is as follows:

During January, the principal efforts have been devoted to setting up the new gas chromatograph and making it operational. New columns have been prepared and are being calibrated for use with this equipment.

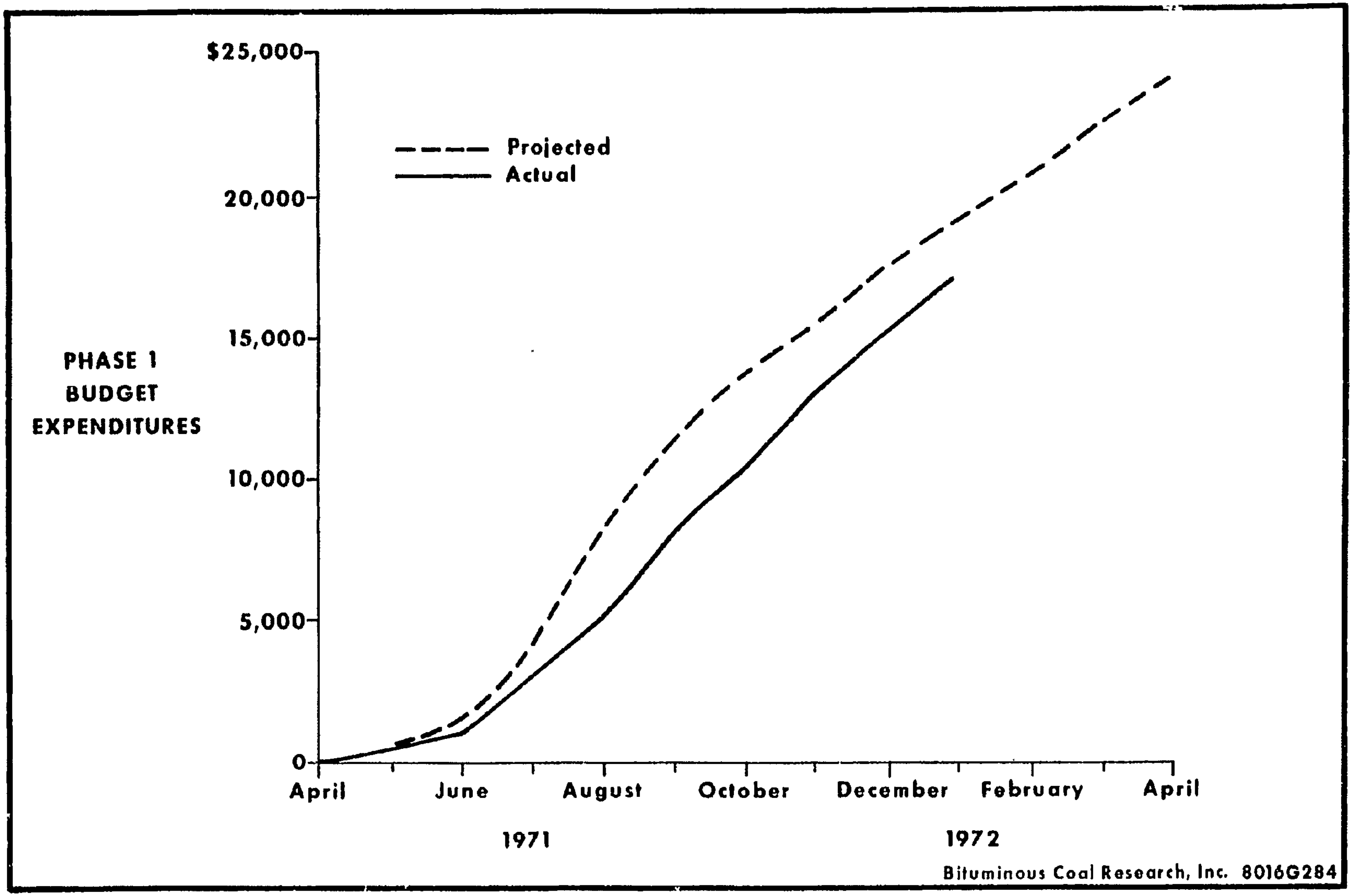


Figure 92. Monthly Progress Chart, Expenditures, Brigham Young University

The Aremcolox machineable ceramic parts in the reactor were replaced with alumina and graphite. These parts, which were located at the point where coal is injected and at the two points where gas samples are withdrawn, had cracked during initial testing. Three test firings with the new parts have shown they function satisfactorily.

A filter is required for the reactor effluent sample collection bottle. This is necessary to trap the fine particles that are not absorbed by the quench water. Porous ceramic filter elements have been ordered for this purpose.

A small fluidizer unit has been designed and fabricated to replace the present auger device in the coal feed line since the latter device does not feed the coal particles uniformly.

4. FPC National Gas Survey - Economics of Manufacturing SNG From Coal: The Synthetic Gas-Coal Task Force, organized by the Federal Power Commission, held a meeting on December 16 and 17 for the purpose of compiling an economic basis which could be used to improve the consistency of cost estimates for the manufacture of SNG from coal.

An evaluation method was developed based upon discussions with individuals who were designated as technical representatives of the Task Force members. Details of the method were presented in the attachments to the letter of January 7, 1972 by T. Kalina.

Using the evaluation method developed by the Synthetic Gas-Coal Task Force, BCR was asked to prepare a report for gas cost estimates for the manufacture of SNG from coal using the BCR/OCR BI-GAS Coal Gasification Process to produce 250 MM scf/day of pipeline gas. As a basis for a commercial plant, the Air Products report was used to calculate investment, operating costs, and gas price information for two coal prices at 15 cents/MM Btu and 30 cents/MM Btu for start-up dates of mid-1971, mid-1975, and mid-1980. These results will be presented in a BCR report and distributed on or about February 1, 1972, to the Synthetic Gas-Coal Task Force for review.

5. Reports and Papers: The paper entitled "Gasification of Lignite by the BCR Two-stage Super-pressure Process," by R. J. Grace, R. A. Glenn, and R. L. Zahradnik was published in the January, 1972, issue of Industrial and Engineering Chemistry Process Design and Development.

R. A. Glenn presented a talk on the status of the BCR/OCR BI-GAS Process at a meeting of the Cleveland Engineering Society, Power Plants Division, in Cleveland, Ohio, on January 4, 1972. A similar talk will be presented by J. W. Tieman on March 23, 1972, at a regional meeting of the Air Pollution Control Association in Buffalo, New York.

6. Patent Matters. Worthwhile ideas continue to be written up as invention disclosures for submission to OCR for consideration.

a. CCR 866 and OCR-1078: A U.S. patent application based on the new process concept (E. E. Donath, December 11, 1970) has been filed and given Serial Number 182,652. The application, entitled "Gasification of Carbonaceous Solids," contains nine claims. As reported last month, the appropriate document assigning rights to the U.S. Government was filed with the patent application on September 22, 1971. BCR has applied for and received a license for foreign filing, and documents have been prepared for filing applications in the following foreign countries: India, Japan, West Germany, France, South Africa, Australia, Great Britain, and Canada.

Confirmatory license to the government was executed by BCR and returned to Mr. Ernest Cohen, Assistant Solicitor, Branch of Patents, under date of January 12, 1972.

b. New Invention Disclosures: Formal Invention Disclosures (Form DI-1217) for six individual BCR suggestions were submitted to OCR on May 7, 1971. These were listed in Progress Report No. 1

Inasmuch as 90 days have elapsed since the submission of these disclosures, in accordance with the patent clause under Contract 14-01-0001-324, BCR is proceeding, as reported last month, to develop patent applications for filing in the U.S., first obtaining the approval of the Solicitor's Office. Action taken on these disclosures is as follows:

(1) OCR-1859: This invention disclosure (BCR Suggestion 178) was submitted to OCR on May 7, 1971. In reviewing this disclosure, entitled "Low-sulfur Char from Coal Gasification," it was decided to combine it with OCR-1078, "Gasification of Carbonaceous Solids," the application for which has already been filed. No further action is required on this disclosure.

(2) OCR-1860 and OCR-1861 As stated last month, OCR Disclosures 1860 and 1861 have been combined into a single patent application entitled "Two-stage Gasification of Pretreated Coal." A copy of this application was mailed to Mr. Howard Silverstein, Branch of Patents, on December 6, 1971, for his review and authorization for filing by BCR. The appropriate document assigning rights to the government has been prepared.

By letter dated December 28, 1971, Mr. George Fumich authorized BCR to file a foreign patent application on the subject invention. This letter was signed by John W. Igoe and returned to Mr. Fumich under date of January 11, 1972, agreeing that BCR will file and prosecute applications, the government will pay the patent filing and issue fees. Other expenses incurred by BCR, including preparation and prosecution of applications, are non-reimbursable. Confirmatory license will be prepared after application is filed in U.S. Patent Office and serial number is received.

(3) OCR-1862: As stated last month, a U.S. patent application has been prepared on disclosure OCR-1862 entitled "Three Stage Gasification of Coal." A copy of this application was sent to Mr. Howard Silverstein,

Branch of Patents, on December 13, 1971, for his review and authorization for filing by BCR. The appropriate document assigning rights to the U.S. Government has been prepared.

By letter dated December 28, 1971, Mr. George Fumich authorized BCR to file a foreign patent application on the subject invention. As stated above, this letter was signed by John W. Igoe and returned to Mr. Fumich on January 11, 1972. Confirmatory license will be prepared after application is filed in U.S. Patent Office and serial number is received.

(4) OCR-1863: As reported last month, a U.S. patent application has also been prepared on disclosure OCR-1863 entitled "Two-stage Downflow Gasification of Coal." A copy of this application was forwarded to Mr. Howard Silverstein, Branch of Patents, on December 13, 1971, for his review and authorization for filing by BCR. The appropriate document assigning rights to the U.S. Government has been prepared.

By letter dated December 28, 1971, Mr. George Fumich authorized BCR to file a foreign patent application on the subject invention. As stated above, this letter was signed by John W. Igoe and returned to Mr. Fumich on January 11, 1972. Confirmatory license will be prepared after application is filed in U.S. Patent Office and serial number is received.

(5) OCR-1864: As reported last month, a U.S. patent application was prepared on disclosure OCR-1864 entitled "Two-stage Gasification of Coal with Forced Reactant Mixing and Steam Treatment of Recycled Char." A copy of this application was mailed to Mr. Howard Silverstein, Branch of Patents, on December 8, 1971, for his review and approval for filing by BCR. The appropriate document assigning rights to the U.S. Government has been prepared.

By letter dated December 28, 1971, Mr. George Fumich authorized BCR to file a foreign patent application on the subject invention. As stated above, this letter was signed by John W. Igoe and returned to Mr. Fumich on January 11, 1972. Confirmatory license will be prepared after application is filed in U.S. Patent Office and serial number is received.

I. Visitors During January, 1972

January 4, 1972

Mr. R. W. Whiteacre
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 7, 1972

Mr. J. Robb
Mr. S. M. Tymiak
Mr. J. D. Rice
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

Mr. Paul Spaite
Mr. D. R. Miller
Processes Research, Inc.
2912 Vernon Place
Cincinnati, Ohio 45219

January 11, 1972

Mr. J. Field
Mr. H. E. Benson
Mr. R. J. Mawhumey
Benfield Corporation
666 Washington Road
Pittsburgh, Pa. 15228

Mr. J. Lindstrom
Mr. D. M. Mitsak
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 12, 1972

Mr. C. E. Packard
The McNally Pittsburg Mfg. Corp.
Pittsburg, Kansas 66762

Mr. James R. Byron
Fluor Corporation
2500 S. Atlantic Blvd.
Los Angeles, California

January 13, 1972

Mr. D. M. Mitsak
Mr. H. F. Leonard
Mr. R. Dorsey
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

Mr. H. A. Dennis
Mr. John H. Lutz
Scientific Design Company, Inc.
Two Park Avenue
New York, New York 10016

January 14, 1972

Mr. Paul Steiner
Visual Industrial Products, Inc.
Indianola, Pennsylvania 15051

Mr. Richard Smith
Mr. H. Gitterman
Burns & Roe
700 Kinderkamack Road
Oradell, New Jersey 07649

Mr. H. F. Leonard
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 17, 1972

Mr. R. O. Skamser
Mr. R. W. Hospodarel
C. F. Braun & Co.
Alhambra, California

Mr. H. F. Leonard
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 18, 1972

Mr. D. M. Mitsak
Mr. H. F. Leonard
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 20, 1972

Mr. Walter Linde
Lotepro Corporation
801 Second Avenue
New York, N. Y.

Mr. Paul Towson
Mr. Jack Ryan
Division of Utilization
Office of Coal Research
U.S. Department of the Interior
Washington, D. C. 20240

January 21, 1972

Mr. R. W. Whiteacre
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 24, 1972

Mr. D. M. Mitsak
Mr. J. F. Farnsworth
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 25, 1972

Mr. Willard Bull
Director of Research
Pittsburg & Midway Coal Mining Co.
9009 West 67th Street
Merriam, Kansas 66202

January 26, 1972

Mr. D. M. Mitsak
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

January 27, 1972

Mr. R. C. Hostert
Mr. A. S. Armstrong
Harshaw Chemical Company
1945 E. 97th Street
Cleveland, Ohio 44106

Mr. Bill Knepschield
Mr. A. Kaczman
Mr. J. P. Matoney
Kaiser Engineers
300 Lakeside Drive
Oakland, California 94604

Mr. F. S. Chalmers
Arthur G. McKee & Company
6200 Oak Tree Blvd.
Independence, Ohio 44131

January 28, 1972

Mr. D. M. Mitsak
Mr. R. W. Whiteacre
Mr. D. Miller
Koppers Company, Inc.
Koppers Building
Pittsburgh, Pa. 15219

J. Trips, Visits, and Meetings during January, 1972

January 19, 1972	Bidders' Conference BCR Laboratory Monroeville, Pa. 15146	R. A. Glenn et al
January 26, 1972	AGA Materials Design Task Group Meeting Pittsburgh, Pa.	R. A. Glenn R. J. Grace J. F. Tassoney

K. Requests for Information

Mr. John Doskey
Chicago Northwestern Railroad Co.
Chicago, Illinois

Mr. Dale Schafer
Meriam Instrument
10920 Madison Avenue
Cleveland, Ohio 44102

III. WORK PLANNED FOR FEBRUARY, 1972

The work planned for February will be basically a continuation of the on-going program which has been underway for the past few months.

The final summary report on the coal composition and beneficiation studies will be completed this month.

The review of the bid package from Koppers for the fluidized-bed gasification PEDU will continue. Suggested design changes for the PEDU will be evaluated to determine whether their inclusion will add substantially to the research program. Reactivity studies of the Consol char have been completed, and a summary report of the procedure and development of the reactivity equations will be drafted. Chars obtained from the Stage 2 PEDU will be evaluated.

Tests will continue in the bench-scale methanator to evaluate suitable catalysts. Emphasis will be placed on non-nickel catalysts as a result of previous experience. Soliciting of bids for equipment for the methanation PEDU is planned, as well as continued work on the model studies.

Data on the Stage 2 PEDU (100 lb/hr) have been compiled and the first draft of a final summary report to cover work completed since September 20, 1970, has been written. Editing of the report will be completed this month.

Tests in Phases II and III of the cold flow model studies for the 5 ton/hr two-stage gasifier will begin. Construction of equipment for Phases IV, V, and VI (Stage 2 tests) is also planned.

Operation of the PDP8/E computer will continue to be studied and the equipment will be set up as soon as it is received. Data from simulation runs will be evaluated as needed.

A. Trips and Meetings Planned

None

B. Papers to be Presented

None

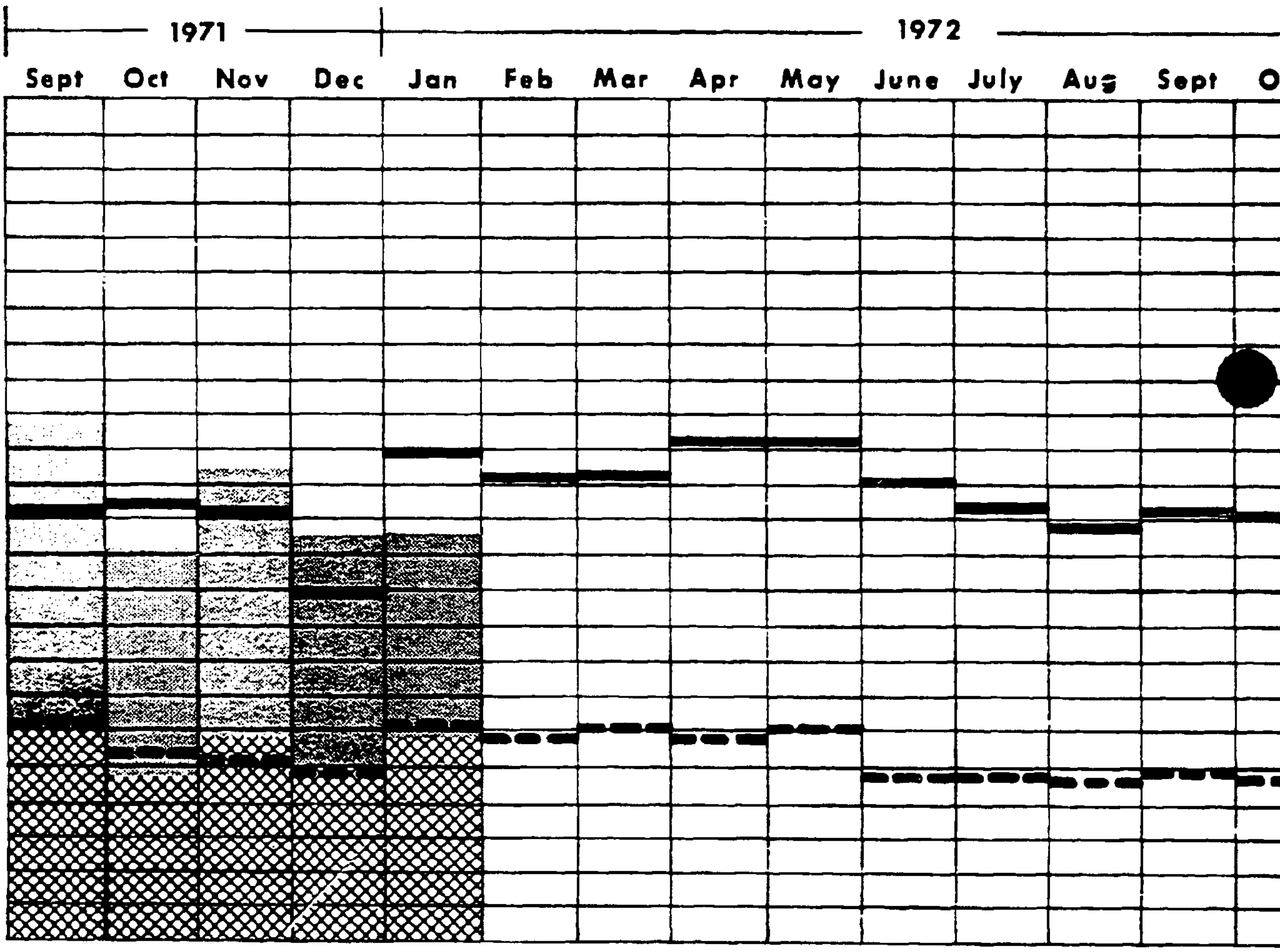
C. Visitors Expected

None

RAG:v

8006

MANHOURS



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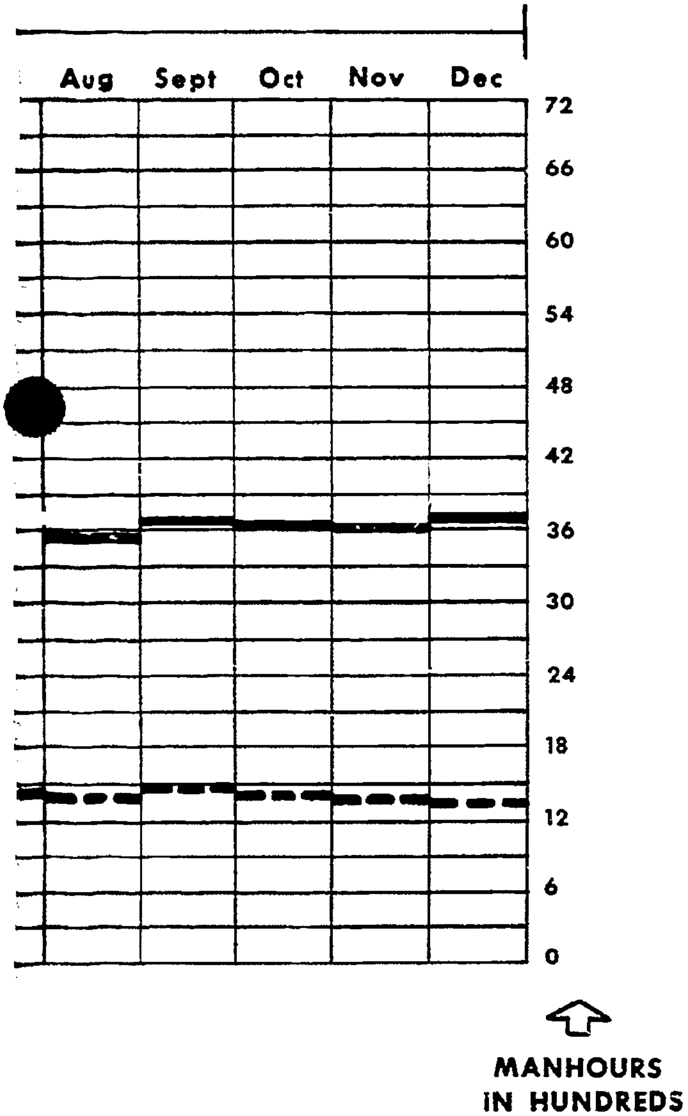


MONTHLY PROGRESS CHART
PART 1 MANHOURS

Bituminous Coal Research, Inc.
350 Hochberg Road Monroeville, Pa.

OFFICE OF COAL RESEARCH
DEPARTMENT OF THE INTERIOR

CONTRACT NO. 14-32-0001-1207

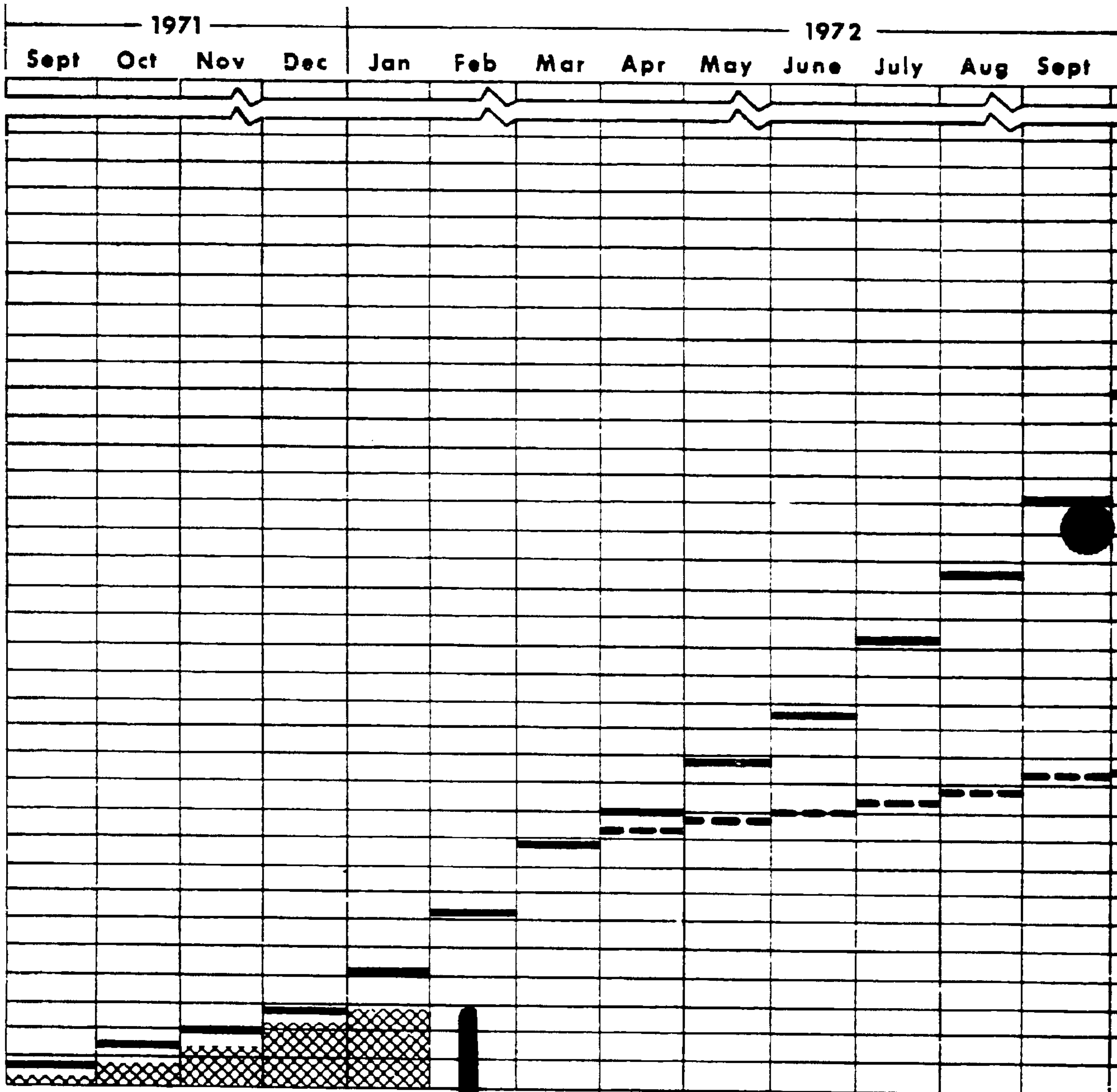
Predicted Professional and Non-professional

Predicted Professional

Actual Non-professional

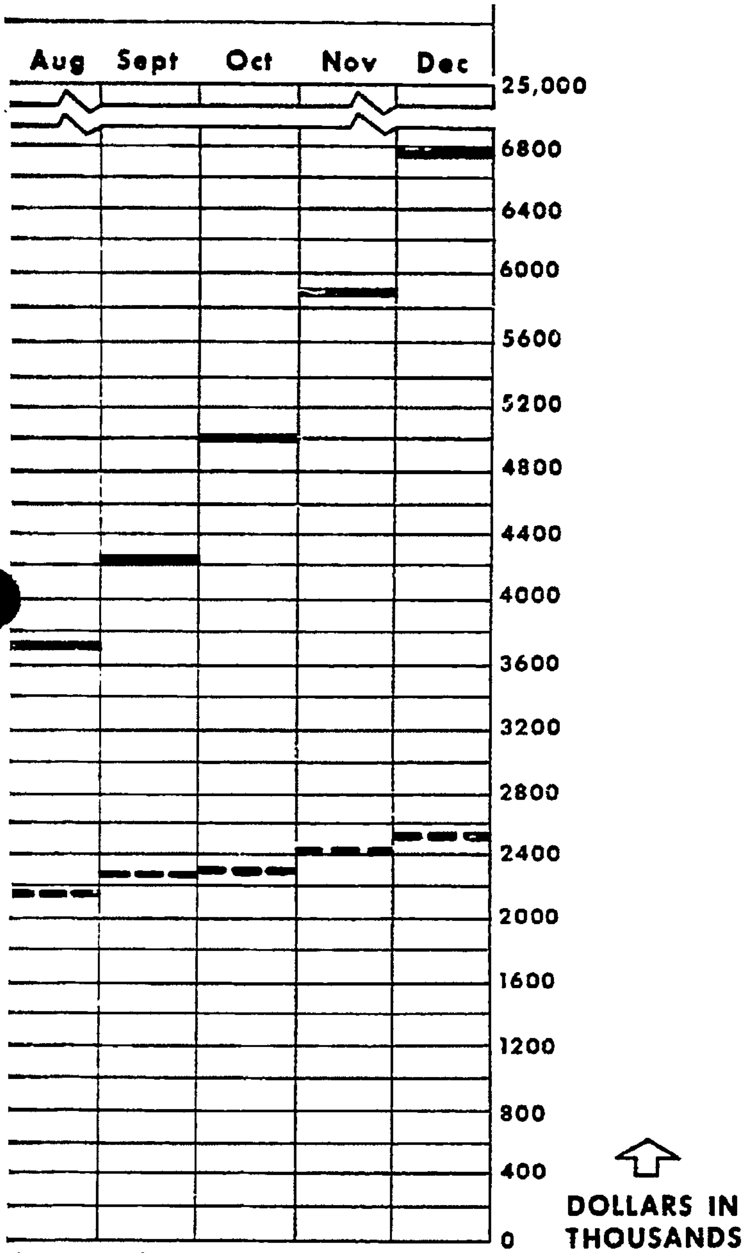
Actual Professional

2



MONTHLY EXPENDITURES (All Costs, in Dollars)

		Sept	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May
Monroeville	Predicted	129,991	129,991	129,991	129,991	323,486	382,228	558,454	105,058	86,238
	Actual	63,610	121,696	146,834	144,590*	103,147				
Homer City	Predicted								154,000	215[illegible]
	Actual									
Total	Predicted	129,991	129,991	129,991	129,991	323,486	382,228	558,454	259,058	301,838
	Actual	63,610	121,696	146,834	144,590*	103,147				



CUMULATIVE EXPENDITURES

MONTHLY PROGRESS CHART
PART 2 EXPENDITURES

Bituminous Coal Research, Inc.
350 Hochberg Road Monroeville, Pa.

OFFICE OF COAL RESEARCH
DEPARTMENT OF THE INTERIOR

CONTRACT NO. 14-32-0001-1207

Expenditures, Cumulative

- Actual, Monroeville
- Actual, Homer City

Predicted Expenditures, Cumulative

- Total, Monroeville and Homer City
- Monroeville

..osts, in Dollars)

..pr	May	June	July	Aug	Sept	Oct	Nov	Dec
..,058	86,238	86,240	65,813	65,813	74,746	62,273	62,273	62,275
..,000	215,600	280,400	444,300	444,300	444,400	760,600	760,600	760,800
..,058	301,838	366,640	510,113	510,113	519,146	822,873	822,873	823,075

* Estimated

2

APPENDIX B

GASIFY: A Computer Simulation of the BCR Two-stage Super-pressure Coal Gasifier

A. Introduction

In the two-stage super-pressure process, fresh coal is introduced into the upper section of the gasifier (See Figure 93). Here, the coal contacts a rising stream of hot synthesis gas produced in the lower section of the gasifier and is partially converted into methane and more synthesis gas. The residual char is swept out of the gasifier together with the gas, is separated, and returned to the bottom section of the gasifier. Here the char is completely gasified under slagging conditions by reaction with oxygen and steam, producing both the synthesis gas required in the upper section of the gasifier and heat needed to complete the endothermic reaction. The following is a complete description of computer program GASIFY which simulates this coal gasification process.

B. General Assumptions for GASIFY

The following general assumptions were made in the gasifier program:

1. The water-gas shift equilibrium describes the gas composition from Stage 1 and Stage 2 adequately.

2. The enthalpies of mixing of the gases are zero.

3. All gas fungacities and activity coefficients are unity.

4. The effect of pressure on the heat of reaction is minor.

The assumptions are subject to some discussion.

According to Thring and Essenhigh[1], at temperatures up to 4000 K, the gasification reactions of carbon will go essentially to completion. Von Fredersdorff and Elliot[2] state that this complete gasification forces the shift reaction towards equilibrium due to the steam disappearance as a result of the steam-carbon reaction. The effect of catalytic agents in the ash as well as the high temperatures present in Stage 1 probably aid in the establishment of equilibrium (2000 F is the suggested temperature where the assumption of equilibrium is legitimate).

The Stage 2 exit temperature is probably lower than 2000 F (nearer 1700 F) but approach to equilibrium may still be a legitimate approximation. PEDU results obtained at BCR show that product (Stage 2) gases are always at a water-gas shift equilibrium corresponding to about 1700 F for the Stage 2 temperature.

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[1] Thring, M. W. and Essenhigh, R. H., "Thermodynamics and Kinetics of Solid Combustion," in "Chemistry of Coal Utilization," Suppl. Vol., H. H. Lowry, Ed., New York: John Wiley & Sons, Inc., 1963. pp. 754-72.

[2] Von Fredersdorff, C. G. and Elliott, M. A., "Coal Gasification," in "Chemistry of Coal Utilization," Suppl. Vol., H. H. Lowry, Ed., New York: John Wiley & Sons, Inc., 1963. pp. 892-1022.

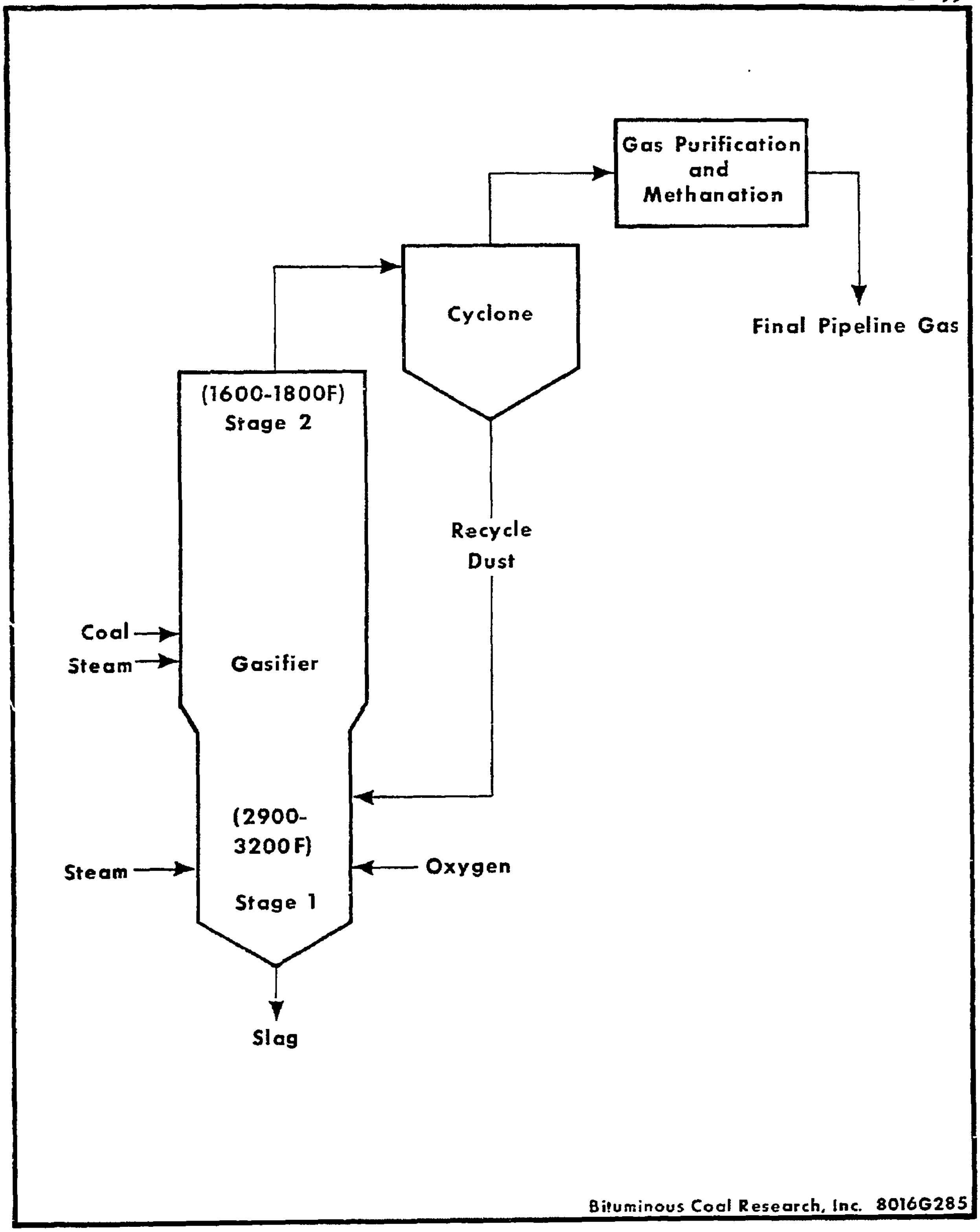

Figure 93. Simplified Flow Diagram for Two-stage Super-pressure Gasifier

Assumptions (2), (3), and (4) may be discussed together. Non-ideal effects tend to be important in low to moderate temperature, high pressure solutions. Fugacities of the components were estimated from the Lydersen correlation (Theorem of Corresponding States) and found to be near to unity in all cases. Likewise, the effect of pressure on the heats of reaction was also estimated and found to amount to only a few hundred Btu/mole of material. This indicates that these components behave like ideal gases at the high temperatures in question.

Mixing effects of gases are small, especially if outside the critical region. This system would probably act in an ideal manner at the very high temperatures found in Stage 1 and Stage 2 and, therefore, activity coefficients and heats of mixing were assumed as unity and zero, respectively, for all subsequent calculations.

C. Sensible Heats and Heats of Formation

For an energy balance in the two-stage gasification process, it is essential that both the sensible heats and heats of formation of all inputs and products be defined. The definitions used in computer program GASIFY for coal and char energies are listed below. Energies of the gaseous components in the system are not defined or discussed here since they are well established and can be found in any thermodynamics text.

Nomenclature:

Q	= heat or energy (Btu)
T	= temperature (K)
QH(x,T)	= sensible energy of component x at temperature T
QF(x)	= heat of formation of component x
GHV(x)	= gross heating value of component x
VM,M,H,S,C,A	= as-received analysis for volatile matter, moisture, hydrogen, sulfur, carbon, and ash

Energy Definitions:

Ash

$$QF(Ash) = 0.0$$

$$QH(Ash,\ T)^{3} = 1.8\left(53.3975\ e^{(.0011466\ T)}\right) \qquad (Btu/lb)$$

Coal

$$QF(Coal) = 1.8\ (GHV(Coal) - 68317\ H/2 - 94054\ C/12 - 70940\ S/32 - 57798\ M/18) \quad (Btu/lb)$$

[3] Glenn, R. A., Special Report No. 3, 27, (1967).

$QH(Coal, T)^{*} = 1.8\ \overline{C}_{P_{coal}}\ (T-298)$ (Btu/lb)

where

$\overline{C}_{P_{coal}} = (1-M-A)\ (0.20 + 0.164VMP - 0.0833VMP^2) + 0.2A + 0.99M + 0.00015(T + 298)$

$VMP = VM/(1-M-A)$

Char

$QF(Char) = 1.8(8024\ C - 68317\ H/2 - 94054\ C/12 - 70940\ S/32 - 57798\ M/18)$ (Btu/lb)

$QH(Char, T) = Ash \times QH(Ash, T) + C\ QH(C,T) + H\ QH(H,T)$ (Btu/lb)

D. GASIFY's Modeling Options

Depending on the type of information desired, the gasifier program may be run with several different calculational schemes for Stages 1 and 2. These options are: (1) the equilibrium mode, (2) the kinetic mode, and (3) the set yield mode. A brief explanation of each mode as it applies to each stage of the gasifier follows.

1. Stage 1 Equilibrium Mode: The equilibrium option in Stage 1 combines the char, oxygen, and steam in Stage 1 into a synthesis gas as dictated by simultaneous equilibrium of the following reactions:

$$2C + O_2 \rightleftarrows 2CO$$

$$2H_2 + O_2 \rightleftarrows 2H_2O$$

$$CO_2 + H_2 \rightleftarrows CO + H_2O$$

$$C + CO_2 \rightleftarrows 2CO$$

$$C + H_2O \rightleftarrows CO + H_2$$

When final equilibrium is achieved, the Stage 1 carbon yield is calculated and a corresponding amount of the ash in Stage 1 is slagged. The remaining char (carbon and ash) is carried into Stage 2 with the synthesis gas.

2. Stage 1 Kinetic Mode: Since no work has been done on the combustion of char at high pressures (80 atmospheres), a Stage 1 expression is not available at this time. When an empirical expression is derived, it will be inserted in the gasifier program and made available as a Stage 1 option.

3. Stage 1 Set Yield Mode: In the set yield mode, the percentage of carbon gasified in Stage 1 is pre-set as a program input. The program combines the oxygen, steam, and a pre-selected percentage of char in Stage 1 into a synthesis gas and brings it to equilibrium by the water-gas reaction:

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* Graboski, M. S., Thermal Properties of Coal, Inter-office Correspondence, BCR, (Aug. 16, 1971) unpublished.

$$CO_2 + H_2 \rightleftarrows CO + H_2O$$

A pre-selected percentage of the ash in Stage 1 is then slagged and the remaining char (carbon and ash) is carried into Stage 2 with the synthesis gas.

4. Stage 2 Equilibrium Mode: The equilibrium option in Stage 2 combines the coal, steam, and synthesis gas from Stage 1 to produce methane and additional synthesis gas as dictated by simultaneous equilibrium of the following reactions:

$$C + 2H_2 \rightleftarrows CH_4$$

$$C + H_2O \rightleftarrows CO + H_2$$

$$C + CO_2 \rightleftarrows 2CO$$

$$CO_2 + H_2 \rightleftarrows H_2O + CO$$

When final equilibrium is achieved, the Stage 2 methane yield and carbon-oxides yield are calculated. The char produced is then calculated as the sum of the carbon in the coal not gasified, the ash in coal, and the char from Stage 1. The product char is carried out of Stage 2 by the methane and synthesis gas.

5. Stage 2 Kinetic Mode: The kinetic option in Stage 2 combines the coal, steam, and synthesis gas from Stage 1 to produce methane and additional synthesis gas as dictated by the simultaneous solution of (1) the water-gas reaction, and kinetic expressions for (2) methane and (3) carbon-oxides formation:

(1) $CO_2 + H_2 \rightleftarrows CO + H_2O$

(2) methane yield $= \dfrac{a_1 + a_2(P_{H_2})}{1 + a_2(P_{H_2})}$

(3) carbon-oxides yield $= b_1$ (Residence time) $\dfrac{(P_{H_2O})}{(P_{H_2})}$.

where

(P_{H_2O}), (P_{H_2}) = partial pressures of H_2O and H_2, respectively

a_1, a_2, b_1 = kinetic constants for the coal being gasified. These constants are pre-set as program inputs.

The char produced is then calculated as described in Section D-4 and is carried out of Stage 2 by the methane and synthesis gas.

6. Stage 2 Set Yield Mode: In the set yield mode, the Stage 2 methane yield and carbon-oxides yield are pre-set as program inputs. The program combines the required amounts of steam, Stage 1 synthesis gas, and coal to produce the pre-set yields of methane and additional synthesis gas. The total synthesis gas is then brought to equilibrium by the water-gas reaction: $CO_2 + H_2 \rightleftarrows CO + H_2O$. The product char is then calculated as described in section D-4 and is carried out of Stage 2 by the methane and synthesis gas.

E. Steam Splitting

In order to maintain a Stage 1 temperature which is appropriate for slagging operation of the gasifier, the amount of steam fed into Stage 1 must be within certain thermodynamically fixed limits. Program GASIFY handles this problem by the following procedure:

1. Accept as inputs to the program a selected Stage 1 temperature and a selected amount of total steam.

2. Add sufficient steam to Stage 1 to achieve the selected temperature.

3. If the amount of steam added to Stage 1 does not exceed the selected total steam, the remainder is put into Stage 2.

Note that Step 2 of the procedure will not be satisfied if the amount of oxygen fed is not sufficient to raise the Stage 1 temperature to the selected temperature. In this case, no steam will be put into Stage 1 and the program will calculate the actual temperature achieved.

F. Program Inputs

Table 72 is a copy of the input sheet required for gasification simulation runs using program GASIFY. The description of each input line on the data sheet follows:

1. Coal Type - Type of coal (Bituminous, lignite, seam, etc.)

2. Flame T. - desired Stage 1 temperature (F)
   Exit T. - desired Stage 2 temperature (F)
   Press. - reactor pressure (atm)

3. Char Pre-heat T. - pre-heat temperature for char fed into Stage 1 (F)
   Char Withdrawl - percent of char produced in Stage 2 that is withdrawn from system (i.e., percent not fed into Stage 1)

4. IMODL1 - Stage 1 option being used

   IMODL1 = 1 = equilibrium option
   IMODL1 = 2 = kinetic option
   IMODL1 = 3 = set yield option

   Carbon Yield - (only if IMODL1 = 3) percent of carbon in Stage 1 that should be gasified.

5. IMODL2 - Stage 2 option being used (sam key as IMODL1)

   Methane Yield - (only if IMODL2 = 3) percent of carbon in coal to be converted to methane.

   Methane Constants - (only if IMODL2 = 2) constants a_1, a_2 as described in Section D-5.

TABLE 72. INPUT DATA SHEET FOR COAL GASIFICATION SIMULATION RUNS

1. (5001) Coal Type ________________ Date ________ Request No. ________

2. (5002) Flame T. ____ Exit T. ____ Press. ____

3. (5002) Char Pre-heat T. ____ Char Withdrawal ____%

4. (5003) IMODL1 ____ Carbon Yield ______%

5. (5003) IMODL2 ____ Methane Yield ______% Methane Constants ____ ____ ____ ____

6. (5003) ITRANA ____ C-oxide Yield ______% C-oxides Constants ____ ____ ____ ____

7. (5003) ITRANV ____ Stage 1 H.L. ______ Stage 2 H.L. ______

8. (5002) Total Steam (lbs.) ______ Pre-heat T. ______

9. (5004) ISTEAM ___ DELSTM ___ IWDRAWL ___ DELDRW ___ IYCH4 ___ DELCH4 ___ IYCO ___ DELYCO ___

10. (5002) Coal (as received, wt percent)

lb ___ Pre-heat T. ___ H ___ O ___ C ___ N ___ S ___ Ash ___ Moist ___ VM ___ G.H.V. ___

Input (5002)	lb	Pre-heat	$\%H_2$	$\%O_2$		%CO	$\%CO_2$	$\%CH_4$	$\%H_2O$	$\%N_2$
11. Stage 1 Oxidizer	0.0	___	___	___	0.0	___	___	___	___	___
12. Char Transport	___	___	___	___	0.0	___	___	___	___	___
13. Coal Transport	___	___	___	___	0.0	___	___	___	___	___

5001 Format (3A4, 8x, 4A4, 4X, A4)
5002 Format (11F7.0)
5003 Format (15, 2X, 10F7.0)
5004 Format (8(15, F5.0))

6. ITRANA - coal transport option

ITRANA = 0 = use coal transport gas analysis as given in line 13 of data sheet.

ITRANA = 1 = use Stage 2 product gas analysis for coal transport.

C-oxide Yield - (only if IMODL2 = 3) percent of carbon in coal to be converted to carbon-oxides.

C-oxide Constants - (only if IMODL2 = 2) residence time and constant b_1 as described in section D-5.

7. ITRANV - 0 - ZERO (not yet available)

Stage 1 H.L. - Total Stage 1 heat loss (Btu)

Stage 2 H.L. - Total Stage 2 heat loss (Btu)

8. Total Steam - total steam to be fed into reactor. Does not include any steam used for transport.

Pre-heat T. - steam pre-heat temperature (F).

9. ISTEAM - number of different steam rates desired.

DELSTM - steam increment (lbs) to be added to total steam (line 8) for additional Total Steam rates.

IWDRWL - number of different withdrawl percentages desired.

DELDRW - percentage increment to be added to Char Withdrawl (line 3) for additional withdrawl rates.

(Complete remainder of line 9 only if IMODL2 = 3)

IYCH4 = number of different methane yields desired.

DELCH4 = percentage increment to be added to methane yield (line 5) for additional methane yields.

IYCO = number of different Stage 2 carbon-oxides yields desired.

DELYCO = percentage increment to be added to C-oxide Yield (line 6) for additional Stage 2 carbon-oxide yields.

10. lbs - pounds of feed coal (as-received basis)
Pre-heat T. - coal pre-heat temperature (F)
G.H.V. - gross heating value (Btu/lb)

11, 12, 13. Pre-heat - pre-heat temperatures (F) percentages - volume percent.

Note: "Pounds of Oxidizer" is set to zero since program GASIFY will calculate it. Column five is also set to zero because of internal program requirements.

G. Flow Chart

Figure 94 shows the flow of operations used in computer program GASIFY to find the solution for a selected set of initial conditions as described in Section E.

The asterisk (*) in the first block of the flow chart (*Guess char feed rate and oxidizer rate) signifies that successive guesses of oxidizer rate are obtained (the secant method is employed).

H. Computer Print-Out

Table 73 is a sample print-out of a simulation run generated by computer program GASIFY. All values are clearly described and dimensioned. The four digit pagination system requires some additional explanation. The page number is determined by the level of each of four input variables being used for a particular print-out (see description of line 9 of Data Input Sheet before continuing). The digits in the page number from left to right correspond to the selected levels of (1) steam, (2) char withdrawl factor, (3) methane yield, and (4) carbon-oxides yield. For example, a 1 in the page number indicates that the print-out is based on the lowest level selected for that variable. A 2 in the page number indicates that the print-out is based on the second level selected for that variable, etc. This approach permits quick location of results for any combination of the four input variables.

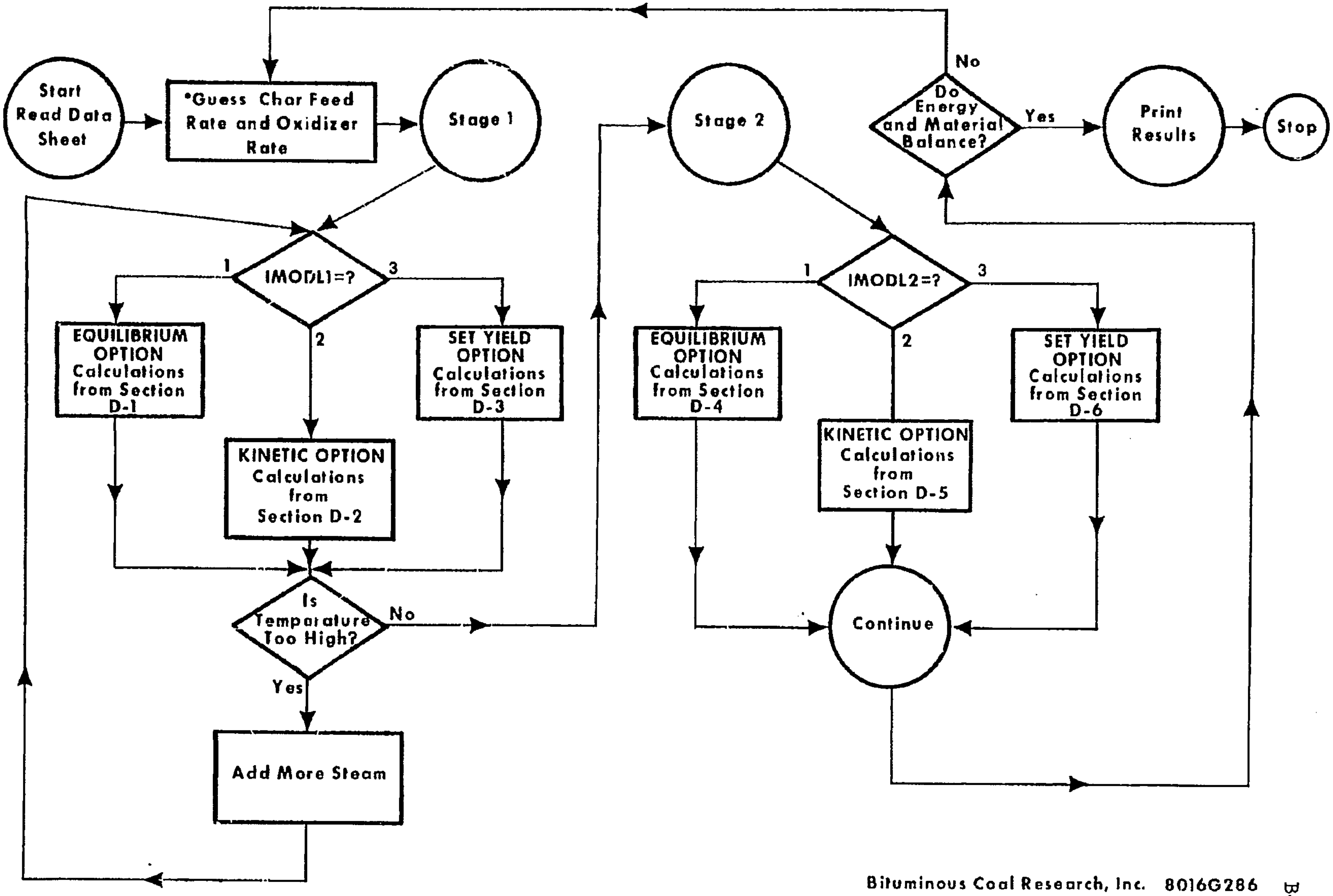

Figure 94. Flow Chart for Program GASIFY

TABLE 73. SAMPLE PRINT-OUT FROM GASIFY

RESULTS FOR GASIFICATION OF PGH. SEAM

NOV. 30,1971 REQUEST # 4 PAGE 2232

STAGE 1, SET YIELD MODEL

YIELD= 60.0 %. COMBUSTION TEMP.= 3000. F

	STREAM	TEMP. F	FLOW, LBS	ENERGY, BTU/1000 SENSIBLE	FORMATION
IN	CHAR	1100.	57.4	14.19	16.55
	TRANSPORT	0.	0.0	0.0	0.0
	STEAM	1200.	63.2	34.71	-365.33
	OXIDIZER	800.	39.5	6.67	0.0
	TOTAL		160.0	55.57	-348.78
OUT	GAS	3000.	132.2	165.43	-499.68
	CHAR	3000.	23.0	25.22	6.62
	SLAG	3000.	4.8	4.20	0.0
	LOSS			5.00	
	TOTAL		160.0	199.85	-493.06

STAGE 2, SET YIELD MODEL

CH4 YIELD= 25.0 %, CO YIELD= 20.0 %, RES. TIME= 0. SEC.

	STREAM	TEMP. F	FLOW, LBS	ENERGY, BTU/1000 SENSIBLE	FORMATION
IN	STAGE 1 GAS	3000.	132.2	165.43	-499.68
	STAGE 1 CHAR	3000.	23.0	25.22	6.62
	STEAM	1200.	26.8	14.75	-155.31
	COAL(AS REC'D)	660.	108.9	20.00	-58.83
	TRANSPORT	0.	0.0	0.0	0.0
	TOTAL		290.9	225.40	-707.20
OUT	GAS	1700.	214.5	158.86	-700.56
	CHAR	1700.	76.5	37.37	22.07
	LOSS			0.50	
	TOTAL		291.0	196.73	-678.50

SOLIDS ANALYSES, WT. PERCENT

	H	O	C	N	S	ASH	H2O	V.M.	BTU/LB GROSS	NET
CHAR	0.0	0.0	86.0	0.0	0.0	14.0	0.0	0.0	12420.	12420.
COAL(AS REC'D)	5.3	6.4	76.9	1.6	1.7	6.9	1.3	37.0	13686.	13174.

GASEOUS ANALYSES, VOL. PERCENT

	M.W.	H2	O2	CO	CO2	CH4	H2O	N2	H2S
STAGE 1 GAS	22.13	15.92	0.0	25.36	15.93	0.0	42.79	0.0	0.0
STAGE 2 GAS	21.19	20.13	0.0	20.78	17.38	17.23	23.30	0.61	0.58
TRANSPORT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRANSPORT	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OXIDIZER	32.00	0.0	100.00	0.0	0.0	0.0	0.0	0.0	0.0

TOTAL DRY GAS, SCF 2943.

GROSS DRY GAS HEATING VALUE, BTU/SCF 402.

NET DRY GAS HEATING VALUE, BTU/SCF 366.

PRESSURE= 80. ATM. WITHDRAWL= 25. %

APPENDIX C

ADDITIONS TO ABSTRACT FILE, JANUARY 1972

Birch, T. J., "Hydrogasification of brown coal:" Pt. 1, "Experiments with 3 ft deep bed co-current reactor-a new assessment" (June 1969); Pt. 2, "Experiments with 19 ft deep bed countercurrent reactor" (Sept. 1969); Pt. 3, "Experiments with a two-stage reactor" (June 1970); CSIRO Rept. No. CE/R25. 540.000 70-24

The results of studies carried out from 1955-1968 are reported. In each part, the problems encountered with a fluidized reactor operated at high temperature and pressure are discussed.

Grace, R. J., Glenn, R. A., and Zahradnik, R. L., "Gasification of lignite by BCR two-stage super-pressure process," I&EC Process Design Develop., 11 (1), 95-102 (1972). 540.000 Journal

This paper was annotated in Progress Rept. No. 81 (Sept. 1970) p. 3148 upon presentation at the AIChE Symposium on Synthetic Hydrocarbon Fuels from Western Coals.

Louis, J. F., *et al.*, "Open cycle coal burning MHD power generation: an assessment and a plan for action," M.I.T. MHD Power Generation Study Group, Final Rept. to U.S. Office Coal Res., R&D Rept. 64 (undated, released 1971). 142 pp. 540.000 OCR-M

In the part of the program relating to coal gasification, the study group proposed an investigation of the most promising coal gasification concepts adaptable to MHD power production including the molten salt and the CO_2 recycling processes.

PATENTS

Johnson, M. M. and Nelson, W. T. (to Phillips Petroleum Company), "Production of methane from carbon monoxide and steam," U.S. Pat. 3,600,145 (Aug. 17, 1971). 2 pp. 540.000 71-10

Carbon monoxide and steam are converted to methane and carbon dioxide in a temperature range of 400-2000°F, a pressure range of 0 to 1,000 psig, gaseous hourly space rates for CO of 200-10,000, and at carbon monoxide to steam ratio (in moles) of about 0.2 to about 20. The conversion is carried out over a nickel catalyst which is promoted with a barium salt of an organic acid and which is supported on an alumina-containing material. (Abstract of the disclosure adapted.)

Spacil, H. S. (to General Electric Company), "Apparatus and method for the hydrogenation of coal," U.S. Pat. 3,556,749 (Jan. 19, 1971). 6 pp. 540.000

71-11

Hydrogen required for conversion of coal to methane at elevated temperatures and pressures in the presence of a catalyst is supplied by dissociation of water vapor. Power for the dissociation is generated in a power station in which carbonaceous char (which is a by-product of the coal hydrogenation) and air (which may be enriched by oxygen produced during the dissociation) are burned. The dissociation is accomplished in solid oxygen-ion electrolyte cells preferably operating at temperatures in excess of 800°C. (Abstract of the disclosure adapted.)

APPENDIX D

PROGRESS REPORT #30

Bituminous Coal Research, Inc.
Coal Gasification

January 1972

Koppers Contract 2415

I. STATUS OF CONTRACT

A. Pilot Plant Engineering Bid Package

1. Koppers submitted to BCR Volume VI of the Bid Package on 14Jan72 (C-289).

2. Two models of the pilot plant facility at Homer City:

   a. Plant site model (scale 1 inch = 20 feet)

   b. Planning/presentation model (scale 1/4 inch = 1 foot)

   were completed by the model maker, accepted by Koppers and BCR and delivered to BCR.

3. BCR (per letter of 24Jan72) deleted the requirement to furnish a set of photographs of the models originally specified to be supplied by Koppers under Amendments #6 and #7.

B. Engineering Assistance and Recommendations for PEDU Program

1. A meeting between BCR and Koppers was held on January 24, 1972, to outline the detail engineering schedule for both PEDUs. Koppers is currently developing schedules and cost data. In the meantime, Koppers has been given approval to proceed with the detail work required to obtain bids on items of equipment on the methanation PEDU.

2. Based on approval to proceed with the solicitation of quotations on the methanation PEDU equipment, Koppers and BCR jointly finalized the specifications on a number of PEDU items, and thus determined where Koppers had to supply further engineering assistance.

3. On January 6, 1972, (C-284) Koppers provided BCR with the necessary specification sheets for BCR to begin soliciting bids on the methanation PEDU. A tabulation of suggested bidders for PEDU units was transmitted to BCR on 13Jan72 (C-287).

4. To provide flexibility in methanation studies, Koppers investigated methods of adding CO_2 and H_2S to the reformer product gas.

Thus, the capability of studying methanation prior to or after acid gas removal will be available. Koppers also investigated the operation of the reformer on propane rather than methane to provide increased flexibility in H_2/CO ratio. (Ref. Koppers memos dated January 10, January 12, and January 12, 1972.)

5. On January 28, 1972, Koppers met with BCR to reinitiate work on the methanation panel board. Approval of the basic panel design was given by BCR.

6. Koppers was asked to check the flexibility of the PEDU with respect to turndown of items. This study was completed and the results indicate that ample flexibility is currently available.

7. Koppers submitted to BCR on 04Jan72 (C-283) recommendations for changes to materials of construction as specified in the 30Sep71 issue of the Methanation PEDU Specifications. These changes are necessary due to customer's decision to add hydrogen sulfide to the methanator feed gas.

8. Preliminary specifications, drawings, and cost estimates for various alternates to the Char Fluidized Bed Gasification PEDU as specified in the 30Sep71 issue were submitted to BCR on 18Jan72 for their review and decision.

II. CONTRACT EVALUATION

A. Four (4) copies of Amendment No. 7 to Amended Subcontract No. 2, including Appendices I through VIII, signed by Mr. J. D. Rice, Vice President, Engineering and Construction Division, Koppers Company, Inc., were transmitted to BCR in our letter C-183 dated 18Oct71. Receipt of these copies was acknowledged by BCR in their letter dated 18Oct71.

B. One (1) set of wash off cloth reproduction for each of one hundred eighty (180) drawings, which were included in the Process Engineering Bid Package dated 01Dec71, revised 17Dec71, and 14Jan72, were transmitted to BCR on 19Jan72 (C-299).

C. BCR in their letter dated 28Jan72 reallocated funds within Part A of Koppers Amendment #6 to cover actual expenditure incurred by Koppers under Part A, Step (a) of our engineering contract.

J. F. Farnsworth
Project Manager