FE-2307-38
Distribution Category UC-90d

RESEARCH AND DEVELOPMENT OF RAPID HYDROGENATION FOR COAL CONVERSION TO SYNTHETIC MOTOR FUELS

(RISER CRACKING OF COAL)

First Quarter Report
For the Period April 1 to June 30, 1978

Dennis A. Duncan
Justin L. Beeson
R. Donald Oberle

Prepared by

Institute of Gas Technology
IIT Center, 3424 S. State Street
Chicago, Illinois 60616

Project No. 8976

Date Published — September 1978

Prepared for the

UNITED STATES DEPARTMENT OF ENERGY

Under Contract No. EX-76-C-01-2307

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

ABSTRACT

Runs were made in the bench-scale unit to investigate hydrocarbon yields from North Dakota lignite at operating pressures of 500 and 1000 psig. The base carbon conversions were reduced to approximately 26% and 33%, and hydrocarbon liquids yields were reduced to 6.4 and 9.2 grams per 100 grams of feed carbon, respectively. These values are considerably lower than those obtained from North Dakota lignite in bench-scale unit operations at 2000 psig. At that pressure, base carbon conversions were approximately 50%, and hydrocarbon liquids yields were 18 grams per 100 grams of feed carbon.

Runs were also made with Illinois No. 6 bituminous coal [free-swelling index (FSI) = 4-1/2]. To avoid plugging the reactor, the coal was mixed with fine silica sand at levels of 10%, 20%, and 30% (by weight) coal with sand. The bench-scale unit was operated using an "upsweeping" temperature profile at coil outlet temperatures of 1450° and 1500°F and a system outlet pressure of 2000 psig. Runs with the 10% and 20% (by weight) coal were successful. The hydrocarbon liquids yields from the bituminous coal were 17.2 grams per 100 grams of feed carbon, approximately 30% more than the average hydrocarbon liquids yield of 12.8 grams per 100 grams of feed carbon obtained from North Dakota lignite under similar processing conditions.

The ramifications of increasing the operating pressure of the process development unit (PDU) to 2600 psig have been investigated, and needed changes in equipment and gas supply have been identified. Procurement and construction of the PDU will begin during the forthcoming quarter.

I. OBJECTIVE AND SCOPE OF WORK

The objective of the research and development program described in this report is to develop the technology of short residence time hydropyrolysis of lignites and coals for optimized yields of high-octane gasoline blending stock constituents. The scope of the investigation will include the design, construction, and operation of a bench-scale unit (5-10 lb/hr) and a process development unit (50-100 lb/hr). The process under development is called "Riser Cracking of Coal." In the final phase of the project, the technical and economic aspects of large-scale operation will be evaluated.

II. ACHIEVEMENT OF PROJECT OBJECTIVES

Task 1 (Planning) has been completed, and Task 2 (Construction and Operation of a Bench-Scale Unit) is continuing in its operating phase. Task 3 (Design of a Process Development Unit) has been completed, and Task 4 (Construction of a Process Development Unit) is in the initial procurement stage.

In the on-going bench-scale unit investigations, lower operating pressures (500 and 1000 psig) have been investigated, and both base carbon conversion and hydrocarbon liquids yields were found to decrease monotonically with a decrease in operating pressure. The decrease in base carbon conversion is consistent with the published results of other investigators.[2] Work with caking coals (Illinois No. 6; FSI = 4-1/2) has been started, and successful runs were obtained with mixtures of 20% (by weight) coal and 80% fine silica sand. Hydrocarbon liquids yields from the Illinois No. 6 coal were found to be significantly greater than the yields obtained from North Dakota lignite under similar processing conditions.

The design of the PDU was reviewed, and, by relatively minor adjustment, the operating pressure was increased from 2000 to 2600 psig. Suppliers of hydrogen, nitrogen, and oxygen at the needed pressures and volumes have been contacted. The investigation of methods for processing caking coals will be continued.

III. SUMMARY OF PROGRESS TO DATE

During the reporting period, 20 runs were made in the bench-scale unit; the overall objectives and results of these runs are summarized in Table 1 and reflect the execution of the near-term program agreed upon in November 1977. Runs at system operating pressures of 500 and 1000 psig were completed, and both base carbon conversion and hydrocarbon liquids yields were found to decrease monotonically with a decrease in operating pressure.

When North Dakota lignite and hydrogen were used as feed materials at a system outlet pressure of 500 psig and a coil outlet temperature of 1500°F the base carbon conversion was approximately 26%, and the hydrocarbon liquids yield was 6.4 grams per 100 grams of feed carbon. At a system outlet pressure of 1000 psig the base carbon conversion increased to approximately 33%, and the hydrocarbon liquids yield increased to approximately 9.2 grams per 100 grams of feed carbon; at a system outlet pressure of 2000 psig base carbon conversions of approximately 50% and liquids yields of 18 grams per 100 grams of feed carbon have been obtained. These runs are described in earlier reports.

Table 1. SUMMARY OF RUNS MADE FROM APRIL 1 THROUGH JUNE 30, 1978

Run/Date	Objective	Results
PP-7/4-4-78	Operate at reduced system pressure of 1000 psig and normal temperature profile to evaluate yields at reduced pressure.	Unsuccessful; aborted because of tar plug in make-gas line after 30 minutes of operation.
PP-8/4-7-78	Operate at reduced system pressure of 500 psig and normal temperature profile to evaluate yields at reduced pressure.	Unsuccessful; aborted because of plug in make-gas line after 15 minutes of operation.
PP-9/4-12-78	Repeat of PP-7.	Successful; operated for 120 minutes with voluntary shutdown.
PP-10/4-15-78	Replication of PP-7.	Unsuccessful; aborted because of plug in carrier gas line after 6 minutes of operation.
PP-11/4-25-78	Repeat of PP-8.	Successful; operated for 180 minutes with voluntary shutdown.
PP-12/4-27-78	Replication of PP-7.	Successful; operated for 180 minutes with voluntary shutdown.
BC-1/5-2-78	Operate with 10% mixture (by weight) of caking coal and sand at coil outlet temperature of 1450°F and pressure of 2000 psig to determine yields from bituminous coal.	Successful; operated for 60 minutes with voluntary shutdown.
BC-2/5-4-78	Operate with 20% mixture (by weight) of caking coal and sand at coil outlet temperature of 1450°F and pressure of 2000 psig to determine yields from bituminous coal.	Unsuccessful; aborted after 30 minutes of operation because of plug in carrier gas line.
BC-3/5-9-78	Repeat of Run BC-2.	Successful; operated for 60 minutes with voluntary shutdown.
BC-4/5-12-78	Operate with 30% mixture (by weight) of caking coal and sand at coil outlet temperature of 1450°F and pressure of 2000 psig to determine yields from bitunous coal.	Unsuccessful; aborted because of plug in coil after 23 minutes of operation.

Table 1, Cont. SUMMARY OF RUNS MADE FROM APRIL 1 THROUGH JUNE 30, 1978

Run/Date	Objective	Results
BC-5/5-16-78	Repeat of Run BC-4.	Unsuccessful; aborted after 10 minutes of operation because of plug in coil.
BC-6/5-18-78	Repeat of Run BC-2.	Unsuccessful; aborted after 19 minutes of operation because of plug in feed hopper.
BC-7/5-25-78	Repeat of Run BC-2.	Successful; operated for 90 minutes with voluntary shutdown.
BC-8/5-31-78	Replication of Run BC-2.	Unsuccessful; aborted after 25 minutes of operation because of plug in coil.
BC-9/6-2-78	Replication of Run BC-2.	Successful; operated for 90 minutes with voluntary shutdown.
BC-10/6-6-78	Operate with mixture of 20% (by weight) caking coal and 80% silica sand at pressure of 2000 psig and coil outlet temperature of 1500°F.	Unsuccessful; aborted after 30 minutes of operation because of plug in coil.
BC-11/6-13-78	Repeat of Run BC-10.	Successful; operated for 90 minutes with voluntary shutdown.
BC-12/6-15-78	Replication of Run BC-10.	Successful; operated for 120 minutes with voluntary shutdown.
BC-13/6-20-78	Replication of Run BC-10.	Successful; operated for 90 minutes with voluntary shutdown.
BC-14/6-22-78	Operate with mixture of 30% (by weight) caking coal and 70% devolatilized char at 2000 psig and coil outlet temperature of 1450°F.	Unsuccessful; coil plugged after 1 minute of operation.

Operations with caking coals were begun; the coal selected for this study is Illinois No. 6 coal, which has an FSI of 4-1/2. The coal was mixed with fine silica sand at levels of 10%, 20%, and 30% (by weight) coal in sand. Successful runs were obtained using the 10% and 20% coal-in-sand mixtures, but the coil reactor plugged when attempts were made to run the 30% coal-in-sand mixture. In these two successful runs the system outlet pressure was maintained at 2000 psig, and the coil outlet temperatures were maintained at 1450° and 1500°F with an "upsweeping" temperature profile (Figure 1) imposed over the length of the reactor.

Although chemical analyses are not yet complete, the yield of hydrocarbon liquids from the bituminous coals was found to be 17.2 grams per 100 grams of feed carbon. The yield of hydrocarbon liquids from North Dakota lignite processed under similar conditions (Runs TP-8, 10, and 11) was 12.8 grams per 100 grams of feed carbon, with the yield of hydrocarbon liquids from the Illinois No. 6 coal being approximately 30% greater.

At the end of the reporting period a single run using devolatilized char as a diluent for the Illinois No. 6 coal had been made with a mixture of 30% (by weight) coal with the char; the reactor plugged after a few minutes of operation.

A computer program has been written for calculating material, component, and elemental balances from operating data and chemical analyses obtained during the runs. In its present form the computer program can make a complete analysis of single runs, and, in its final form, the tables of information customarily given in the quarterly and annual reports will be obtained as a part of the output of the computer program. This will help reduce the time required for the compilation of these tables.

Work on the correlation of data was continued; a model proposed by Johnson[2] was examined for its ability to describe the kinetics of the hydropyrolysis of North Dakota lignite; this required a substantial extrapolation above the pressure at which the data were taken. The model predicted base carbon conversion and the total methane and ethane yield reasonably well, but the calculation of oil yields was less satisfactory.

The design of the PDU was reviewed, and, by making minor changes, it was found that the design operating pressure could be increased from 2000 to 2600 psig; these changes are being incorporated into the PDU. In addition, a low-pressure version of the combustor sections of the PDU has been built and will be operated to test the operation of the design concept and to uncover any potential problems in construction methods and materials of construction.

Our approximate position in the technical program is shown on the progress chart (Figure 2).

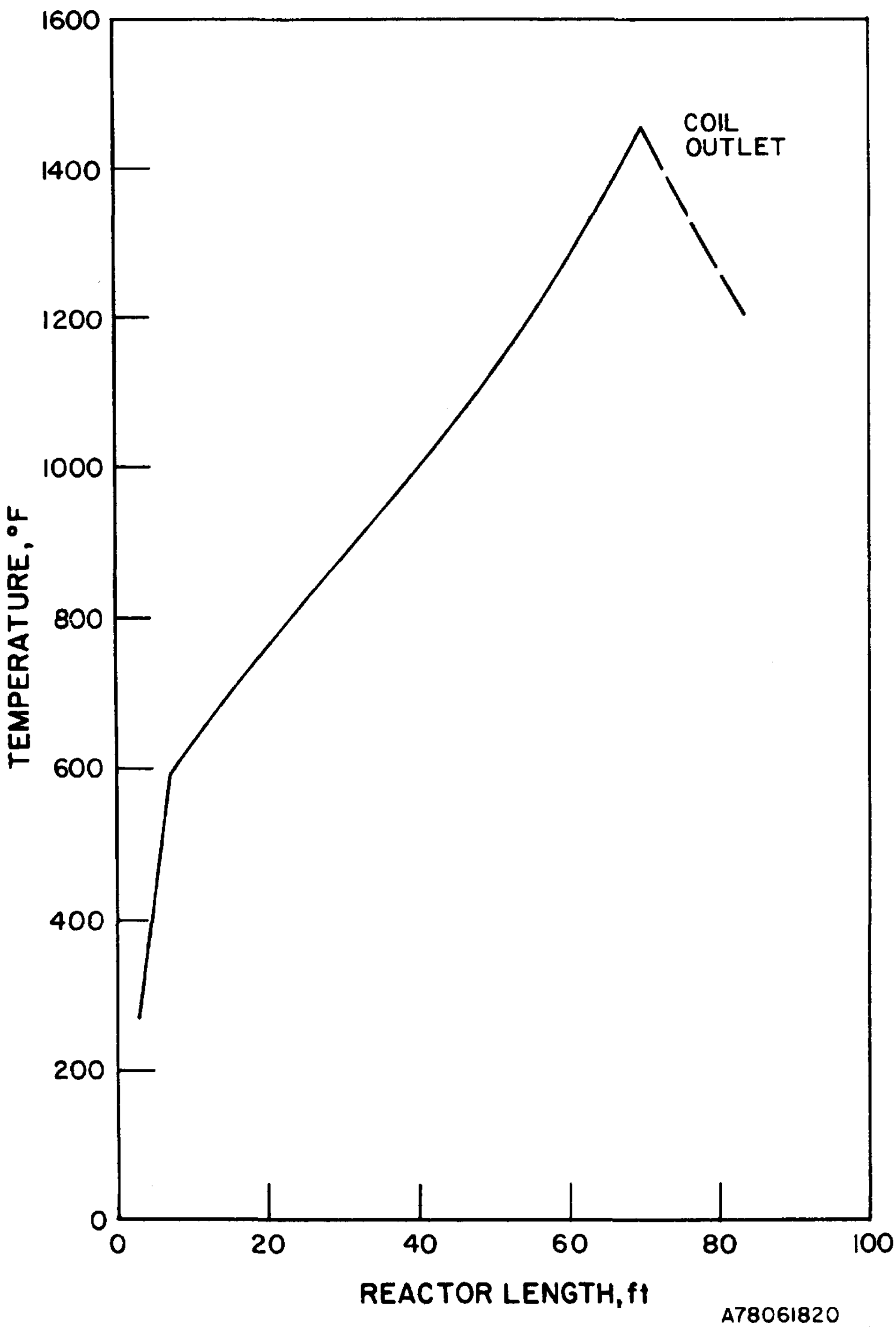

Figure 1. IMPOSED TEMPERATURE PROFILE USED IN SERIES BC RUNS

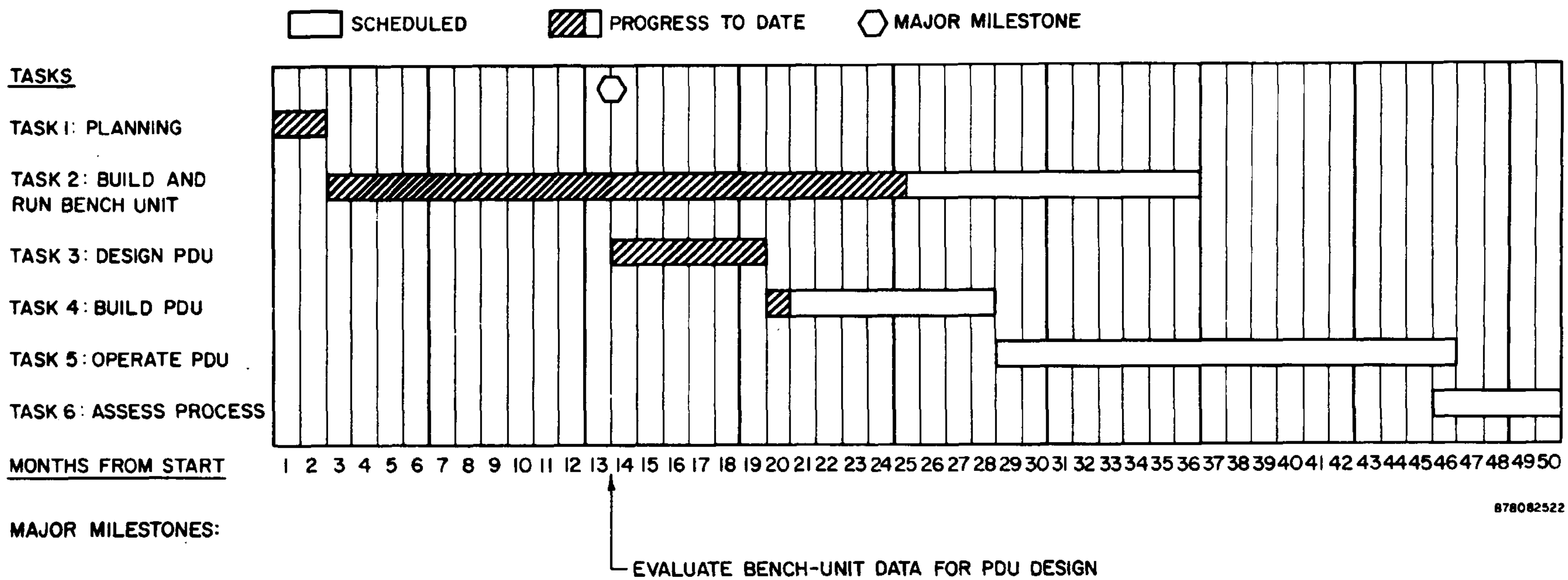

Figure 2. PROGRESS CHART

IV. DETAILED DESCRIPTION OF TECHNICAL PROGRESS

A. Task 2. Build and Operate a Bench-Scale Unit

1. Work Accomplished

a. Bench-Scale Unit Operations

During the reporting period, 20 runs were made in the bench-scale unit (Figure 3) using North Dakota lignite, mixtures of Illinois No. 6 coal and silica sand, and mixtures of Illinois No. 6 coal and devolatilized char as feed solids. The sieve analyses of these materials are shown in Table 2, and the operating conditions and main results are summarized in Table 3.

The planned runs using a reduced system operating pressure were completed (Runs PP-5 through PP-12), and exploratory work for processing caking coals was started. Although analyses are not yet complete, the proximate and ultimate analyses of the feed solids and spent solids are shown in Tables 4 and 5. The mass balances and product distributions are shown in Table 6, and the average make-gas compositions are shown in Table 7. The available chemical analyses of the main liquid product, the gasoline fraction of the main liquid product, light liquids condensed in the freeze-out train, and fuel oil fraction of the main liquid product are summarized in Tables 8, 9, 10, and 11.

From the data taken from the runs conducted at a reduced system operating pressure, it was found that both the base carbon conversion and hydrocarbon liquids yields decreased with a decrease in operating pressure. At a system outlet pressure of 1000 psig, the average base carbon conversion was 33%, and the hydrocarbon liquids yield was 9.2 grams per 100 grams of feed carbon. At a 500 psig system outlet pressure, the base carbon conversion was 26%, and the hydrocarbon liquids yield was 6.4 grams per 100 grams of feed carbon. Base carbon conversions of 50% and hydrocarbon liquids yields of as high as 18 grams per 100 grams of feed carbon have been obtained in runs at a 2000 psig system outlet pressure with similar residence times and temperature profiles.

Prior to starting work with caking coals, the connections to the char trap were changed to allow the char trap to be disconnected from the coil outlet immediately after a run. This allows the coil to be steamed out in the event of a plug. In the initial work with caking coal, the feed coal was mixed with fine silica sand, and the fraction of coal mixed with the sand was increased in successive runs until plugging of the reactor occurred. Successful runs were obtained using 10% and 20% (by weight) coal in sand, but the reactor plugged when the fraction of coal was increased to 30%.

An upsweeping temperature profile similar to that used in Runs TP-8, 10, and 11 was used in these runs (Figure 2). The average liquids yield from the caking coal was 17.2 grams per 100 grams of feed carbon, while the average hydrocarbon liquids yield using North Dakota lignite under similar processing conditions was 12.8 grams per 100 grams of feed carbon. This shows that the Illinois No. 6 coal will yield approximately 30% more hydrocarbon liquids than will North Dakota lignite.

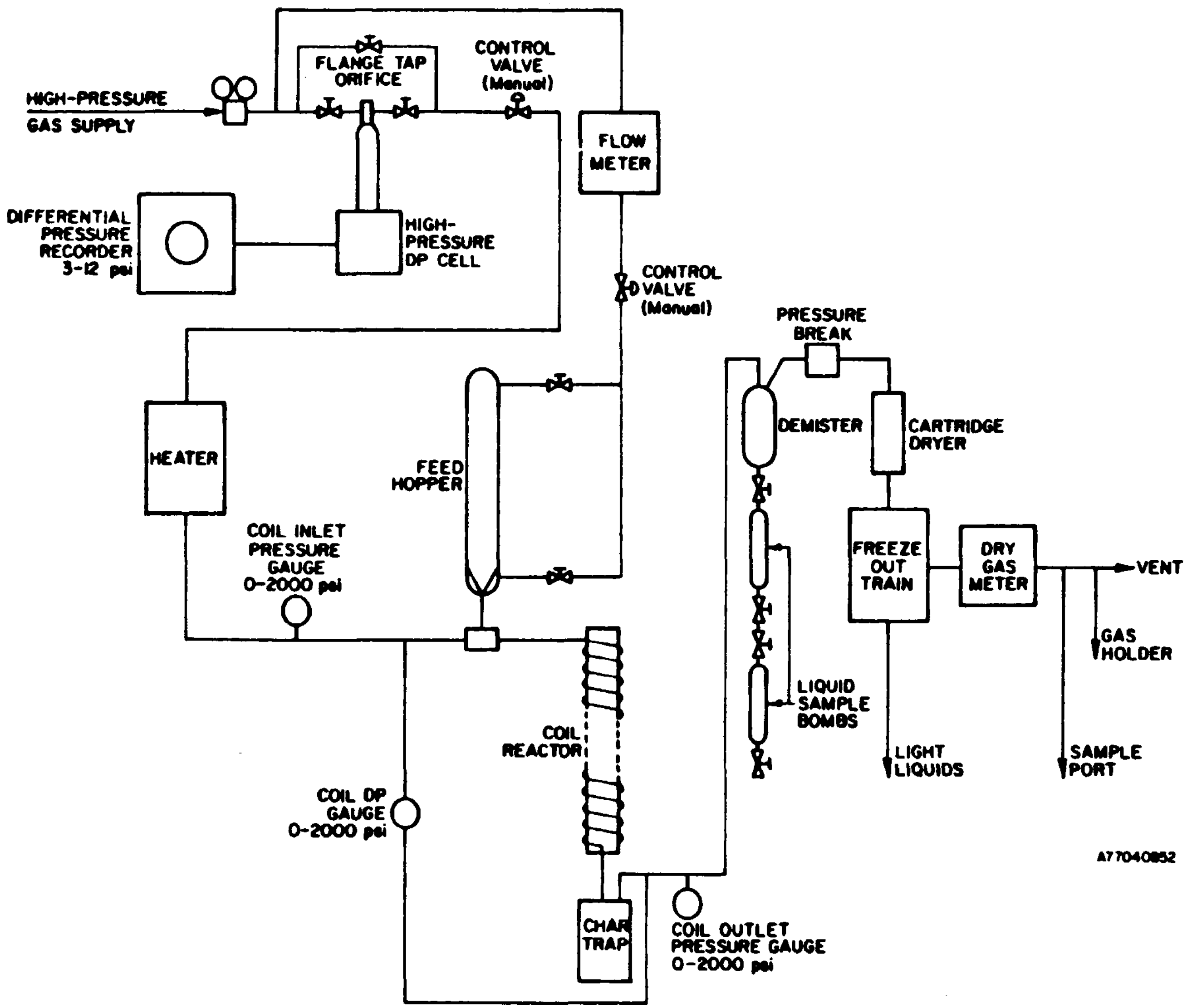

Figure 3. BENCH-SCALE UNIT

Table 2. SCREEN ANALYSES OF MATERIALS USED FROM APRIL 1 THROUGH JUNE 30, 1978

Size, U.S. Mesh	North Dakota Lignite	Illinois No. 6 Coal	Coal* and Silica Sand	Coal** and Devolatilized Char
> 60	0	0	2.8	3.4
60 x 80	1.2	24.1	11.6	13.3
80 x 100	1.9	12.0	18.0	18.4
100 x 200	13.6	40.5	35.7	33.3
200 x 325	34.4	21.4	15.7	17.3
pan	48.9	1.5	16.2	14.3
	100.0	100.0	100.0	100.0

*20% (by weight) Illinois No. 6 coal with 80% silica sand.

**20%(by weight) Illinois No. 6 coal with 80% devolatized char.

Table 3. OPERATING CONDITIONS AND RESULTS OF RUNS MADE FROM MARCH 1 THROUGH JUNE 30, 1978

Run No.	PP-5	PP-9	PP-11	PP-12	BC-1	BC-3	BC-7	BC-9	BC-11	BC-12	BC-13
System Outlet Pressure, psig	500	1000	500	1000	2000	2000	2000	2000	2000	2000	2000
Coil Outlet Temperature, ^{o}F	1500	1500	1500	1500	1450	1450	1450	1450	1500	1500	1500
Residence Time, s	2.6	2.7	2.9	0	3.2	3.1	3.5	3.4	3.5	3.2	3.4
Solids Feed Rate, lb/hr	1.9	2.4	1.4	0.74	6.0	6.7	6.0	4.0	3.1	2.5	2.5
Run Length, min	70	120	180	180	55	60	90	90	90	120	90
Solids in Feed Gas, wt %	76.9	75.8	85.0	49.7	81.1	80.8	81.1	72.4	67.7	60.0	0
H_2/MAF Coal Weight Ratio	0.19	0.23	0.23	0.76	1.34	0.77	0.71	--	--	--	
Balances, wt %											
Ash	88.2	98.6	96.9	93.0	98.5	97.9	100.2	--	--	--	
Carbon	--	--	--	--	--	--	--	--	--	--	
Hydrogen	--	--	--	--	--	--	--	--	--	--	
Overall	90.5	99.2	95.0	95.8	100.8	98.0	100.4	98.2	98.9	99.0	97.3
Carbon Distribution, wt %											
Liquids	--	--	--	--	--	--	--	--	--	--	--
Carbon Oxides	8.06	7.51	6.12	9.34	6.00	3.71	5.50	--	--	--	--
Methane	7.75	9.57	5.86	13.95	10.80	9.92	9.66	--	--	--	--
Light Gases	3.56	4.45	3.27	6.25	7.33	7.26	7.73	--	--	--	--
Char	66.00	68.71	74.25	60.23	63.25	66.18	62.88	--	--	--	--

A78072385

Table 4. ANALYSIS OF FEED SOLIDS

Run No.	PP-5*	PP-9*	PP-11*	PP-12*	BC-1**	BC-3†	BC-7†	Illinois No. 6 Coal	Devolatilized Char
	wt %								
Proximate Analysis									
Moisture	10.1	12.9	15.9	15.7	0.3	1.0	1.1	5.3	0.7
Volatile Matter	37.1	36.0	35.2	34.8	3.9	7.5	8.3	37.6	1.7
Ash	10.1	8.9	8.8	8.8	90.7	81.6	80.5	10.2	27.5
Fixed Carbon	42.7	42.2	40.1	40.7	5.1	9.9	10.1	46.9	70.1
Total	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Ulimate Analysis (Dry Basis)									
Ash	11.24	10.27	10.43	10.40	90.99	82.40	81.39	10.76	27.72
Carbon	60.5	61.3	61.1	61.9	7.00	13.7	14.4	68.8	69.40
Hydrogen	4.02	4.13	4.13	4.15	0.53	1.02	1.01	5.03	0.34
Sulfur	0.88	0.79	0.80	0.78	0.37	0.74	0.77	4.16	1.91
Nitrogen	0.78	0.81	0.82	0.79	0.12	0.10	0.24	1.16	0.72
Oxygen (by difference)	22.58	22.70	22.72	21.98	0.99	2.04	2.19	10.09	0
Total	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.0	100.0

*North Dakota lignite.

**10% (by weight) Illinois No. 6 coal with 90% silica sand.

†20% (by weight) Illinois No. 6 coal with 80% silica sand.

B78072386

Table 5. ANALYSIS OF SPENT SOLIDS

Run No.	PP-5	PP-9	PP-11	PP-12	BC-1	BC-3	BC-7
	wt						
Proximate Analysis							
Moisture	0.5	0.9	0.9	0.90	0.10	0.10	0.1
Volatile Matter	11.3	12.1	12.1	11.7	0.9	1.7	1.9
Ash	18.3	17.6	16.5	18.9	95.0	88.9	88.9
Fixed Carbon	69.9	69.4	70.5	68.5	4.0	9.3	9.1
Total	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Ultimate Analysis (Dry Basis)							
Ash	18.41	17.8	16.67	19.06	95.12	89.01	89.01
Carbon	74.2	74.0	74.8	73.5	4.70	10.0	9.9
Hydrogen	2.36	2.43	2.43	2.34	0.19	0.41	0.42
Sulfur	0.79	0.64	0.68	0.76	0.13	0.27	0.25
Nitrogen	0.60	0.67	0.65	0.57	0.08	0.03	0.13
Oxygen (by difference)	3.64	4.46	4.77	3.77	0	0.28	0.29
Total	100.00	100.00	100.00	100.00	100.00	100.00	100.00

B78072387

Table 6. MASS BALANCES AND PRODUCT DISTRIBUTIONS IN RECENT RUNS

Run No.	PP-5	PP-9	PP-11	PP-12	BC-1	BC-3	BC-7	BC-9	BC-11	BC-12	BC-13
Component	g										
Feed Solids	981	2207	1968	1008	2474	3025	4071	2729	2076	2227	1692
Feed Hydrogen	150	400	333	582	310	407	534	564	538	765	564
Feed Methane	8	16	1	35	9	15	19	23	26	36	10
Feed CO	7	17	0	0	9	6	23	16	23	11	66
Feed Nitrogen	11	17	9	35	23	24	31	25	23	34	8
Feed Argon	119	256	4	370	226	269	343	410	380	638	422
Total Mass In	1276	2913	2315	2030	3051	3746	5021	3767	3066	3711	2762
Spent Char/Solids	477	1104	1013	435	2326	2718	3686	2469	1848	1986	1470
Liquids	244	701	521	330	59	144	211	127	106	111	88
Light Liquids	5	21	13	22	4	8	9	4	30	12	13
Gases	429	1065	652	1158	685	800	1136	1099	1055	1565	1117
Total Mass Out	1155	2891	2199	1945	3074	3670	5042	3699	3039	3674	2688
Distribution of Products											
Hydrogen	115	346	313	518	336	380	501	528	510	745	524
Nitrogen	26	24	13	35	56	34	55	23	13	22	21
Argon	98	253	7	346	227	256	363	381	368	628	442
Methane	55	151	79	98	25	54	75	52	56	62	43
Ethane	21	62	41	41	8	26	38	23	24	29	19
Propane	1	0	0	0	6	10	13	7	0	0	0
Light Gases (C_2-C_4)	1	4	0	0	1	1	4	3	0	1	2
Carbon Oxides	111	225	174	119	24	39	80	61	95	78	66
Hydrocarbon Liquids											
Main Liquid Product (MLP)	29	96	52	22	26	68	99	53	45	40	26
Freeze-Out	5	19	13	21	1	5	6	4	10	11	9
Make-Gas	0	0	0	0	0	0	0	0	0	0	0
Gases (MLP work-up)	8	14	11	7	0	0	0	1	3	1	3
Char	477	1104	1013	435	2326	2718	3686	2469	1848	1986	1470
Water (by difference)	207	593	483	303	37	79	122	94	67	71	63
Total Mass Out	1155	2891	2199	1945	3073	3670	5042	3699	3039	3674	2688

A78072388

Table 7. AVERAGE MAKE-GAS COMPOSITIONS

Run No.	PP-5	PP-9	PP-11	PP-12	BC-1	BC-3	BC-7	BC-9	BC-11	BC-12	BC-13
	mol % (wet basis)										
Component											
CO	3.56	2.45	1.88	1.13	0.34	0.37	0.65	0.56	0.86	0.65	0.72
CO_2	0.83	0.45	0.62	0.09	0	0 07	0.10	0.07	0.10	0	0
Hydrogen	72.22	75.03	79.81	87.74	93.39	92.11	90.72	92.95	93.05	93.08	92.78
Methane	4.10	3.66	2.43	1.73	0.62	1.19	1.43	0.97	1.04	0.87	0.82
Ethane	0.84	0.80	0.52	0.31	0.12	0.30	0.40	0.24	0.26	0.22	0.21
Propane	0.03	0	0.02	0	0.06	0.08	0.09	0.05	0	0	0
Butane	0	0	0	0	0	0	0	0.03	0	0	0
Ethylene	0.04	0.05	0.06	0.03	0.01	0.01	0.01	0.0	0.02	0.01	0.02
Propylene	0	0	0.01	0	0	0	0.02	0	0	0	0
Acetylene	0	0	0	0	0.01	0	0.01	0	0	0	0
Benzene	0.01	0	0	0	0	0	0	0	0	0	0
Argon	3.16	2.77	0.02	3.04	3.18	3.13	3.32	3.38	3.39	3.99	3.95
Nitrogen	0.57	0.38	0.13	0.24	1.13	0.59	0.72	0.30	0.17	0.20	0.27
Steam	14.63	14.39	14.46	5.69	1.13	2.14	2.45	1.43	1.12	0.98	1.23
Total	99.99	99.98	99.96	100.00	99.98	100.00	99.97	99.98	100.00	100.00	100.00

B78072389

Table 8. ANALYSES OF MAIN LIQUID PRODUCT

Run No.	RT-3	PS-1	PP-2	PP-4	PP-9	PP-11	PP-12	BC-1	BC-3	BC-7,9	BC-11,12,13
Specific Gravity	1.028	1.058	1.061	0.999	1.010	1.051	1.051	1.093	1.065	1.079	*
IBP, °F	160	145	154	154	153	*	*	*	156	149	153
Ultimate Analysis, wt%											
C	88.63	82.65	80.65	80.68	85.36	*	*	82.80	*	80.00	81.56
H	6.68	7.15	6.53	6.17	6.54	*	*	6.47	*	6.62	6.05
S	0.79	0.30	2.01	0.72	0.79	*	*	2.72	3.26	2.57	2.71
N	0.46	0.59	0.61	0.37	0.69	*	*	*	*	*	*
O (by difference)	2.84	7.81	10.2	12.06	6.62	*	*	*	*	*	*
Ash	0.6	1.5	0	0	0	*	*	*	*	0	0.2
C/H Weight Ratio	13.27	11.56	12.35	13.08	13.05	*	*	*	*	12.08	13.48
Fraction, wt%											
C_5-400°F	40.7	38.3	38.3	**	49.7	*	*	*	41.6	44.8	29.9
400°F +	56.0	58.0	57.5	**	44.9	*	*	*	56.1	55.2	64.5

* In process.
** Insufficient sample.

B78072390

Table 9. ANALYSES OF GASOLINE FRACTION OF MAIN LIQUID PRODUCT

Run No.	RT-3	PS-1	PP-2	PP-4	BC-3	BC-7, 9
	wt %					
Component						
Benzene	36.1	3.19	10.4	33.4	4.77	4.36
Toluene	25.4	9.28	17.0	23.9	15.5	15.6
Ethylbenzene	1.24	2.56	1.13	0.59	3.99	3.51
Xylenes	3.23	7.82	5.06	2.63	7.22	9.32
C_9 Aromatics	0.40	5.40	2.32	0.55	3.35	4.80
Indans	2.25	4.62	3.88	2.42	5.47	6.94
Indene	0.28	0.53	0.24	0.07	0.13	0.08
Naphthalenes	13.9	5.41	21.15	17.48	10.56	12.78
Phenol	14.5	31.0	28.4	17.0	30.90	21.6
Cresols	0.44	20.0	7.98	0.73	13.12	14.21
C_8 Phenols	0	1.33	0.47	0	0.41	0.63
Unidentified	2.26	8.86	1.87	1.23	4.58*	6.17*
Total	100.00	100.00	100.00	100.00	100.00	100.00

* 75% or more thiophene and thiophene derivatives.

Table 10. ANALYSES OF COLD-TRAP LIQUIDS

Run No.	PP-5	PP-9	PP-11	PP-12	BC-1	BC-3	BC-7	BC-9	BC-11	BC-12	BC-13
Component	wt %										
Benzene	84.0	89.1	82.4	90.4	7.70	56.6	49.2	41.8	80.5	85.3	64.8
Toluene	13.4	9.56	15.0	7.77	60.50	30.5	34.7	39.5	13.8	10.5	27.6
Xylene	0.63	0.24	0.68	0.50	12.48	3.48	4.74	5.47	0.67	0.82	2.10
Indene & Indan	0.60	0.12	0.41	0.14	2.97	0.72	1.08	1.68	0.38	0.21	0.40
Ethylbenzene	0.14	0.05	0.16	0.11	7.19	2.52	3.25	3.84	0.59	0.41	1.14
Naphthalenes	0.11	0.06	0.54	0.10	3.21	1.26	1.03	1.37	0.75	0.26	0.94
Unidentified	1.12	0.87	0.81	0.98	5.95*	4.42	5.28	6.34	3.31	2.50	3.02
Total	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

* Unidentified fraction 90% thiophene and derivatives of thiophene.

B78072391

Table 11. ANALYSES OF FUEL OIL FRACTION OF MAIN LIQUID PRODUCT

Run No.	RT-3	PS-1	PP-2	PP-4	PP-9	BC-3	BC-7	BC-11*
Ultimate Analysis, wt%								
C	88.27	87.09	85.78	**	91.99	84.64	83.43	87.40
H	5.85	6.80	6.14	**	5.97	5.98	5.80	5.68
S	0.12	0.13	0.23	0.15	0.11	**	1.17	**
N	0.43	0.16	0.15	0.09	0.66	**	**	**
O (by difference)	4.26	3.23	7.70	**	1.77	**	**	**
Ash	1.07	2.59	0	**	0	**	**	0.31
C/H Weight Ratio	15.09	12.81	13.97	**	15.32	14.15	14.38	15.39
CC Residue, wt%	3.8	13.5	20.9	8.3	6.19	19.1	18.8	**

* Combined product from Runs BC-11, 12, and 13.

** In process.

B78072392

The composition of the gasoline fraction of the main liquid product from Illinois No. 6 coal (Table 9, Runs BC-3, 7, and 9) is generally similar to that obtained from North Dakota lignite under similar processing conditions except that the sulfur content is higher. The gasoline fraction is rich in oxygenated compounds, toluene, xylenes, and ethyl benzene.

b. Data Analysis

A computer program has been written that will compile material and component balances from operating data and will also calculate the research octane number of the liquids in the gasoline boiling range. In its present form, the program analyzes single runs, and, in a further phase, it will store data from single runs "on disk" so that information needed for monthly, quarterly, and annual reports can be recalled and printed directly into tables.

In further investigations of mathematical models, a preliminary investigation of the model proposed by Johnson[2] was made. In making the analysis, it was necessary to extrapolate beyond the range of Johnson's data. The model appears to be a good predictor of total carbon conversion and methane plus ethane yields, but prediction of oil yields was less satisfactory. The ability of the model to account for variations in conversion with hydrogen partial pressure is of interest, and further efforts will be made to correlate data with this model.

c. Simulation of PDU Combustor

A low-pressure version of the combustor section of the PDU has been built; it will be used to explore the operation of the design concept and to uncover potential construction and materials of construction problems prior to incorporation into the PDU.

2. Work Forecast

Work on processing of caking coals will be continued; devolatilized char will be evaluated as a diluent. Following this, a low-temperature entrained-flow hydrotreatment analogous to that described by Kawa, *et al.*[3] will be tried. Other methods, such as the use of alkali metal carbonates (also described by Kawa, *et al.*[3]) will be considered.

B. Task 3. Design a PDU

The PDU design has been issued and approved.

C. Task 4. Construction of a PDU

The design of the PDU has been reviewed, and, with minor changes, the operating pressure can be increased from 2000 to 2600 psig. The task is now in the initial procurement stage; the construction site within the pilot plant is being readied, and suppliers of large-volume hydrogen, oxygen, and nitrogen at high pressure have been contacted to provide the needed gases for the eventual operation of the PDU.

V. CONCLUSIONS

The main findings from the work performed during the reporting period can be summarized as follows:

1. Both base carbon conversions and hydrocarbon liquids yields are reduced as system operating pressure is reduced.

2. Caking coals can be processed by mixing the caking coal with sand of the same particle size range as that of the coal. The coal fraction that can be processed will depend also on the reactor geometry. The 1/8-inch ID reactor could handle a 20% (by weight) coal-in-sand mixture.

3. Hydrocarbon liquids yields from Illinois No. 6 coal are significantly greater than the liquids yields obtained from North Dakota lignite.

4. The operating pressure of the PDU can be increased from 2000 to 2600 psig.

PATENT STATUS

The work performed during the reporting period is not considered patentable.

LITERATURE CITED

1. Hiteshue, R. W., Friedman, S. and Madden, R., "Hydrogasification of High-Volatile A Bituminous Coal," Report of Investigations 6376. Washington, D.C: 1964.

2. Johnson, James L., "Kinetics of Initial Coal Hydrogasification Stages." Paper presented at the 173rd National Meeting of the American Chemical Society, New Orleans, La., March 1977.

3. Kawa, W. et al., "Agglomeration Studies in the Low Pressure Hydrogenation of Coal in a Fluidized Bed," Bulletin 579. Washington, D.C.: U.S. Bureau of Mines, 1959.

*U.S. GOVERNMENT PRINTING OFFICE: 1979-640-014/4492. Region 4.