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IMPACT OF HYDROGEN PARTIAL PRESSURE ON
COAL LIQUEFACTION

Final Technical Report

By
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MASTER

June 1984

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Air Products and Chemicals, Inc.
Allentown, Pennsylvania

and

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FINAL TECHNICAL REPORT:
IMPACT OF HYDROGEN PARTIAL PRESSURE
ON COAL LIQUEFACTION

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UNITED STATES DEPARTMENT OF ENERGY
Office of Solvent-Refined Coal Products
under Contract DE-AC05-78-OR-03054

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ABSTRACT

This program was conducted to determine the effects of hydrogen partial pressure on the SRC-I direct coal liquefaction process and SRC-I Demonstration Plant design. A native solvent was produced in quantity and slurried with Kentucky #9 Mulford coal in a series of coal liquefaction runs under varying hydrogen gas rates, temperatures, residence times, and hydrogen partial pressures. The results showed that hydrogen partial pressure significantly affected product distribution; the magnitude of the effect was comparable to changes in temperature and residence time. Also, the impact of hydrogen partial pressure was enhanced by increases in both temperature and residence time. Operating at low hydrogen partial pressure did not show any apparent advantage; it reduced coal conversion, reduced oil yield, and had a detrimental effect on the yield distribution of other products.

EXECUTIVE SUMMARY

Because hydrogen partial pressure is one of the least understood process variables in SRC-I coal liquefaction, a study was conducted to determine its effects. Kentucky #9 Mulford coal was slurried with native solvent and processed through Air Products' continuous coal process development unit under wide ranges of hydrogen gas rates (7.5-60 M scf/ton of coal), temperatures (760-840°F), residence times (20-60 min), and hydrogen partial pressures (400 to 1,800 psia).

This study provides an investigation into how hydrogen partial pressure affects product distribution from coal liquefaction over a wide range of hydrogen partial pressures. The results show that changes in hydrogen partial pressure significantly impact the product distribution; the magnitude of the effect is comparable to that of temperature and residence time. Furthermore, the effect is enhanced when temperature and/or residence time increase. Decreases of the hydrogen partial pressure below 700 psia cause severe coking reactions when the temperature is raised to 840°F.

An increase in hydrogen partial pressure had the following effects:

- o increased coal conversion
- o increased conversion of asphaltenes and preasphaltenes to lighter products
- o significantly increased the oil yield
- o increased light gas yields
- o decreased sulfur content in the SRC
- o increased hydrogen content of the recycle solvent
- o increased hydrogen consumption

This study strongly suggests that further studies should be conducted to optimize the effects of hydrogen partial pressure on the process, both within and, preferably, beyond the constraints of the current basic SRC-I design, considering the major impact of this variable on the process.

1.0 INTRODUCTION

One of the least understood variables in the SRC-I process is the impact of hydrogen partial pressure and how it interacts with dissolver temperature, slurry residence time, and product distribution. Hydrogen partial pressure is not an explicit part of ICRC's current sequential or parallel kinetic model of the SRC-I process (Givens et al., 1983), but it will be included in future versions.

The purpose of this program was to determine the effects of hydrogen partial pressure on coal liquefaction in a native solvent, and to develop a data base that would enable this parameter to be incorporated into ICRC's kinetic model. This data base will also enable ICRC to evaluate an optional operating mode, based on low hydrogen partial pressure operation, which may result in substantial capital and operating cost savings. In addition, the data base can be used to predict dissolver behavior should hydrogen flow into the dissolvers be inadvertently interrupted and reduced below the normal SRC-I operating range. Therefore, these data will also provide a guideline for developing a trouble-shooting strategy should such adverse situations arise.

The specific objectives of the program were:

- o to determine liquefaction behavior under a wide range of hydrogen partial pressures falling within SRC-I process conditions.
- o to determine whether coking occurs at low hydrogen partial pressures.
- o to determine the effect of hydrogen partial pressure on product distribution and solvent hydrogen content.
- o to address hydrogen partial pressure as a design variable.

2.0 EXPERIMENTAL PROGRAM

2.1 Experimental Conditions for Process Runs

Process runs were conducted with 40 wt % Kentucky #9 Mulford coal in a native solvent derived from the same Mulford coal in Air Products' coal process development unit (CPDU) (see Figure 1 for a schematic). A detailed flow diagram and description of the CPDU have been documented by International Coal Refining Co. (ICRC, 1979).

The following ranges of process conditions were studied in these runs:

Run number	BCL-71
Coal	Kentucky #9 Mulford coal
Slurry concentration (wt %)	40
Temperature (°F)	760/800/840
Total pressure (psig)	2,000
Feed gas composition	Hydrogen and mixture of 50% hydrogen and 50% diluent gas
Hydrogen rates (M scf/ton of coal)	7.5-60
Hydrogen partial pressure (psia)	400-1,800
Nominal residence time (min)	20-60
Space rate (lb of coal/ft ³ -hr)	28-85

During run BCL-71, 17 data points were obtained under wide ranges of hydrogen partial pressure (400-1,800 psia), residence time (20-60 min), and temperature (760-840°F). The hydrogen partial pressure was controlled by changing feed gas rates and by diluting feed hydrogen gas with nitrogen (50% hydrogen-50% diluent gas). Feed compositions and specific experimental conditions for each data point are summarized in Table 1.

Operating data for run BCL-71 are detailed in Appendix A-1 and complete material-balance and sample work-up data are included in Appendix A-2.

Figure 1

**APCI COAL PROCESS DEVELOPMENT UNIT
(COAL LIQUEFACTION SYSTEM #1)**

Table 1

Feed Compositions and Specific Experimental Conditions of
Runs with Pure Hydrogen and Nitrogen-Diluted Hydrogen Feed Gas

Run no.	Coal concentration (wt %)	Feed gas ^a composition	Temp (°F)	Residence time (min)	Total feed gas rate (M scf/ton)	H ₂ gas rate (M scf/ton)	H ₂ pressure in feed (psia)	Total pressure (psig)
1	40	H ₂ /N ₂	760	60	30	15	1007	2000
2	40	H ₂	760	60	15	15	1975	2000
3	40	H ₂	760	60	60	60	1975	2000
4	40	H ₂ /N ₂	800	20	15	7.5	1007	2000
5	40	H ₂ /N ₂	800	20	30	15	1007	2000
6	40	H ₂	800	20	15	15	1975	2000
7	40	H ₂	800	20	60	60	1975	2000
8	40	H ₂ /N ₂	800	60	30	15	1007	2000
9	40	H ₂	800	60	15	15	1975	2000
10	40	H ₂	800	60	60	60	1975	2000
11	40	H ₂ /N ₂	840	20	15	7.5	1007	2000
12	40	H ₂ /N ₂	840	20	30	15	1007	2000
13	40	H ₂	840	20	15	15	1975	2000
14	40	H ₂	840	20	60	60	1975	2000
15	40	H ₂ /N ₂	840	60	30	15	1007	2000
16	40	H ₂	840	60	15	15	1975	2000
17	40	H ₂	840	60	60	60	1975	2000

^a H₂/N₂ = Mixture of 50 mol % H₂ and 50 mol % diluent gases.

H₂ = Mixture of 98 mol % H₂ and 2 mol % reference gas.

2.2 Feed Materials

2.2.1 Coal. Kentucky #9 Mulford coal is a western Kentucky high-volatile C bituminous coal that meets SRC-I base-case specifications. This coal is from the same source as that used for the liquefaction parametric studies conducted over the past two years, including the native solvent liquefaction study of Kang et al. (1984); however, the batches differ. Proximate and ultimate analyses of the representative coal samples used for this run (BCL-71) are compared in Table 2 with a Mulford coal sample used in an earlier native solvent liquefaction run (BCL-69), to illustrate the variations in the feed coal compositions.

These data show that elemental compositions of the feed coals used in this and previous studies were apparently uniform; however, a significant difference in ash concentration for different batches was noticeable. Feed coal was one of the major variables affecting product distribution during the development of our data base. We observed variations not only among different sources of Kentucky #9 coal, but also among different batches of the same coal. Therefore, throughout the study the feed coal was riffled before use in order to ensure its uniformity.

Unexpectedly, the yields from liquefaction of Mulford coal in native solvent obtained in this study (run BCL-71) deviate significantly from those obtained in the previous run (BCL-69) performed with Mulford coal and native solvent. Unfortunately, detailed analyses of the feed coals and solvents could not be made due to time constraints. However, we speculate that higher reactivity of the new batch of Mulford coal might have been caused by more reactive macerals in this coal compared with that of the earlier batch, which probably resulted from inconsistent coal cleaning. Significant differences in the ash

Table 2

Proximate and Ultimate Analyses of Kentucky #9 Mulford Coal

Proximate analysis (wt %)		
Coal sample no.	FSK9-196/197	FSK9-157/178
Run no.	BCL-71	BCL-69
Moisture	2.36 (4.04 ^a)	* NNAB
Volatile matter	39.88	NDA
Fixed carbon	49.61	NDA
Ash	8.51	NDA
Ultimate analysis (wt %, moisture-free basis)		
Coal sample no.	FSK9-196/197	FSK9-157/178
Run no.	BCL-71	BCL-69
Carbon	71.30	71.59
Hydrogen	4.99	4.97
Oxygen	10.73	10.58
Nitrogen	1.55	1.63
Sulfur	3.08	3.02
Organic	1.76	NDA
Pyritic	0.96	NDA
Sulfate	0.36	NDA
Ash	8.35	9.66

a Karl Fisher titration method.

b No data available.

concentration between the batches tend to support this conclusion. Therefore, the interpretations in this study were based primarily on data from BCL-71.

2.2.2 Process Solvent. Native solvent was prepared by processing Kentucky #9 Mulford coal through 2- and 1-gal continuous stirred tank reactors (CSTRs) (Hoover et al., 1983) with a Ft. Lewis SRC-I process-derived solvent as the starting solvent.

The starting solvent (derived from Kentucky #9 Fies coal) was transformed to native solvent by completing approximately 5 passes (a mixture of solvents from passes 2, 3, 6, and 7) through the process unit under the following conditions:

Coal	Kentucky #9 Mulford
Coal concentration (wt %)	40
Reaction temperature (°F)	840
Nominal residence time (min)	40
Hydrogen pressure (psig)	2000
Hydrogen feed rate (M scf/ton)	30

The process solvent (450-850°F boiling cut) was recovered from the product slurry from each pass by batch distillation and recycled to the process unit to obtain the native solvent.

The native process solvent derived from processing Mulford coal in the CPDU consisted of 99.7% pentane-soluble oils and 0.3% asphaltenes, with a total hydrogen content of 7.9%. Table 3 compares the native solvent used for this study with those used for the earlier Mulford coal liquefaction studies.

Ft. Lewis solvent was used to develop most of the earlier Mulford coal liquefaction data base developed by ICRC (Kang and Givens, 1983; Sivasubramanian and Givens, 1983). This starting solvent and the earlier Ft. Lewis solvent contained a significant amount of asphaltenes (5.31% and 3.82%,

Table 3

Comparison of Solvent Properties

Process solvents	Composition (wt %)						
	Solvent fraction		Elemental				
	Oils	Asphaltenes	C	H	N	S	O
Start-up solvent for native solvent preparation run (HCL-68) (Ft. Lewis)	94.69	5.31	88.09	7.90	1.00	0.46	2.64
Pass 1 solvent	99.90	0.10	87.75	<u>8.12</u>	0.80	--	--
Pass 2 solvent	99.84	0.16	87.92	<u>8.04</u>	0.78		
Native solvent I (passes 3 and 6 solvent blend) ^a	99.76	0.24	88.72	<u>7.87</u>	0.84	0.48	2.09
Native solvent II (passes 2, 3, 6, and 7 solvent blend) ^b	99.74	0.26	88.33	<u>7.89</u>	0.79	0.49	--
Ft. Lewis solvent ^c	96.18	3.82	87.76	<u>8.24</u>	0.85	0.36	2.95

a Kentucky #9 coal derived solvent used for Mulford coal parametric study with native solvent through CPDU runs 69 and 70.

b Kentucky #9 coal derived solvent used for this study (Run BCL-71). Solvents from passes 3-7 were not analyzed.

c Used for Mulford coal CPDU runs 55-66.

respectively) compared to the trace amounts present in the freshly distilled solvents. The Ft. Lewis solvents may have developed these heavier materials during storage or the distillation cut points at the Ft. Lewis plant may have differed significantly from the native solvent batch-distillation cut points. Hydrogen content in the first pass solvent increased due mainly to the removal of heavyasphaltenic materials, which carry significantly less hydrogen compared with the remaining oil components. With additional recycle passes, the hydrogen content of the solvent tended to decrease, indicating the CSTR in the CPDU is less effective at hydrogenating the solvent than was the tubular reactor in the Ft. Lewis plant. This assumes that the hydrogen content of the CPDU recycle solvent shifted to a level below the Ft. Lewis steady-state hydrogen concentration during preparation of the native solvent. However, these differences in solvent properties also may have been due to the two different feed coals, namely, Mulford and Fies, or to the differences in both reactor hydrodynamics and feed coals. The higher oxygen content of the Ft. Lewis solvents may have been due to oxidation during storage.

Boiling-cut distributions determined by simulated gas chromatographic (GC) distillation (modified ASTM D2886, Wilsonville method) (Schweighardt et al., 1983) for the start up solvent and the Mulford-derived native solvent mixture are compared in Table 4. No significant differences were observed, except that the start-up solvent contained heavier asphaltenic materials, which could not be detected by simulated distillation.

2.3 Preparation of Feed Gases and Measurement of Gas Streams

Feed gases for this study were prepared by admixing pure hydrogen gas with either ~2 mol % reference gas or 48 mol % nitrogen diluent and 2 mol % reference gas in tube trailers. Because enough gas was stored

Table 4

Comparison of GC Simulated Distillation Cuts (wt %)
(Wilsonville Method)

Distillation cut (°F)	Start-up solvent (Ft. Lewis, Fies)	Passes 3/6 solvent blend ^a (CPDU, Mulford native)	Passes 2/3/6/7 solvent blend ^b (CPDU, Mulford native)
<350	1.28	0.34	0.90
350-450	5.39	7.18	8.20
450-550	23.17	23.98	24.67
550-650	40.63	44.97	39.53
650-750	23.14	21.15	22.46
750-850	6.39	2.39	4.24
>850	N.D. ^c	N.D.	N.D.

^a Mulford-derived native solvent used for previous Runs 69 and 70.

^b Mulford-derived native solvent used during Run BCL-71 for current study.

^c Not determined and unknown.

In the trailers before each process run to keep the feed gases uniform, hydrogen purities were maintained at either 98 or 50%. In order to assure complete mixing of the diluent gases, the feed gases were blended long before their use. Feed gas flow rates to the CPDU were determined by means of a known volume of liquid (glycol) displaced by incoming feed gas flow to the reactor (ICRC, 1979). The feed gas rate at run conditions of volume, pressure, and temperature was converted to that at a standard gas state (0°C and 1 atm) by using the modified Peng-Robinson equation-of-state correlation that is incorporated in ICRC's current ASPEN Plus SRC-I computer simulation program. Examples 1 and 2 illustrate physical properties of feed gases calculated at typical run conditions:

	<u>Example 1</u>	<u>Example 2</u>
Feed gas composition (H ₂ /Reference Gas/N ₂)	98/2/0	50/2/48
Temperature (°F)	70	70
Pressure (psia)	2014.7	2014.7
Density (lb/ft ³)	0.8783	5.2291
Avg. molecular weight (g/g-mol)	2.6890	15.7896
Molar volume (mL/mol)	190.398	185.699
Compressibility factor	1.0807	1.0540

To ensure uniformity, the feed gases were analyzed periodically using gas chromatography, especially during material-balancing. Product gas samples were simultaneously analyzed to determine gas-balance closure based on the reference gas. Product gas rates determined by a dry test meter were not usually reliable because unaccountable gas leaks often developed during the runs. Although accurate determination of hydrogen consumption and gas production is significantly affected by the accuracy of the gas flow rate measurement, other yield data are not as significantly impacted. This is due to the relative weights of these components in the product stream.

2.4 Product Work-up

2.4.1 Gas Products. Gas chromatography was used to analyze all feed and product gas components except water and ammonia. The product off-gas water concentration was assumed to be in equilibrium with the liquids (mainly aqueous condensate with trace amounts of light oils) in the ice-bathed light-oil knock-out condenser. Ammonia gas in the off-gas was scrubbed in 0.1 N sulfuric acid by passing product gases through an on-line scrubber system specially developed for this study. Subsequently, ammonia gas abducted by sulfuric acid was quantified by use of an ammonium ion selective electrode.

2.4.2 Condensed Products. Condensed products recovered from the unit were aqueous and light-oil condensates and product slurry. Condensates were not analyzed in detail because the relative amounts were insignificant compared to the large amount of product slurry. Elemental compositions of these condensates were assumed to be those of water and light oils that had been typically observed during previous Mulford coal process runs. The boiling cuts of light condensates were assumed to be those of typical light-oil condensates.

Dissolved water in feed and product slurries was quantified by the Karl-Fisher titration method to determine the water balance between feed and product. The product slurry was solvent-fractionated to oils, asphaltenes, preasphaltenes, and residues by sequentially dissolving product slurry with pentane, benzene, and pyridine, and by filtering the insolubles from each step through a Millipore® filter with an average pore size of 5 μm (Schweighardt et al., 1983). Elemental compositions of all fractions and ashes in the residue were further analyzed to determine the elemental balance between feeds and products and to determine coal conversion. Oils recovered from solvent separation were further subjected to

simulated GC distillation (a modified ASTM D2886, Wilsonville method) (Schweighardt et al., 1983). Distillate cut points were necessary to evaluate hydrogen partial pressure and other thermophysical properties of fluids under reaction conditions. Subsequently, the hydrogen partial pressure for each data point was evaluated using the modified Peng-Robinson equation of state. This system was developed by ICRC for SRC-I process studies, based on the most current experimental data base available on thermophysical properties of coal-derived fluids. This equation of state (Mathias and Stein, 1983) is currently incorporated in the ICRC/ASPEN computer simulation program. All residue samples produced under low hydrogen partial pressures were petrographically analyzed to determine if coke formation occurred as a result of hydrogen starvation (Davis et al., 1983).

3.0 RESULTS AND DISCUSSION

3.1 Liquefaction of Mulford Coal in Native Solvent

The native solvent was significant not only because it was derived from the feed coal being studied, but also because it was indigenous to the continuous stirred tank reactor hydrodynamics of the CPDU. Preparing solvent in this way was an attempt to avoid possible variations in hydrogen content and other solvent properties caused by different reactor configurations or hydrodynamic behaviors.

Tables 5 and 6 summarize the yield and partial pressure data and Table 7 summarizes reactor effluent compositions obtained from reacting Kentucky #9 Mulford coal in single-pass runs in either one or two CSTRs in series at various process conditions. Yield structures were calculated on the basis of the actual composition of the starting solvent, which was analyzed by solvent separation (Table 5), and also based on the assumption that the starting solvent contained 100% oils (Table 6). The starting solvent, which was freshly distilled before use, contained only

Table 5

Effect of Hydrogen Partial Pressure on Yield Distribution of Kentucky #9 Mulford Coal in Native Solvent
(Yield Calculation Based on the As-Analyzed Compositions of Feed Solvent)

Sample no.	71-117 ^a	71-99 ^a	69-47 ^b	71-90 ^a	71-163 ^b	71-142 ^b	71-14 ^a	69-7 ^b	71-7 ^a	71-126 ^a	71-54 ^a
Temperature (°F)	760	760	760	760	800	800	802	800	800	800	800
Nominal residence time (min)											
Target	30+30	30+30	30+30	30+30	20	20	20	20	20	30+30	30+30
Actual	61.6	64.2	61.6	60.1	19.7	21.8	20.3	19.8	20.5	60.1	64.5
Feed gas rate (M scf/ton of coal)											
Total	30	15	30	60	15	30	15	30	60	30	15
H ₂	15	15	30	60	7.5	15	15	30	60	15	15
Diluent gas	Yes	No	No	No	Yes	Yes	No	No	No	Yes	No
Hydrogen consumption (wt % MMF coal)	1.52	1.45	1.15	1.70	1.01	1.11	1.26	0.84	1.74	1.48	1.96
Yield (wt % MMF coal)											
Total	92.32	93.02	92.12	93.43	87.88	90.84	90.99	89.83	92.83	92.07	95.26
C ₁ -C ₄	2.31	1.74	3.06	2.16	1.92	3.10	2.01	2.29	2.61	5.78	3.98
CO + CO ₂	0.97	0.85	1.80	0.85	0.85	1.13	1.00	1.53	1.00	1.31	1.20
H ₂ S	1.62	1.18	2.11	1.44	1.22	1.51	1.21	1.14	1.32	1.67	1.19
NH ₃	0.0067	0.0032	ND	0.0350	0.0024	0.0116	0.0016	ND	0.0179	0.0110	0.0024
H ₂ O	3.63	2.56	2.00	4.56	2.95	4.09	2.33	1.85	3.41	2.80	3.74
Oil	17.20	30.29	12.45	33.36	21.11	16.42	24.14	10.62	32.21	24.37	35.21
SRC	66.59	56.38	70.69	51.03	59.83	64.59	60.30	72.40	52.27	56.13	49.92
Asphaltene	32.89	34.85	36.30	30.11	21.73	30.47	33.68	37.35	29.56	30.41	33.45
Preasphaltene	33.71	21.53	34.38	20.92	38.10	34.11	26.62	35.05	22.71	25.72	16.47
Unc. coal	8.65	8.46	9.30	8.44	13.10	10.13	10.21	11.08	8.90	9.25	6.63
Conversion of coal	91.34	91.54	90.70	91.56	86.90	89.87	89.75	88.92	91.10	90.75	93.37
S in SRC (wt %)	1.07	1.13	1.08	0.94	1.18	1.06	1.22	1.08	1.00	0.86	0.85
H in feed solvent (wt %)	7.89	7.89	7.87	7.89	7.89	7.89	7.89	7.87	7.89	7.89	7.89
H in prod. solvent (wt %)	8.02	8.07	7.85	8.01	7.90	7.95	7.89	7.78	7.94	7.92	8.02
H ₂ partial pressure (psia)	793	1451	1681	1750	489	699	1422	1696	1750	671	1259
H ₂ conc. in liquid (wt % H ₂ in liquid phase)	0.0727	0.1470	0.1503	0.1533	0.0533	0.0678	0.1531	0.1586	0.1613	0.0684	0.1491

^a Yield data based on single analysis

^b Yield data based on duplicate analyses

Table 5 (continued)

Sample no.	69-37 ^b	71-44 ^a	71-156 ^b	71-149 ^a	71-29 ^a	69-14 ^b	71-21 ^a	71-135 ^a	71-71 ^b	69-26 ^b	71-80 ^b
Temperature (°F)	800	800	840	840	840	840	840	840	840	840	840
Nominal residence time (min)											
Target	30+30	30+30	20	20	20	20	20	30+30	30+30	30+30	30+30
Actual	61.3	61.0	19.6	20.5	20.4	20.4	20.2	61.0	61.8	60.7	59.5
Feed gas rate (M scf/ton of coal)											
Total	30	60	15	30	15	30	60	30	15	30	60
H ₂	30	60	7.5	15	15	30	60	15	15	30	60
Diluent gas	No	No	Yes	Yes	No	No	No	Yes	No	No	No
Hydrogen consumption (wt % MMF coal)	1.76	2.39	1.05	1.30	1.94	1.39	2.63	2.18	2.12	2.44	3.58
Yield (wt % MMF coal)											
Total	92.87	96.80	81.34	88.42	92.84	90.53	95.43	84.30	94.77	94.53	98.33
C ₁ -C ₄	5.17	4.84	4.48	6.21	4.44	5.68	6.53	12.43	5.93	10.53	10.86
CO + CO ₂	2.20	1.15	1.23	1.39	1.39	2.09	1.44	1.76	1.45	2.36	1.27
H ₂ S	1.49	1.86	1.10	1.75	1.43	1.58	1.98	2.30	1.80	2.00	1.31
NH ₃	ND	0.0315	0.0032	0.0126	0.0033	ND	0.0336	0.0080	0.0025	ND	0.0778
H ₂ O	2.09	3.80	2.67	4.27	1.69	2.64	3.45	0.82	4.27	3.86	2.41
Oil	15.02	43.56	13.60	15.05	34.97	18.56	49.78	22.34	37.38	26.03	57.82
SRC	66.90	41.56	58.25	59.74	48.92	59.97	32.20	44.62	43.95	49.74	24.59
Asphaltene	37.69	31.38	21.97	27.43	24.86	32.78	22.30	23.27	29.96	31.65	15.44
Preasphaltene	29.21	10.17	36.29	32.31	24.06	27.19	9.90	21.35	13.99	18.10	9.14
Unc. coal	8.92	6.11	19.77	13.05	8.72	10.74	7.57	17.79	7.80	8.09	5.58
Conversion of coal	91.08	93.89	80.23	86.95	91.28	89.26	92.43	82.21	92.20	91.91	94.42
S in SRC (wt %)	0.80	0.63	0.99	0.86	1.01	0.92	0.74	0.70	0.66	0.59	0.54
H in feed solvent (wt %)	7.87	7.89	7.89	7.89	7.89	7.87	7.89	7.89	7.87	7.87	7.89
H in prod. solvent (wt %)	7.79	8.16	7.76	7.84	7.84	7.76	7.88	7.71	7.75	7.81	8.12
H ₂ partial pressure (psia)	1606	1685	440	622	1324	1565	1664	546	1115	1387	1579
H ₂ conc. in liquid (wt% H ₂ in liquid phase)	0.1568	0.1640	0.0518	0.0657	0.1644	0.1640	0.1725	0.0614	0.1562	0.1607	0.1769

^a Yield data based on single analysis

^b Yield data based on duplicate analyses

Table 6

Effect of Hydrogen Partial Pressure on Yield Distribution of Kentucky #9 Mulford Coal in Native Solvent
(Yield Calculation Based on the Assumption That Feed Solvent Is 100% Oils)

Sample no.	71-117	71-99	69-47	71-90	71-163	71-142	71-14	59-7	71-7	71-126	71-54
Temperature (°F)	760	760	760	760	800	800	802	800	800	800	800
Nominal residence time (min)											
Target	30+30	30+30	30+30	30+30	20	20	20	20	20	30+30	30+30
Actual	61.6	64.2	61.6	60.1	19.7	21.8	20.3	19.8	20.5	60.1	64.5
Feed gas rate (M scf/ton of coal)											
Total	30	15	30	60	15	30	15	30	60	30	15
H ₂	15	15	30	60	7.5	15	15	30	60	15	15
Diluent gas	Yes	No	No	No	Yes	Yes	No	No	No	Yes	No
Hydrogen consumption (wt % MMF coal)	1.32	1.45	1.15	1.70	1.01	1.11	1.26	0.84	1.74	1.48	1.96
Yield (wt % MMF coal)											
Total	92.32	93.02	92.12	93.43	87.88	90.84	90.99	89.83	92.83	92.07	95.26
C ₁ -C ₄	2.31	1.74	3.06	2.16	1.92	3.10	2.01	2.29	2.61	5.78	3.98
CO + CO ₂	0.97	0.85	1.80	0.85	0.85	1.13	1.00	1.53	1.00	1.31	1.20
H ₂ S	1.62	1.18	2.11	1.44	1.22	1.51	1.21	1.14	1.32	1.67	1.19
NH ₃	0.0067	0.0032	ND	0.0350	0.0024	0.0116	0.0016	ND	0.0179	0.0110	0.0024
H ₂ O	3.63	2.56	2.00	4.56	2.95	4.09	2.33	1.85	3.41	2.80	3.74
Oil	16.73	29.83	12.05	32.90	20.65	15.96	23.67	10.22	31.75	23.91	34.75
SRC	67.06	56.84	71.09	51.49	60.30	65.05	60.76	72.80	52.73	56.59	50.38
Asphaltene	33.35	35.32	36.70	30.57	22.20	30.93	34.14	37.75	30.02	30.88	33.92
Preasphaltene	33.71	21.53	34.38	20.92	38.10	34.11	26.62	35.05	22.71	25.72	16.47
Unc. coal	8.66	8.46	9.30	8.44	13.10	10.13	10.21	11.08	8.90	9.25	6.63
Conversion of coal	91.34	91.54	90.70	91.56	86.90	89.87	89.79	88.92	91.10	90.75	93.37
S in SRC (wt %)	1.07	1.13	1.08	0.94	1.18	1.06	1.22	1.08	1.00	0.86	0.85
H in feed solvent (wt %)	7.89	7.89	7.87	7.89	7.89	7.89	7.89	7.87	7.89	7.89	7.89
H in prod. solvent (wt %)	8.02	8.07	7.85	8.01	7.90	7.95	7.89	7.78	7.94	7.92	8.02
H ₂ partial pressure (psia)	793	1451	1681	1750	489	699	1422	1696	1750	671	1259
H ₂ conc. in liquid (wt % H ₂ in liquid phase)	0.0727	0.1470	0.1503	0.1533	0.0533	0.0678	0.1531	0.1586	0.1613	0.0684	0.1491

Table 6 (continued)

Sample no.	69-37	71-44	71-156	71-149	71-29	69-14	71-21	71-135	71-71	69-26	71-80
Temperature (°F)	800	800	840	840	840	840	840	840	840	840	840
Nominal residence time (min)											
Target	30+30	30+30	20	20	20	20	20	30+30	30+30	30+30	30+30
Actual	61.3	61.0	19.6	20.5	20.4	20.4	20.2	61.0	61.8	60.7	59.5
Feed gas rate (M scf/ton of coal)											
Total	30	60	15	30	15	30	60	30	15	30	60
H ₂	30	60	7.5	15	15	30	60	15	15	30	60
Diluent gas	No	No	Yes	Yes	No	No	No	Yes	No	No	No
Hydrogen consumption (wt % MWF coal)	1.76	2.39	1.04	1.30	1.94	1.39	2.63	2.18	2.12	2.44	3.58
Yield (wt % MWF coal)											
Total	92.87	96.80	81.34	88.42	92.84	90.53	95.43	84.30	94.77	94.53	98.33
C ₁ -C ₄	5.17	4.84	4.48	6.21	4.44	5.68	6.53	12.43	5.93	10.53	10.86
CO + CO ₂	2.20	1.15	1.23	1.39	1.39	2.09	1.44	1.76	1.45	2.36	1.27
H ₂ S	1.49	1.86	1.10	1.75	1.43	1.58	1.98	2.30	1.80	2.00	1.31
NH ₃	ND	0.0315	0.0032	0.0126	0.0033	ND	0.0336	0.0080	0.0025	ND	0.0778
H ₂ O	2.09	3.80	2.67	4.27	1.69	2.64	3.45	0.82	4.27	3.86	2.41
Oil	14.62	43.10	13.14	14.59	34.51	18.16	49.32	21.88	36.92	25.64	57.36
SRC	67.30	42.02	58.72	60.21	49.38	60.37	32.66	45.09	44.41	50.14	25.05
Asphaltene	38.09	31.85	22.43	27.89	25.32	33.18	22.76	23.74	30.42	32.05	15.91
Preasphaltene	29.21	10.17	36.29	32.31	24.06	27.19	9.90	21.35	13.99	18.10	9.14
Unc. coal	8.92	6.11	19.77	13.05	8.72	10.74	7.57	17.79	7.80	8.09	5.58
Conversion of coal	91.08	93.89	80.23	86.95	91.28	89.26	92.43	82.21	92.20	91.91	94.42
S in SRC (wt %)	0.80	0.63	0.99	0.86	1.01	0.92	0.74	0.70	0.66	0.59	0.54
H in feed solvent (wt %)	7.87	7.89	7.89	7.89	7.89	7.87	7.89	7.89	7.87	7.87	7.89
H in prod. solvent (wt %)	7.79	8.16	7.76	7.84	7.84	7.76	7.88	7.71	7.75	7.81	8.12
H ₂ partial pressure (psia)	1606	1685	440	622	1324	1565	1664	546	1115	1387	1579
H ₂ conc. in liquid (wt % H ₂ in liquid phase)	0.1568	0.1640	0.0518	0.0657	0.1644	0.1640	0.1725	0.0614	0.1562	0.1607	0.1769

Table 7
Component Rates in the CPDU Reactor Effluent Stream (g/hr)

Sample ID	71-117	71-99	69-47	71-90	71-163	71-142	71-14	69-7	71-7	71-126	71-54
Temp. (°F)	760	760	760	760	800	800	800	800	800	800	800
Pres. (psig)	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000
Component											
H ₂	24.39	18.56	45.07	93.76	13.13	36.31	29.14	72.04	145.0	20.98	15.97
N ₂ ^a	364.90	0.34	2.96	0.42	364.90	680.30	0.52	7.45	0.66	382.5	0.23
x	24.02	10.27	11.56	40.17	17.06	37.48	14.34	18.31	57.96	24.3	9.74
C ₁	4.29	3.51	5.59	4.39	5.85	8.58	6.41	9.14	8.18	11.88	8.37
C ₂	4.09	2.6	3.38	3.72	4.84	7.27	4.78	5.12	6.59	8.97	5.19
C ₃	3.05	2.05	2.52	2.73	3.82	4.73	3.82	4.16	5.34	6.97	4.28
C ₄	0.93	0.83	5.23	0.84	1.48	2.61	1.31	1.10	1.33	4.0	2.56
C ₅	0.19	0.15	0.17	0.35	0.31	0.65	0.35	0.27	0.0	0.38	0.40
CO	0.9	0.71	2.96	0.94	0.95	1.76	2.80	3.83	3.2	1.48	2.25
CO ₂	4.36	3.76	6.98	3.80	6.26	6.92	5.46	9.37	5.02	5.82	4.03
H ₂ S	8.84	6.20	11.63	8.02	10.41	11.64	10.05	9.84	10.89	9.28	6.24
NH ₃	0.05	0.02	0.0	0.16	0.04	0.08	0.0	0.0	0.13	0.05	0.02
H ₂ O	47.09	36.60	28.97	51.45	64.55	67.78	59.0	37.81	62.17	44.99	44.38
100-150 (°F cut)	0.10	3.99	0.10	0.23	8.49	6.05	0.31	0.15	0.32	3.51	0.95
150-200	0.28	7.98	0.24	0.11	0.40	0.44	0.83	0.22	0.64	0.05	0.29
200-250	0.69	9.82	0.84	8.46	2.11	1.81	1.27	0.53	2.06	1.01	1.03
250-300	1.15	1.18	1.97	0.45	1.67	1.05	2.13	0.89	2.65	3.34	1.72
300-350	5.39	10.56	12.33	9.06	17.77	14.50	20.38	15.94	19.08	32.46	17.18
350-400	33.96	39.70	45.71	40.72	70.49	61.41	66.27	63.40	77.50	38.83	59.96
400-450	47.28	60.11	51.96	62.57	86.27	76.73	98.17	85.28	95.57	62.62	63.98
450-500	119.20	113.00	117.90	121.30	202.10	174.70	189.90	179.00	197.00	130.80	134.50
500-550	134.60	120.60	127.20	132.50	222.40	190.60	201.50	198.70	212.60	138.70	137.60
550-600	154.10	156.40	146.80	171.20	240.30	217.60	230.70	224.80	238.80	153.60	153.70
600-650	245.40	257.80	236.80	282.30	382.70	330.00	367.20	361.50	385.50	239.00	240.70
650-700	153.40	162.30	145.00	161.80	236.90	207.70	230.70	220.70	233.40	151.00	147.10
700-750	82.04	68.22	74.09	93.44	117.00	107.00	126.80	121.30	129.20	80.35	77.04
750-800	57.49	48.98	46.82	63.28	61.25	67.35	92.19	79.06	82.86	59.21	51.27
800-850	3.31	2.31	1.89	3.07	1.44	1.87	6.29	5.05	4.33	9.66	2.42
Asphaltene	181.50	184.90	202.40	170.40	188.80	238.00	282.70	326.10	246.70	171.90	177.30
Preasphaltene	183.40	112.70	189.60	116.50	324.10	262.50	220.40	302.80	186.70	143.10	86.08
ION	47.13	44.27	51.32	47.01	111.50	77.94	84.53	95.75	73.16	51.49	34.64
Ash	46.31	47.96	52.90	53.70	81.81	74.62	69.86	79.52	71.54	49.57	40.88

^a reference gas

Table 7 (continued)

Sample ID	69-36	71-44	71-156	71-149	71-29	69-14	71-21	71-135	71-71	69-26	71-80
Temp. (°F)	800	800	840	840	840	840	840	840	840	840	840
Pres. (psig)	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000
Component											
H ₂	43.69	88.25	11.94	31.44	27.6	69.67	138.30	16.96	13.64	37.05	80.03
N ₂ ^a	2.83	0.32	357.10	641.20	0.37	7.14	0.50	384.40	0.26	4.48	0.30
x	11.60	38.98	16.95	37.37	14.91	18.34	60.10	24.13	10.50	10.57	39.08
C ₁	11.54	10.70	13.05	18.85	13.45	17.88	19.05	26.11	2.00	22.15	22.70
C ₂	7.44	6.62	10.58	14.44	9.39	11.99	13.92	17.81	12.77	15.32	15.72
C ₃	6.45	6.80	8.22	10.58	9.48	10.18	14.56	14.43	9.58	14.14	14.11
C ₄	2.80	2.18	5.92	5.90	3.96	6.13	6.01	8.54	6.94	6.36	7.69
C ₅	0.52	0.34	0.61	0.91	0.58	0.82	1.06	1.14	0.96	0.95	0.95
CO	3.30	3.03	1.53	2.61	4.27	4.58	5.58	2.13	1.78	3.37	2.47
CO ₂	8.90	3.31	8.97	8.74	7.28	12.73	6.49	7.51	6.13	9.82	4.66
H ₂ S	8.28	10.24	9.46	14.26	11.83	13.10	16.59	12.61	9.78	11.19	7.36
NH ₃	0.0	0.16	0.04	0.07	0.03	0.0	0.25	0.04	0.02	0.0	0.45
H ₂ O	28.97	47.14	60.42	73.70	48.50	52.63	65.28	32.47	47.93	40.44	41.54
100-150 (°F cut)	0.29	0.82	0.16	0.30	0.16	0.31	0.88	2.71	0.44	0.11	8.89
150-200	0.92	0.22	7.76	0.16	0.80	1.97	0.80	0.24	0.43	0.99	0.59
200-250	2.05	1.48	5.50	1.61	4.73	2.52	9.01	1.63	1.05	3.13	2.09
250-300	4.93	4.06	1.01	2.80	3.32	6.36	4.02	3.60	1.77	7.57	5.68
300-350	20.67	24.37	14.59	25.39	23.78	27.6	28.68	22.72	15.47	26.3	27.57
350-400	53.33	70.03	70.55	80.99	86.15	75.81	94.52	68.77	62.62	60.11	79.25
400-450	68.34	70.68	85.93	88.40	107.70	101.50	118.60	73.27	71.76	80.34	94.50
450-500	125.20	145.20	183.50	190.50	198.40	186.70	208.80	145.30	149.90	143.50	170.50
500-550	126.20	150.50	195.80	195.10	197.70	193.90	210.30	137.20	147.20	139.20	168.50
550-600	142.50	167.30	237.20	215.70	246.90	217.80	264.40	145.10	157.80	155.10	183.80
600-650	224.00	259.60	394.00	341.40	397.80	344.90	420.20	229.20	243.80	240.00	269.60
650-700	136.80	156.70	243.20	210.90	237.70	212.90	267.10	135.40	155.30	139.00	146.80
700-750	72.21	83.21	121.70	108.30	121.80	114.10	118.50	65.45	69.41	68.98	90.42
750-800	50.36	56.10	97.00	74.89	87.27	81.33	106.00	40.52	57.41	35.91	52.47
800-850	2.74	3.27	5.88	1.37	4.70	3.54	7.04	1.98	9.39	1.09	2.14
Asphaltene	211.7	175.30	133.00	227.80	210.00	274.60	190.20	129.90	165.50	179.30	89.58
Preasphaltene	162.30	56.00	302.50	263.90	199.50	225.00	82.79	116.80	76.11	101.20	51.49
IOM	49.60	33.62	168.00	106.50	72.28	88.87	63.27	97.34	42.19	45.24	31.40
Ash	51.95	44.45	83.96	78.74	74.06	82.20	72.95	53.88	49.08	52.89	49.34

^a Reference gas.

trace amounts of pentane-insoluble asphaltenes (0.26%). The yield distributions calculated by either method (as compared in Tables 5 and 6) do not differ significantly. This can be a problem with solvent containing a large amount of pentane-insoluble asphaltenes in the starting solvent, as discussed previously (Sivasubramanian and Givens, 1983; Kang and Givens, 1983).

Due to time constraints and high costs, error analyses were not conducted on the data developed in this study. However, the following summarizes the results of a recent variability study (Sivasubramanian, 1983) performed on the yield data of oils, asphaltenes, preasphaltenes, and conversions of Mulford coal, which was based on the solvent separation technique (Schweighardt, 1983).

Statistically Permissible Maximum Differences
Confidence Level - 95%
Based on Total Product Yield

Fractions	Differences (wt %)			df
	<u>Single analysis</u>	<u>Two analyses</u>	<u>Four analyses</u>	
Oils	2.59	1.83	1.30	6
Asphaltenes	3.15	2.23	1.59	7
Preasphaltenes	1.44	1.02	0.72	7
Residue or Conversion	2.33	1.65	1.17	7

df = degree of freedom

Most of the yield data was based mainly on a single analysis of product slurries, as indicated in Table 5.

The discussion and conclusions are based mainly on the yield data from Run BCL-71 due to inconsistencies between the data from BCL 71 and BCL-69.

3.2 Evaluation of Hydrogen Partial Pressure and Hydrogen Solubility

Hydrogen gas is one of the major reactants that must be precisely determined and correlated with other process parameters. Hydrogen in the dissolver may be defined as either hydrogen partial pressure or dissolved hydrogen concentration in the liquid phase (or hydrogen solubility). However, expressing it as the concentration of dissolved hydrogen is actually more appropriate for coal conversion because the major hydrogenation reactions of coal take place in the liquid phase, whereas vapor phase hydrogenation reactions involve the lighter conversion products and solvents. However, the hydrogen partial pressure in the SRC-I dissolver, as in any other process, is not an independent variable. Instead, it depends on all the other reactor variables, including temperature, pressure, and the rate and composition of feed materials. Therefore, the evaluation of hydrogen partial pressure and hydrogen solubility during the SRC-I process development depended upon various thermophysical correlations, because direct experimental determination of the physical properties of reactor fluids at particular reaction conditions was impractical, not only in terms of cost and resources, but also unavailability of the data base.

Development of the experimental data base on the physical properties of the SRC-I-derived coal liquids and its correlations is currently being performed under another ICRC/APCI program (ASPEN Plus Modeling) and is beyond the scope of this study. The thermodynamic correlations developed under this program are being incorporated in the ASPEN computer program. This final version of the phase equilibrium model for the SRC-I process uses the modified Peng-Robinson equation of state for vapor/liquid equilibrium calculations based on the most recent experimental data base (Mathias, 1983 and 1984). Table 7 lists the composition data for the reactor effluents that were used to calculate the partial pressure and solubility of hydrogen gas and other reactor physical properties by use of this correlation. The partial pressure and solubility of hydrogen gas are shown in Tables 5 and 6.

Relationships of hydrogen partial pressure and hydrogen solubility to

other process variables are illustrated in Figures 2-5 and Table 8. APCI/VLE computer calculations used to evaluate hydrogen partial pressure and hydrogen solubility data are provided in Appendix A-3.

3.2.1 Temperature Dependency of Hydrogen Partial Pressure. Figure 2 illustrates that an increase in temperature decreases hydrogen partial pressure. However, hydrogen solubility increases or decreases with an increase in temperature, depending on the purity of feed gas. In this particular case, hydrogen solubility increased with an increase in temperature. For example, at a specified hydrogen gas rate of 60 M scf/ton of coal with no diluent gases, a nominal residence time of 60 min (a given slurry pumping rate), and a system pressure of 2,000 psig, the increase in temperature from 760 to 800°F and to 840°F decreased hydrogen partial pressure from 1,750 to 1,690 and finally, to 1,580 psia, respectively. At the same time, hydrogen solubility increased from 0.153 wt % (grams of dissolved hydrogen gas per 100 g of liquid-phase materials, excluding mineral matter in the reactor) to 0.164 and 0.177 wt %, respectively, at the corresponding temperatures. In the presence of 50 mol % of diluent gas, however, an increase in temperature not only decreased hydrogen partial pressure but also hydrogen solubility at the same time (see Table 8), illustrating a certain difficulty in interpreting the data when a large amount of diluent gas is added. Note that the impartial coal conversion due to different temperatures (impartial liquid properties and their compositions) had significant effects on the hydrogen partial pressure and hydrogen solubility in these data, even if process conditions other than temperature were fixed.

3.2.2 Residence Time Dependency of Hydrogen Partial Pressure. Figure 3 shows that an increase in nominal residence time, with other conditions such as temperature and gas rate fixed, decreases the hydrogen partial pressure. The changes are less

Table 8

Effect of Diluent Gas on Hydrogen Partial Pressure and Hydrogen Solubility in Dissolver

Sample no.	71-117	71-99	71-142	71-14	71-126	71-54	71-149	71-29	71-135	71-71
Temperature (°F)	760	760	800	800	800	800	840	840	840	840
Nominal residence time (min)	60	60	20	20	60	60	20	20	60	60
Total pressure (psig)	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000
Total gas rate (M scf/ton of coal)	30	15	30	15	30	15	30	15	30	15
Mol % diluent gas	50	2	50	2	50	2	50	2	50	2
Hydrogen rate (M scf/ton of coal)	<u>15</u>	<u>15</u>	<u>15</u>	<u>15</u>	<u>15</u>	<u>15</u>	<u>15</u>	<u>15</u>	<u>15</u>	<u>15</u>
Hydrogen partial pressure (psia)	790	1450	700	1420	670	1260	620	1320	550	1120
Hydrogen solubility (wt % H ₂ in reactor liquid phase)	0.073	0.147	0.068	0.153	0.068	0.149	0.066	0.164	0.061	0.156

Figure 2 - Effects of temperature on hydrogen partial pressure and hydrogen solubility

Basis: Kentucky #9 Mulford coal

60 minute residence time

60 mscf/ton total gas rate

98 mol % H_2

Figure 3 - Effects of time on hydrogen partial pressure and hydrogen solubility

**Basis: Kentucky #9 Mulford coal, 840° F,
60 MSCF H₂ rate/ton of coal
Purity 98 mol %**

significant than the changes with temperature. At 60 M scf of hydrogen/ton of coal without diluent gas and 2,000 psig of system pressure, an increase in residence time from 20 to 60 min decreased hydrogen partial pressure from 1,660 to 1,580 psia. However, hydrogen solubility is not a straightforward linear function of residence time, but increases or decreases depending upon other process conditions such as feed gas rates. At the high hydrogen rate of 60,000 scf/ton of coal, an increase in residence time from 20 to 60 min increased hydrogen solubility (71-21 and 71-80 in Table 5), whereas at the low hydrogen rate of 15,000 scf/ton of coal, the same change in residence time decreased hydrogen solubility (71-14 and 71-54 in Table 5).

3.2.3 Hydrogen Feed Rate Dependency of Hydrogen Partial Pressure.

Figure 4 illustrates the effects of hydrogen gas rate (without diluent) on hydrogen partial pressure and hydrogen solubility. In general, the increase in hydrogen feed rate tends to increase both hydrogen partial pressure and solubility. For a given set of process conditions (800°F, 60-min residence, and 2,000 psig), the increase in hydrogen rate from 15,000 to 30,000 and then to 60,000 scf per ton of coal increased the hydrogen partial pressure from 1,260 to 1,610 and then to 1,690 psia, respectively, and hydrogen solubility from 0.149 to 0.157 and then to 0.164 wt %, respectively. An inconsistency in the data points of 71-29 and 69-14 at 840°F and 20 min between 15 and 30 M scf/ton was probably due to the inconsistency in the yield data generated from the different batches of Mulford coal, as discussed earlier.

3.2.4 Pressure Dependency of Hydrogen Partial Pressure. Figure 5 illustrates the effects of system pressure on hydrogen partial pressure and hydrogen solubility. The data shown in this figure were simulated using ICRC's VLE correlation described earlier, based on a typical product composition (BCL71-80) obtained from this study.

Figure 4 - Effects of hydrogen flow rate with no
diluent gas on hydrogen partial
pressure and hydrogen solubility
Basis: Kentucky #9 coal
800⁰ F
60 minute nominal residence time

Figure 5 - Effects of total pressure on hydrogen
partial pressure and hydrogen solubility

Basis: Kentucky #9 Mulford coal

840° F

60 minute residence time

60 MSCF H₂ rate per ton of coal

The total system pressure obviously affects both hydrogen partial pressure and hydrogen solubility, although the relative changes of hydrogen concentration (mol % of hydrogen) in the vapor phase are insignificant. Decreasing the total pressure from 2,000 to 1,000 psig decreases, almost linearly, both hydrogen partial pressure and hydrogen solubility to less than one-half of their values at 2,000 psig. Partial pressure dropped from 1,580 to 770 psia, and solubility from 0.177 to 0.076 wt %, respectively. In contrast, the hydrogen concentration in the vapor phase dropped insignificantly, only about 2% (from 78.4 to 76.2 mol %).

3.2.5 Dependency on Diluent Gas of Hydrogen Partial Pressure. Data shown in Table 8 illustrate the effects of diluent gas on hydrogen partial pressure and hydrogen solubility at various process conditions. Diluent gas in feed gas had a major impact on hydrogen partial pressure and hydrogen solubility, the magnitude of which is similar to the effect of total pressure. For a given set of process conditions, the diluent gas almost proportionately decreased both partial pressure and solubility. For example, at 840°F, 60-min residence time, and a hydrogen flow rate of 15,000 scf/ton of coal (but with varying total gas rates of 30,000 scf with 50% nitrogen diluent and 15,000 scf without diluent), the hydrogen partial pressure and the hydrogen solubility decreased from 1,120 to 550 psia and from 0.156 to 0.061 wt %, respectively, in the presence of 50 mol % inert diluent gas.

This study clearly illustrates that the diluent gas in the feed gas stream and total system pressure are more sensitive control variables affecting hydrogen partial pressure and hydrogen solubility (both vapor- and liquid-phase hydrogen concentrations) than feed gas rate.

3.3 Effects of Hydrogen Partial Pressure on Yield Distribution

Figures 6-37 illustrate the distribution of products obtained from the liquefaction of Kentucky #9 Mulford coal in native solvent as a function of hydrogen partial pressure (or, intrinsically, hydrogen solubility) at various temperatures and residence times. The discussions in Section 3.2 showed how hydrogen partial pressure depends upon the parameters of feed gas purity, hydrogen rate, pressure, temperature, and residence time. Therefore, when the data in these figures are interpreted, it should be understood that the hydrogen partial pressure is not an independent variable; it also depends on all other parameters.

3.3.1 Conversion of Coal. Figures 6-9 show the effects of hydrogen partial pressure on the conversion of Mulford coal at various temperatures and residence times. In general, increasing the hydrogen partial pressure increased the conversion of coal, regardless of any changes in other process variables (an exception with 69-47 may be due to different batches of coal). However, the degree to which hydrogen partial pressure impacted conversion was strongly dependent upon temperature and also affected by residence time. At lower temperatures and shorter residence times, hydrogen partial pressure had less of an impact on conversion. For example, at 60-min residence time (Figure 6), coal conversions at 760°F were nearly constant (about 91.5%) under a wide range of hydrogen partial pressures (between 800 and 1,750 psia). However, the increase in temperature from 760 to 800 and 840°F increased the coal conversion by about 2-3%, from 91.5 to 94.5% when the hydrogen partial pressure was sufficiently high, i.e., above 1,200 psia. In contrast, conversion decreased by 3% (from 93.9 to 90.8%) at 800°F and by 12% (from 94.4 to 82.2%) at 840°F when the partial pressure dropped from 1,690 to 670 psia at 800°F from 1,580 to 550 psia at 840°F, respectively. The loss of conversion upon lowering the hydrogen partial pressure below

Figure 6 - Effects of hydrogen partial pressure and temperature on coal conversion
Basis: Kentucky #9 Mulford coal
60 minutes nominal residence time

800 psia was profoundly accelerated with an increase in temperature, resulting in the higher coal conversion with lower temperature. This result clearly demonstrates that hydrogen partial pressure becomes increasingly important at elevated process temperatures in order to obtain higher conversions of coal.

Similar effects of hydrogen partial pressure are illustrated in Figure 7, which plots data obtained at 20 min and two different temperatures. These data show that reducing the residence time from 60 to 20 min diminished the effects of hydrogen partial pressure on the conversion of coal. Coal conversion at 800°F remained at 90-91% as the hydrogen partial pressure dropped from 1,750 to about 700 psia, but it decreased sharply to 87% when hydrogen partial pressure dropped to 500 psia. Conversion at 840°F was higher than that at 800°F when the hydrogen partial pressure was above 1,100 psia, but it decreased rapidly by about 6% below the level of conversion obtained at 760°F with a further decrease of hydrogen partial pressure below 1,100 psia (80.3% at 840°F and 440 psia v. 86% at 800°F and 490 psia).

Figures 8 and 9 show the effects of hydrogen partial pressure and residence time on conversion at constant temperatures. At a given process temperature, the effects of hydrogen partial pressure on conversion tend to increase as the residence time increases; this is similar to the effects observed with temperature increases. The conversions obtained at 60-min residence and at constant temperatures of 800 and 840°F changed more rapidly with changes in hydrogen partial pressure than those obtained at 20-min residence at the same constant temperatures. The effects of hydrogen partial pressure together with the effects of residence time on conversion were accelerated with the increase in temperature. At 840°F, conversions at 60-min residence were greater than those at 20

Figure 7 - Effects of hydrogen partial pressure and temperature on coal conversion
Basis: Kentucky #9 Mulford coal
20 minutes nominal residence time

Figure 8 - Effects of hydrogen partial pressure and
residence time on coal conversion
Basis: Kentucky #9 Mulford coal
840° F process temperature

Figure 9 - Effects of hydrogen partial pressure and
residence time on coal conversion
Basis: Kentucky #9 Mulford coal
800° F process temperature

min when the hydrogen partial pressure was maintained above 800 psia. Conversion then rapidly decreased below the conversion level of 20 min when hydrogen partial pressure was reduced below 800 psia. In other words, the sensitivity of conversion to hydrogen partial pressure was greater at the longer residence times. The effects of residence time were less profound at 800 than at 840°F. Overall, residence time affected conversion more than hydrogen partial pressure at lower temperatures, but hydrogen partial pressure affected conversion more than did residence time at elevated temperatures (840°F).

3.3.2 Oil Yields. The data plotted in Figures 10-13 illustrate the effects of hydrogen partial pressure on oil yields from Mulford coal liquefaction at various process conditions. The maximum affordable hydrogen partial pressures based on the current plant design are indicated by dashed lines in the figures. These lines were generated from interpolations between the data points associated with no diluent gas. Oil yields were also a complex function of hydrogen partial pressure, temperature, and residence time. Oil yields increased when hydrogen partial pressure increased, regardless of other process conditions. However, the increased oil yields caused by the increased hydrogen partial pressure were further enhanced by temperature increases (Figures 10 and 11) and residence time (Figures 12 and 13). Temperature appears to play a more significant role.

Figure 10 shows that at 60-min residence, the oil yield increased 16% (from 17 to 33%) at 760°F, 19% (from 24 to 43%) at 800°F, and 36% (from 22 to 58%) at 840°F with corresponding increases in hydrogen partial pressures (from 800 to 1,750 psia at 760°F, from 670 to 1,690 psia at 800°F, and from 550 to 1,580 psia at 840°F, respectively). Similarly, at a residence time of 20 min, the oil yield increased 11% (from 21 to 32%) at 800°F and 36% (from 14 to 50%) at 840°F when hydrogen partial pressure increased (from 490 to 1,750 psia at 800°F and from 440 to 1,670

Figure 10 - Effects of hydrogen partial pressure and temperature on oil yield
Basis: Kentucky #9 Mulford coal
60 minute residence time

Figure 11 - Effects of hydrogen partial pressure and temperature on oil yield

Basis: Kentucky #9 Mulford coal
20 minute nominal residence time

Figure 12 - Effects of hydrogen partial pressure and residence time on oil yield
Basis: Kentucky #9 Mulford coal
840° F process temperature

Figure 13 - Effects of hydrogen partial pressure and residence time on oil yield
Basis: Kentucky #9 Mulford coal
800° F process temperature

psia at 840°F) (see Figure 11). Another example, graphed in Figure 12, shows that at 840°F, oil yields increased 36% (from about 14 to 50%) at 20 min and about 36% (from 22 to 58%) at 60 min when hydrogen partial pressure increased from 440 to 1,670 psia and from 550 to 1,580 psia, respectively. Similarly, at 800°F (Figure 13) the oil yield increased from 21 to 32% (a net increase of 11%) at 20 min and from 24 to 43% (a net increase of 19%) at 60 min, with corresponding increases in hydrogen partial pressure from 490 to 1,750 psia and from 670 to 1,690 psia, respectively.

These results show that at a given residence time the increase in oil yields caused by increasing the hydrogen partial pressure was progressively magnified by increases in temperature. On the other hand, at a given temperature the increase of oil yield caused by an increase in hydrogen partial pressure was progressively magnified by residence time. Thus, hydrogen partial pressure becomes even more influential as both temperature and residence time increase.

3.3.3 Asphaltene Yields. The data plotted in Figures 14-17 illustrate the effects of hydrogen partial pressure on asphaltene yields, also at various temperatures and residence times. Asphaltene yield is strongly dependent on hydrogen partial pressure as well as temperature and residence time, and in an extremely complicated manner. At any given temperature or residence time, the asphaltene yields passed through a maximum as the hydrogen partial pressure was varied between 400 and 1,800 psia.

Asphaltene yields appeared to be much less sensitive to hydrogen partial pressure than other product yields unless the temperature was elevated to 840°F. Also, under the influence of hydrogen partial pressure, temperature affected the asphaltene yields more than residence time (see Figures 14-17). For example, at 60-min residence (Figure 14), the asphaltene yields

Figure 14 - Effects of hydrogen partial pressure and temperature on asphaltene yield
Basis: Kentucky #9 Mulford coal
60 minute residence time

initially increased and then decreased (from 15 to 30 to 23% at 840°F, from 31 to 33 to 30% at 800°F, and from 30 to 35 to 33% at 760°F) upon corresponding decreases of hydrogen partial pressure (from 1,590 to 550 psia at 840°F, from 1,690 to 670 psia at 800°F, and from 1,750 to 790 psia at 760°F, respectively). At 20-min residence (Figure 15), asphaltene yields also increased and then decreased (from 22 to 27 to 22% at 840°F and from 30 to 34 to 24% at 800°F) with corresponding decreases in hydrogen partial pressure (from 1,670 to 440 psia at 840°F and from 1,750 to 490 psia at 800°F, respectively). In both cases, temperature increases progressively decreased the asphaltene yields, and the effects of hydrogen partial pressure became more significant when the temperature was increased from 800 to 840°F.

Figures 16 and 17 depict the effects of hydrogen partial pressure on asphaltene yields at varying residence times. At all conditions studied, the hydrogen partial pressure strongly impacted the conversion of asphaltenes; the effects were most noticeable at elevated temperatures (840°F). However, the effects of residence time were apparently less significant than those of temperature. Even at 840°F, any changes in asphaltene yields caused by increasing residence time from 20 min to 60 min were minor for most of the hydrogen partial pressures studied, until the pressure exceeded 1,400 psia. Above this pressure, however, asphaltene yields varied significantly, by as much as 7% at 1,600 psia (22% at 20 min vs. 15% at 60 min). At lower

Figure 15 - Effects of hydrogen partial pressure and temperature on asphaltene yield
Basis: Kentucky #9 Mulford coal
20 minute residence time

Figure 16 - Effects of hydrogen partial pressure and residence time on asphaltene yield
Basis: Kentucky #9 Mulford coal
840° F process temperature

Figure 17 - Effects of hydrogen partial pressure and
residence time on asphaltene yield
Basis: Kentucky #9 Mulford coal
800° F process temperature

temperatures (800°F), residence time affected asphaltene yields insignificantly over the ranges of hydrogen partial pressure studied (400 to 1,800 psia); see Figure 17. This result suggests that to increase the conversion of asphaltenes, increasing hydrogen partial pressure and temperature would be much more effective than increasing residence time.

3.3.4 Preasphaltene Yields. Figures 18-21 illustrate the effects of hydrogen partial pressure on preasphaltene yields; they decreased uniformly with the increased severity of hydrogen partial pressure, temperature, and residence time. Hydrogen partial pressure strongly impacted preasphaltene yields, as did temperature and residence time. At 60-min residence time, an increase in hydrogen partial pressure from about 800 to 1,600 psia decreased preasphaltene yields by about one-half at both 800 and 840°F (from 18 to 9% at 840°F and from 23 to 11% at 800°F) and by about one-third at 760°F (from 33 to 21%) (Figure 18). At 20-min residence, corresponding pressure changes decreased preasphaltene yields by one-third at 840°F (from 27 to 17%) and by one-quarter at 800°F (from 32 to 25%) (Figure 19).

In terms of temperature, at 840°F an increase in hydrogen partial pressure from 800 to 1,600 psia decreased the preasphaltene yield by one-third at 20-min residence (from 28 to 17%) and by one-half at 60 min (from 17 to 9%) (Figure 20). Likewise, at a constant temperature of 800°F, corresponding changes in hydrogen partial pressure decreased the preasphaltene yield by one-third (from 33 to 24%) at 20-min residence and by one-half (from 23 to 11%) at 60 min (Figure 21). This result shows that all three process variables studied (hydrogen partial pressure, temperature, and residence time) jointly affected preasphaltene conversion in a similar manner.

Figure 18 - Effects of hydrogen partial pressure and temperature on preasphaltene yield
Basis: Kentucky #9 Mulford coal
60 minute residence time

Figure 19 - Effects of hydrogen partial pressure and temperature on preasphaltene yield
Basis: Kentucky #9 Mulford coal
20 minute residence time

D

Figure 20 - Effects of hydrogen partial pressure and residence time on preasphaltene yield

Basis: Kentucky #9 Mulford coal

840° F process temperature

Figure 21 - Effects of hydrogen partial pressure and
residence time on preasphaltene yield
Basis: Kentucky #9 Mulford coal
800° F process temperature

3.3.5 Light Hydrocarbon Gas Yields. Figures 22-25 illustrate the effects of hydrogen partial pressure on the yields^a of light hydrocarbon gases (C_1-C_4), as a function of temperature and residence time. Unexpectedly, the yields varied considerably, depending on whether or not diluent gas was added to the feed gas. The gas yields obtained in the presence of excessive amounts of diluent gas (nitrogen) systematically deviated far from the trend of the data obtained in the absence of the diluent gas. Other yield data were probably also influenced by the addition of diluent gas to the reaction system, but the impacts were not as easily recognized. The hydrocarbon gas yields observed upon addition of diluent gas were probably higher than expected because the added gas approximately doubled the gas flow rate in the reactor. This would shorten the gas-phase residence time to half of that which would occur without diluent gas, under the same hydrogen flow rate. The shorter gas residence time induced by the addition of diluent gas may cause preferential stripping of the vapor phase components, including light gas products, relative to the liquid phase components, thereby further increasing the formation of light gases. Also, the presence of diluent gas dilutes not only hydrogen gas, but also other reacting species in the system. Therefore, the deviations in gas yield in the presence of diluent gas were probably due to artifacts attributable to the diluent gas. Furthermore, the diluent gas may have changed other reactor hydrodynamic properties such as true residence time, in addition to thermochemical and physical properties of the reactor contents, due to the shift in vapor/liquid phases.

The data plotted in Figures 22-25 assume that the artifacts created by the diluent gas were influential and indicate that the effects of an increase in hydrogen partial pressure were magnified by an increase in temperature and residence time.

Figure 22 shows that at 60-min residence an increase of hydrogen partial pressure from 1,200 to 1,600 psia would appear to increase the gas yields from 1.5 to 1.9% at 760°F, from 3.8 to 4.6% at 800°F, and from 6.6 to as much as 11% at 840°F. In contrast, Figure 23 shows that at 20-min residence an increase in hydrogen partial pressure from 1,300 to 1,700 psia would appear to increase the gas yields from 1.8 to 2.5% at 800°F and from 4.3 to 6.8% at 840°F. Another example (Figures 24 and 25) illustrates that at a steady temperature of 840°F an increase of hydrogen partial pressure (from 1,200 to 1,600 psia) appears to increase the hydrocarbon gas yield from 3.7 to 6.1% at 20-min residence and from 6.7 to 11% at 60 min. This is similar to the effects observed with temperature changes. The gas yields with diluent gas (data points below 800 psia in the figures) are internally consistent; they increased with an increase in hydrogen partial pressure similarly to the gas yields without diluent gas.

3.3.6 Hydrogen Consumption. Data in Figures 26-29 illustrate the effects of hydrogen partial pressure on the hydrogen consumption of Mulford coal at various temperatures and residence times. An increase in hydrogen partial pressure increased hydrogen consumption at all temperatures and residence times studied. The effects of hydrogen partial pressure were sharply accelerated by an increase in temperature and, to a lesser degree, by an increase in residence time. Hydrogen partial pressure was a major parameter that affected the consumption of hydrogen as much as temperature and residence time. The superimposed effect of temperature on hydrogen consumption appeared to be much greater than that of residence time. For example, at a fixed residence time of 60 min (see Figure 26), hydrogen consumption increased from 1.3 to 1.7% at 760°F, from 1.5 to 2.4% at 800°F, and from 2.1 to 3.6% at 840°F with corresponding increases in hydrogen partial pressure (from 790 to 1,750 psia at 760°F, from 670 to 1,690 psia at 800°F, and

Figure 22 - Effects of hydrogen partial pressure and temperature on hydrocarbon gas (C_1-C_4) yield
 Basis: Kentucky #9 Mulford coal
 60 minute residence time

Figure 23 - Effects of hydrogen partial pressure and temperature on hydrocarbon gas (C_1-C_4) yield
Basis: Kentucky #9 Mulford coal
20 minute residence time

Figure 24 - Effects of hydrogen partial pressure and
residence time on hydrocarbon gas (C_1 - C_4) yield
Basis: Kentucky #9 Mulford coal
840° F process temperature

Figure 25 - Effects of hydrogen partial pressure and residence time on hydrocarbon gas (C_1 - C_4) yield
Basis: Kentucky #9 Mulford coal
800° F process temperature

Figure 26 - Effects of hydrogen partial pressure and temperature on hydrogen consumption
Basis: Kentucky #9 Mulford coal
60 minute residence time

from 1,120 to 1,590 psia at 840°F). Hydrogen consumption increased progressively with increasing temperature. One data point, obtained at 840°F, 60 min, and 450 psia, shows an outstanding deviation from the trends observed with the other data obtained in the absence of diluent gas, apparently due to the combined effects of temperature and diluent gas. A diluent gas effect may exist with other data obtained at lower temperatures, but to a lesser extent.

At a fixed residence time of 20 min, hydrogen consumption also increased--from 1.0 to 1.7% at 800°F and from 1.2 to 2.6% at 840°F with corresponding increases in hydrogen partial pressure (from 490 to 1,750 psia at 800°F and from 440 to 1,670 psia at 840°F) (Figure 27).

Rearrangement of these data (Figures 28 and 29) illustrates that at a fixed temperature of 840°F the increase in hydrogen partial pressure from 440 to 1,670 psia at 20 min and from 1,200 to 1,580 psia at 60 min increased hydrogen consumption from 1.2 to 2.6% and from 2.1 to 2.6%, respectively. At a lower fixed temperature (800°F), increases of hydrogen partial pressure from 490 to 1,750 psia at 20 min and from 670 to 1,680 psia at 60 min also increased hydrogen consumption, from 1.0 to 1.7% and from 1.5 to 2.4%, respectively. Evidently, hydrogen partial pressure is one of the major parameters affecting hydrogen consumption.

3.3.7 Sulfur Content in SRC. The data plotted in Figures 30-33 illustrate how hydrogen partial pressure influences the sulfur content of SRC products. As with the light gas yields, the sulfur contents were affected by the absence or presence of diluent gas, which complicates interpretation of the data.

The sulfur content in the SRC appears to decrease with an increase in hydrogen partial pressure at all conditions if the data with and without diluent gas are treated separately. The data obtained with diluent gas are indicated by broken lines.

Figure 27 - Effects of hydrogen partial pressure and temperature on hydrogen consumption
Basis: Kentucky #9 Mulford coal
20 minute residence time

Figure 28 - Effects of hydrogen partial pressure and residence time on hydrogen consumption
Basis: Kentucky #9 Mulford coal
840° F process temperature

Figure 29 - Effects of hydrogen partial pressure and
residence time on hydrogen consumption
Basis: Kentucky #9 Mulford coal
800° F process temperature

Figure 30 - Effects of hydrogen partial pressure and temperature on sulfur content in SRC

Basis: Kentucky #9 Mulford coal
60 minute residence time

Figure 31 - Effects of hydrogen partial pressure and temperature on sulfur content in SRC
Basis: Kentucky #9 Mulford coal
20 minute residence time

Figure 32 - Effects of hydrogen partial pressure and residence time on sulfur content in SRC
Basis: Kentucky #9 Mulford coal
840° F process temperature

Figure 33 - Effects of hydrogen partial pressure and
residence time on sulfur content in SRC
Basis: Kentucky #9 Mulford coal
800° F process temperature

3.3.8 Hydrogen Content in Product Solvent. Figures 34-37 illustrate the effects of hydrogen partial pressure on the product-solvent hydrogen content at various temperatures and residence times. The hydrogen content of the starting solvent was 7.89%. Overall, the hydrogen contents of the product solvent increased with an increase in hydrogen partial pressure; the degree of changes depended upon other process conditions. The increase was accelerated by both temperature and residence time, temperature having a greater effect. The effect of diluent gas is indicated in the figures by a broken line.

3.3.9 Effect of Nitrogen Diluent Gas on Ammonia Gas Formation.

Another question to be resolved was whether the nitrogen gas used as a diluent was chemically active in the coal reaction system and, if so, how much it would impact the yield distribution of coal. Various minerals found naturally in coal may be able to catalytically convert nitrogen gas to ammonia under the highly reductive coal liquefaction environment.

In order to verify this hypothesis, ammonia gas produced by liquefying Mulford coal in the presence and absence of nitrogen gas was carefully quantified (see Table 9). Overall, the ammonia gas in the products occurred only in trace amounts, usually in the range of hundredths of a percent on a mineral- and moisture-free (MMF) coal basis; it never exceeded 0.1 wt % MMF coal under the conditions investigated in this study.

Figure 34 - Effects of hydrogen partial pressure and temperature on hydrogenation of solvent

Basis: Kentucky #9 Mulford coal

60 minute residence time

Figure 35 - Effects of hydrogen partial pressure and temperature on hydrogenation of solvent
Basis: Kentucky #9 Mulford coal
20 minute residence time

Figure 36 - Effects of hydrogen partial pressure and residence time on hydrogenation of solvent
Basis: Kentucky #9 Mulford coal
840° F process temperature

Figure 37 - Effects of hydrogen partial pressure and residence time on hydrogenation of solvent
Basis: Kentucky #9 Mulford coal
800° F process temperature

-17-

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Table 9

Effect of N₂ Diluent Gas on NH₃ Gas Formation

Sample no.	71-117	71-99	71-163	71-142	71-4	71-126	71-54	71-156	71-149	71-29	71-135	71-71
Temp (°F)	760	760	800	800	800	800	800	840	840	840	840	840
Time (min)												
Target	30+30	30+30	20	20	20	30+30	30+30	20	20	20	30+30	30+30
Actual	61.6	64.2	19.7	21.8	20.3	60.1	64.5	19.6	20.5	20.4	61.0	61.8
Feed gas rate (M scf/ton)												
Total gas rate	30	15	15	30	15	30	15	15	30	15	30	15
H ₂ gas rate	15	15	7.5	15	15	15	15	7.5	15	15	15	15
N ₂ gas rate	15	0	7.5	15	0	15	0	7.5	15	0	15	0
NH ₃ gas (wt% MMF coal)	0.0067	0.0032	0.0024	0.0116	0.0016	0.0110	0.0024	0.0032	0.0126	0.0033	0.0080	0.0025

However, these data did show that the presence of nitrogen gas consistently increased the formation of ammonia gas several-fold, indicating that the nitrogen gas used as a diluent did form additional ammonia gas, but not enough to perturb the overall yield distribution. At a given hydrogen gas rate of 15,000 scf/ton of coal, the additional 15,000 scf of nitrogen gas injected per ton of coal to the feed-gas stream increased the formation of ammonia gas from 0.003 to 0.007 wt % MMF coal at 760°F and 60-min residence time, from 0.002 to 0.012 wt % at 800°F and 20-min residence, from 0.002 to 0.011 wt % at 800°F and 60 min, from 0.003 to 0.013 wt % at 840°F and 20 min, and from 0.003 to 0.008 wt % at 840°F and 60 min. These data do not reveal any definitive trends in relation to the process conditions, primarily because of the trace concentrations involved. Therefore, from a practical viewpoint, the nitrogen gas added to the feed gas stream may be considered chemically inert.

3.3.10 Evidence of Coke Formation under Hydrogen-Starved Conditions.

This program also determined whether coke would form under low hydrogen partial pressures and the limiting hydrogen partial pressure that would induce coke formation under SRC-I process conditions. Table 10 summarizes the results based on investigation of selected samples of product residue that were obtained under low hydrogen partial pressures. Coke formation was determined petrographically by examining samples under a microscope through polarized light beams and by measuring the refractive index of the sample, similar to the procedure used by Davis et al.(1983).

Residues produced below 800°F showed no more than a trace amount of coke formation, even under hydrogen partial pressures of about 500 psia. However, at 840°F significant coke was formed when the hydrogen partial pressure was reduced below about 600 psia. Under these conditions, residence times became a major

Table 10

Coke Formation in Unconverted Coal under Hydrogen Starvation Conditions

Sample no.	117	163	142	126	156	149	135
Temperature (°F)	760	800	800	800	840	840	840
Residence time (min)							
Target	30+30	20	20	30+30	20	20	30+30
Actual	61.6	19.7	21.8	60.1	19.6	20.5	61.0
Feed gas rate (M scf/ton)							
Total gas rate	30	15	30	30	15	30	30
H ₂ rate	15	7.5	15	15	7.5	15	15
N ₂ rate	15	7.5	15	15	7.5	15	15
Unc. coal (wt % MMF)	8.66	13.07	10.13	9.25	19.62	13.05	17.79
Coke formation in unc. coal	None	None	Trace	Trace	40%	10%	50%
H ₂ partial pressure (psia)	793	489	699	671	440	622	546

parameter involved in the process of coke formation. For example, a drop in hydrogen partial pressure from 620 to 440 psia at 840°F and 20-min residence increased coke formation from 10 to 40%; at a longer residence time (60 min) under similar pressure conditions (starting at 550 psia) and the same temperature, coke increased from 10 to 50%. These data indicate that, to prevent coke formation, a partial pressure of at least 700 psia or higher must be maintained in the dissolver at the SRC-I process conditions of 840°F and 60-min residence. However, note that this limiting hydrogen partial pressure will probably also depend upon the type of feed coal used.

3.3.11 Effects of Hydrogen Partial Pressure on Plant Design. As stated previously, hydrogen partial pressure has been the least studied variable in SRC-I process. The results of this program have shown that hydrogen partial pressure affects the product distribution of coal under various SRC-I operating conditions as much as temperature and residence time. Also, the effect of hydrogen partial pressure is not independent; rather, it is dependent upon every other process variable related to the reactor, which makes its analysis extremely complicated.

Temperature and residence time have a negative influence on hydrogen partial pressure, i.e., increasing these variables decreases the hydrogen partial pressure. However, these variables are not normally used to directly control hydrogen partial pressure; they are usually dictated by yield considerations. Process variables that more directly control hydrogen partial pressure are system pressure, feed-gas flow rate, and feed gas purity. Pressure and gas purity have almost rectilinear relationships with hydrogen partial pressure, whereas gas flow rate has a nonlinear relationship. Increasing the hydrogen gas rate at first increases hydrogen partial pressure, but it then levels off at higher rates.

This study strongly indicates that operating the SRC-I plant under low hydrogen partial pressure would significantly decrease the yields of desirable products, especially liquid products, although it would be accompanied by a decline in hydrogen consumption. Because of the significant effect of this parameter on yield distribution, a trade-off study is recommended to determine the costs and benefits of increasing hydrogen partial pressure in the current SRC-I plant design.

4.0 CONCLUSIONS

- Hydrogen partial pressure in the dissolver is controlled mainly by pressure, feed gas purity, and hydrogen flow rate; its sensitivity to gas flow rate is less than its sensitivity to the other variables.
- Reducing the hydrogen partial pressure drastically decreased the coal conversion when process temperatures were above 800°F and hydrogen partial pressures were below 800 psia. Increases in temperature and, to a lesser degree, residence time, significantly amplified this effect. In order to avoid coke formation, hydrogen partial pressure should be maintained at or above 800 psia under typical SRC-I process conditions (840°F, 2,000 psig, and 20-60 min residence).
- Hydrogen partial pressure is one of the major process parameters, comparable to temperature and residence time, affecting oil yields at all process conditions. The effect of hydrogen partial pressure increased synergistically with increases in temperature and residence time. Accordingly, maintenance of an acceptable hydrogen partial pressure is increasingly important as the temperature and residence time increase.
- Hydrogen partial pressure is a key variable that affects the conversion of asphaltenes to oils and lighter products at higher temperatures (840°F).

- Hydrogen partial pressure significantly impacted the conversion of preasphaltenes to a degree comparable to that of temperature and residence time at all process conditions. Also, the increase in preasphaltene conversion as the partial pressure increased was amplified by increases in both temperature and residence time.
- Light hydrocarbon gas yields increased with increases in hydrogen partial pressure as well as temperature and residence time at a given feed hydrogen composition; dilution with nitrogen appeared to cause increased gas yields at a given hydrogen partial pressure.
- A rise in hydrogen partial pressure increased hydrogen consumption; also, the effects of partial pressure increased when both temperature and residence time were raised. Dilution with nitrogen appears to increase hydrogen consumption at a given partial pressure.
- Increasing the hydrogen partial pressure significantly enhanced the removal of sulfur from the SRC products at a given feed hydrogen composition.
- The hydrogen partial pressure had to be high enough to alleviate coking reactions (for example, above 800 psia).
- Hydrogen partial pressure also had a direct impact on the hydrogen content of the recycle solvent; an increase in hydrogen partial pressure increased the hydrogen content at a given hydrogen feed composition. The effect was further enhanced by increases in temperature and residence time, but more significantly by temperature.
- The results strongly suggest that operating at a low hydrogen partial pressure with the system pressure and hydrogen feed rate below design specifications (i.e., below 2,000 psig of pressure and 28,000 scf of hydrogen/ton of coal), would significantly degrade

the yield distribution. Decreases to 800-psia hydrogen partial pressure would cause an unacceptable, major reduction in coal conversion due to coking, with further losses as the pressure dropped below 800 psia. In contrast, increasing the pressure, feed gas purity, and hydrogen gas rate beyond the design base (2,000 psig, 85%, and 28,000 scf/ton of coal) would enhance the yield distribution, with concomitant increases in hydrogen consumption.

Overall, hydrogen partial pressure is a key variable, comparable to temperature and time in its impact on product yield distributions. A trade-off study of these three major design variables, within and beyond the framework of the basic SRC-I design, is highly recommended, considering the major impact of hydrogen partial pressure on yield distribution.

5.0 LITERATURE CITED

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APPENDIX A-1

CPDU Run BCL-71 Operating Data Summary

Date D/M/Y/HR	Balance Period	Pressure psig	Temperature °F		Slurry Rate g/hr		Gas Rates ^a slph		Condensate rate, g/hr		Remarks _g	
			RX-1	RX-2	Feed	Product	Feed	Product	H ₂ O	Organic		
2-19-84	0800	1	2000	800	--	2364.6	1020	1824.0	2060.8			
	0900	2	2000	803	--	2270.2	2300	1839.5	2030.4			
	1000	3	2000	803	--	2293.7	2240	1829.5	2030.2	0.50	1.73	
	1100	4	2000	801	--	2389.0	2380	1811.95	2025.7			
	1200	5	2000	802	--	2329.8	2820	1813.0	2004.5			
	1300	6	2000	800	--	2418.1	2300	1814.9	2012.7	11.87	1.53	
	1400	7	2000	802	--	2389.9	2354.1	1857.5	1992.5	13.2	2.4	NH ₃ -1 A/B 15.12/850-840 mmHg/19.5°C
	1500	8	2000	802	--	2384.9	2200	439.1	743.5			
								447.5				
	1600	9	2000	801	--	2420.1	2340	454.9	470.8			
								458.2				
	1700	10	2000	801	--	2385.5	2320	465.8	479.0	7.71	0.83	
								456.7				
	1800	11	2000	802	--	2439.7	1360	478.0	479.1			
								482.5				
	1900	12	2000	801	--	2422.7	3260	465.2	474.2			
								459.1				
	2000	13	2000	802	--	2452.7	2380	448.9	454.6	5.00	1.10	NH ₃ -2 A/B 15.02/845/803 mmHg/19°C
2100	14	2000	802	--	2442.8	2081.1	441.9	434.1	7.6	1.3		
2200	15	2000	836	--	2407.0	2680	1862.1	1680.1				
							1787.7					
2300	16	2000	841	--	2424.0	2200	1850.3	1986.6				
							1878.1					
2400	17	2000	841	--	2415.1	2300	1849.3	2001.7	10.60	0.40		
							1855.3					
2-20-84	0100	18	2000	842	--	2372.7	2200	1860.8	1932.5			
								1851.7				
	0200	19	2000	842	--	2443.2	2280	1858.0	2340.6			
								1850.3				
	0300	20	2000	842	--	2421.4	2300	1853.2	1707.5	10.17	0.90	
							1854.3					

^a Gas rates are unadjusted raw data with feed rates determined by glycol system and product rates determined by dry test meter.

APPENDIX A-2

**A Summary of Material Balance Data
for Native Solvent Liquefaction Runs
BCL-69 and BCL-71**

Key For Raw Data Matrix

Column #	<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>	<u>5</u>	<u>6</u>	<u>7</u>	<u>8</u>	<u>9</u>
Run #	Run #	Sample #	Month	Day	Year	Hr Start	Hr End		
Conditions	Temp 1 ^a	Temp 2 ^b	Pressure	H ₂ Feed ^c	Slurry Rate ^d				
	Receiver ²	H ₂ O ²	Lights ²	Gas Produced ¹					
Gas	C ₃	C ₃ =	IC ₄	H ₂ S	nC ₄	C ₄ =	H ₂	CO ₂	
Analysis (%)	C ₂ =	C ₂	NH ₃	O ₂	N ₂	C ₁	CO	C ₅ ⁺	H ₂
Solvent	Lights	C	H	N	S	O			
Breakdown	Oils	C	H	N	S	O			
In Slurry	Asph.	C	H	N	S	O			
	Preash.	C	H	N	S	O			
Coal	Wt. %	C	H	N	S	O			
	Lights	C	H	N	S	O			
Added SRC	Oils	C	H	N	S	O			
	Asph.	C	H	N	S	O			
	Preash.	C	H	N	S	O			
These rows not utilized									
Product	Lights	C	H	N	S	O			
Liquid	Oils	C	H	N	S	O			
Analysis	Asph.	C	H	N	S	O			
	Preash.	C	H	N	S	O	Ash		
	Residue	C	H	N	S	O	Ash		
Not Utilized									

All pressures in PSIG, All Temperatures °F, All Fractions Wt. %

^a Temp 1: temperature for reactor 1

^b Temp 2: temperature for reactor 2

^c SLPH

^d gm/hr

THIS ARRAY CONTAINS INITIAL DATA

71.00	7.00	2.00	19.00	1981.00	1400.00	1500.00	0.0	0.0
800.00	0.0	2000.00	1783.70	2404.00	0.0	0.0	0.0	0.0
2257.50	55.45	1.75	1704.80	0.0	0.0	0.0	0.0	0.0
0.14	0.02	0.0	0.42	0.03	0.0	94.59	0.15	0.0
0.03	0.26	0.01	1.91	0.03	0.67	0.15	0.0	0.49
0.0	85.23	10.01	0.27	1.09	2.54	0.0	0.0	0.0
59.84	88.33	7.89	0.79	0.49	2.50	0.0	0.0	0.0
0.16	88.33	7.89	0.79	0.49	2.50	0.0	0.0	0.0
0.0	82.93	5.37	2.73	1.03	8.40	0.0	0.0	0.0
40.00	68.73	5.21	1.49	1.45	13.55	9.63	3.61	0.0
0.0	86.71	9.39	0.27	1.09	2.54	0.0	0.0	0.0
0.0	88.09	8.32	0.74	0.51	2.83	0.0	0.0	0.0
0.0	86.00	5.68	2.17	1.03	4.11	0.18	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3.42	86.14	11.25	0.17	0.38	1.67	0.0	0.0	0.0
70.97	88.11	7.94	0.83	0.56	2.56	0.0	0.0	0.0
10.93	83.82	6.20	2.34	0.96	6.68	0.0	0.0	0.0
8.27	80.37	5.32	3.00	1.05	10.26	0.0	0.0	0.0
6.41	36.64	1.99	0.65	0.84	10.44	54.03	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

APPENDIX A-3

Example of VLE computer calculations used to evaluate the hydrogen partial pressure and hydrogen solubility data.

(IHTMO 17 VLE Models are equivalent to those used in ASPEN Plus)

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FA0	STAR	NAME=010, CUMM=10					
FA0	STAR	NAME=010, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=011, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=012, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=013, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=014, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=015, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=016, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=017, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=018, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=019, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=020, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=021, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=022, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=023, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=024, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10
FA0	STAR	NAME=025, CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10	CUMM=10

 SELECTED PROPERTIES OF HYPOTHETICAL COMPONENTS
 NOTE : * AFTER PROPERTY VALUE INDICATES IT IS USER-INPUT

NAME	COMPAR	TEMP, F	SPGR	MOL WT	TC, F	PC, PSI	OMEGA	ETALK	IDEAL 77, F	CP, BTU/LB, F 400, F	800, F
5010	65-150(SAC)	125.0 *	0.080 *	76.55	428.6	495.69	0.252	0.0	0.377	0.564	0.747
5011	150-200(SAC)	175.0 *	0.136 *	90.61	498.4	503.74	0.283	-0.000	0.352	0.544	0.722
5012	200-250(SAC)	225.0 *	0.172 *	104.39	561.1	482.82	0.317	-0.074	0.340	0.529	0.704
5013	250-300(SAC)	275.0 *	0.214 *	117.41	626.4	473.20	0.345	-0.145	0.324	0.506	0.673
5014	300-350(SAC)	325.0 *	0.252 *	125.90	694.7	472.15	0.365	-0.212	0.304	0.475	0.634
5015	350-400(SAC)	375.0 *	0.293 *	134.75	767.0	510.90	0.400	-0.266	0.274	0.430	0.578
5016	400-450(SAC)	425.0 *	0.366 *	143.16	830.4	505.64	0.432	-0.310	0.269	0.422	0.566
5017	450-500(SAC)	475.0 *	0.470 *	152.19	894.4	452.29	0.418	-0.320	0.273	0.429	0.577
5018	500-550(SAC)	525.0 *	0.588 *	162.24	949.0	425.65	0.455	-0.275	0.272	0.428	0.576
5019	550-600(SAC)	575.0 *	1.012 *	187.62	1006.9	408.43	0.455	-0.200	0.269	0.423	0.570
5020	600-650(SAC)	625.0 *	1.033 *	200.34	1061.3	387.77	0.520	-0.150	0.269	0.423	0.568
5021	650-700(SAC)	675.0 *	1.068 *	216.31	1126.5	384.08	0.534	-0.132	0.269	0.421	0.559
5022	700-750(SAC)	725.0 *	1.097 *	236.11	1186.3	374.35	0.556	-0.122	0.269	0.419	0.552
5023	750-800(SAC)	775.0 *	1.117 *	257.41	1238.9	354.54	0.549	-0.114	0.264	0.419	0.552
5024	800-850(SAC)	825.0 *	1.137 *	279.10	1291.6	327.76	0.606	-0.105	0.269	0.418	0.550
5025	850-900(SAC)	875.0 *	1.227 *	380.63	1517.8	229.30	0.680	-0.050	0.269	0.416	0.542

 2 4117, 4=2014.7, T=700, F=24.39, 364.92, 24.018, 4.29, 4.09, 3.05,
 5.93, 1.19, 1.90, 2.36, 8.84, 47.09, 10041, 1.27815, 6.668, 1.1534,
 5.3856, 33.963, 47.278, 110.51, 134.64, 154.13, 245.41, 153.34, 62.036,
 57.466, 3.5136, 412.09,
 3 471-117, FLASH, 117, -118, 119,
 4=2014.7, T=700,
 4 END PROGRAM

ORDER OF CALCULATION:

1 - 471-117

THERMO INPUT SUMMARY
VERSION 84.262-A

AIR PRODUCTS & CHEMICALS, INC -- CYCLE SYNTHESIS

KANG
97-1-1540

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*** INPUT SUMMARY FOR THERMO ID (TRID) = 'DEFAULT' ***

CAPP THERMODYNAMIC SYSTEM - VERSION 84.249-A

** SPECIFIED THERMODYNAMIC CORRELATION **

TRID: 17

EQUATION OF STATE: LOCAL CORRELATION
Peng-Robinson

APPLICATIONS:

- 1) HIGH PRESSURE CRUDE OIL, HYDROCARBON SYSTEMS
- 2) WATER - ALCOHOL - HYDROCARBON SYSTEMS

LIMITATIONS:

- 1) COMPOUND LISTING ARE APPROXIMATE - USE WITH CAUTION

THERMO - EQUATION OF STATE

00: 0.5 EQUATION OF STATE DEFAULTED

EXTENDED CORRESPONDING-STATES THEORY DEVELOPED AT THE NATIONAL BUREAU OF STANDARDS

APPLICATIONS:

- 1) ATOM PRESSURE SYSTEMS
- 2) HYDROCARBONS UP TO C20
- 3) LIGHT ORGANIC GASES

LIST OF COMPOUNDS: COMPOUND NAME

24	METHANE	30	CARBON DIOXIDE
25	ETHANE	31	CARBON MONOXIDE
26	PROPANE	32	HYDROGEN SULFIDE
1	METHANE	29	WATER
2	ETHANE	5010	65-150(S&C)
3	PROPANE	5011	150-200(S&C)
4	BUTANE	5012	200-250(S&C)
5	PENTANE	5013	250-300(S&C)
		5014	300-350(S&C)
		5015	350-400(S&C)
		5016	400-450(S&C)
		5017	450-500(S&C)
		5018	500-550(S&C)
		5019	550-600(S&C)
		5020	600-650(S&C)
		5021	650-700(S&C)
		5022	700-750(S&C)
		5023	750-800(S&C)
		5024	800-850(S&C)
		5025	850-900(S&C)

FLASH CALCULATION FOR 1271-117

HEAT DUTY = 0.0 BTU/HR
 FLASH TEMP = 760.00 DEG F
 FLASH PRESS = 2014.70 PSIA

STEAM PROPERTIES -- TRIP = DEFAULT, THERMO = CAPP, IMRMO = 17, TRANS = RMS

T O T A L	STEAM NUMBER	* 117 118 119		
		2014.70	2014.70	2014.70
	PRESSURE PSIA	2014.70	2014.70	2014.70
	TEMPERATURE DEG F	760.00	760.00	760.00
	DEG C	1150.20	760.00	760.00
	ENTHALPY BTU/LB	690043.50	395879.19	294204.31
	AVE. MOL WT	54.136261	75.149334	194.361115
	COMPOSITION MOLE %			
	HYDROGEN	33.818848	39.367519	7.000001
	HYDROGEN	36.395545	42.567947	6.541696
	ARGON	1.679360	1.937838	0.431906
	ETHANE	0.747173	0.857132	0.215232
	ETHANE	0.360037	0.424799	0.163500
	PROPANE	0.133251	0.211129	0.106760
	BUTANE	0.044705	0.077450	0.031428
	PENTANE	0.007350	0.007564	0.006360
	CARBON MONOXIDE	0.089774	0.104803	0.017047
	CARBON DIOXIDE	0.276001	0.315985	0.087244
	HYDROGEN SULFIDE	4.724834	0.600322	0.359650
	WATER	7.303239	8.015524	3.712410
	CS-150 (SFC)	0.003571	0.003566	0.003502
	150-200 (SFC)	0.008577	0.006240	0.010206
	200-250 (SFC)	0.018383	0.016707	0.026491
	250-300 (SFC)	0.027450	0.024215	0.047971
	300-350 (SFC)	0.115440	0.089296	0.244396
	350-400 (SFC)	0.704200	0.448920	1.745580
	400-450 (SFC)	0.422701	0.363841	2.658694
	450-500 (SFC)	2.053013	1.042502	6.944591
	500-550 (SFC)	2.154490	0.891624	8.146888
	550-600 (SFC)	2.292800	0.755040	9.731793
	600-650 (SFC)	3.422428	0.856596	15.825402
	650-700 (SFC)	1.981176	0.364154	9.803438
	700-750 (SFC)	0.470763	0.127130	5.051983
	750-800 (SFC)	0.623962	0.050394	3.369592
	800-850 (SFC)	0.033171	0.002013	0.183895
	850-900 (SFC)	3.024928	0.026147	17.531631
	Flow Rate S LBS/Hr			
	HYDROGEN	24.369984	23.524948	0.864881
	HYDROGEN	361.918070	353.681641	11.235934
	ARGON	24.017975	22.959991	1.057637
	ETHANE	4.289999	4.078276	0.211696
	ETHANE	4.069397	3.788545	0.301426
	PROPANE	3.049996	2.761323	0.288653
	BUTANE	0.930000	0.617994	0.112000
	PENTANE	0.190000	0.161803	0.028130

	CARBON MONOXIDE	0.900070	0.870719	0.029275
	CARBON DIOXIDE	4.159937	4.174559	0.235409
	HYDROGEN SULFIDE	8.839946	8.088556	0.751383
	WATER	47.084931	42.989106	4.100493
	CS-150(SRC)	0.100410	0.083540	0.016869
	150-200(SRC)	0.278150	0.221447	0.056702
	200-250(SRC)	0.686050	0.517253	0.169343
	250-300(SRC)	1.153746	0.808455	0.345326
	300-350(SRC)	5.385198	3.439279	1.946486
	350-400(SRC)	33.907982	19.541031	14.367742
	400-450(SRC)	17.211985	23.941254	23.336441
	450-500(SRC)	119.209970	50.152054	69.057175
	500-550(SRC)	134.649984	16.607315	68.031815
	550-600(SRC)	154.174974	42.061234	112.007780
	600-650(SRC)	245.409882	51.018890	194.369481
	650-700(SRC)	153.319974	23.363594	130.014450
	700-750(SRC)	62.038971	8.903020	73.135466
	750-800(SRC)	57.465977	4.305519	53.180054
	800-850(SRC)	3.313549	0.165519	3.146900
	850-900(SRC)	412.089500	2.951798	409.135254
	TOTAL FLOWS LBS/HR	35.791330	22.059943	6.131206
		1937.808587	745.927734	1191.667725
	ENTHALPY BTU/HR	294204.31	0.0	294204.31
	DENS. DENSITY LBS/CU-FT	43.903013	0.0	43.903013
	Avg. Mol. Wt.	194.301115	0.0	194.301115
	COMPOSITION MOLE %			
	HYDROGEN	7.000001	0.0	7.000001
	WATER	6.541090	0.0	6.541090
	WATER	0.431906	0.0	0.431906
	WATER	0.215232	0.0	0.215232
	WATER	0.103500	0.0	0.103500
	WATER	0.106760	0.0	0.106760
	WATER	0.031428	0.0	0.031428
	WATER	0.006360	0.0	0.006360
	CARBON MONOXIDE	0.017047	0.0	0.017047
	CARBON DIOXIDE	0.087244	0.0	0.087244
	HYDROGEN SULFIDE	0.359050	0.0	0.359050
	WATER	3.712410	0.0	3.712410
	CS-150(SRC)	0.003502	0.0	0.003502
	150-200(SRC)	0.010200	0.0	0.010200
	200-250(SRC)	0.026491	0.0	0.026491
	250-300(SRC)	0.047971	0.0	0.047971
	300-350(SRC)	0.244300	0.0	0.244396
	350-400(SRC)	1.745580	0.0	1.745580
	400-450(SRC)	2.656094	0.0	2.656094
	450-500(SRC)	6.944591	0.0	6.944591
	500-550(SRC)	8.146888	0.0	8.146888
	550-600(SRC)	4.731793	0.0	4.731793
	600-650(SRC)	15.825402	0.0	15.825402
	650-700(SRC)	9.803438	0.0	9.803438
	700-750(SRC)	5.051993	0.0	5.051993
	750-800(SRC)	3.369592	0.0	3.369592
	800-850(SRC)	0.183895	0.0	0.183895
	850-900(SRC)	17.531631	0.0	17.531631
	FLOWS LBS/HR			
	HYDROGEN	0.804061	0.0	0.804061
	WATER	11.235934	0.0	11.235934

2	ARGON	1.057837	0.0	1.057837
3	ETHANE	0.211896	0.0	0.211896
4	ETHANE	0.301426	0.0	0.301426
5	PROPANE	0.288653	0.0	0.288653
6	BUTANE	0.112000	0.0	0.112000
7	PENTANE	0.028136	0.0	0.028136
8	CARBON MONOXIDE	0.029275	0.0	0.029275
9	CARBON DIOXIDE	0.235409	0.0	0.235409
10	HYDROGEN SULFIDE	0.751383	0.0	0.751383
11	WATER	4.100493	0.0	4.100493
12	C5-150 (SRC)	0.016869	0.0	0.016869
13	150-200 (SRC)	0.056702	0.0	0.056702
14	200-250 (SRC)	0.169543	0.0	0.169543
15	250-300 (SRC)	0.345376	0.0	0.345376
16	300-350 (SRC)	1.946446	0.0	1.946446
17	350-400 (SRC)	14.421742	0.0	14.421742
18	400-450 (SRC)	23.336441	0.0	23.336441
19	450-500 (SRC)	69.057175	0.0	69.057175
20	500-550 (SRC)	88.031815	0.0	88.031815
21	550-600 (SRC)	112.067780	0.0	112.067780
22	600-650 (SRC)	194.389481	0.0	194.389481
23	650-700 (SRC)	130.014450	0.0	130.014450
24	700-750 (SRC)	73.135468	0.0	73.135468
25	750-800 (SRC)	53.180054	0.0	53.180054
26	800-850 (SRC)	3.146900	0.0	3.146900
27	850-900 (SRC)	409.135254	0.0	409.135254
28	TOTAL LTC. NOU/HR	6.131206	0.0	6.131206
29	NOU/HR	1191.667725	0.0	1191.667725
30	ENTHALPY NOU/HR	395879.19	0.0	395879.19
31	AVP. ENTHALPY NOU/HR	3.710474	0.0	3.710474
32	AVP. NOU/HR	25.149338	0.0	25.149338
33	COMPOSITION NOU/HR	39.362579	0.0	39.362579
34	HYDROGEN	42.567947	0.0	42.567947
35	ARGON	1.937838	0.0	1.937838
36	ETHANE	0.857132	0.0	0.857132
37	ETHANE	0.424799	0.0	0.424799
38	PROPANE	0.211129	0.0	0.211129
39	BUTANE	0.047450	0.0	0.047450
40	PENTANE	0.007564	0.0	0.007564
41	CARBON MONOXIDE	0.104808	0.0	0.104808
42	CARBON DIOXIDE	0.315945	0.0	0.315945
43	HYDROGEN SULFIDE	0.800322	0.0	0.800322
44	WATER	8.045524	0.0	8.045524
45	C5-150 (S-C)	0.003586	0.0	0.003586
46	150-200 (SRC)	0.008240	0.0	0.008240
47	200-250 (SRC)	0.016707	0.0	0.016707
48	250-300 (SRC)	0.023216	0.0	0.023216
49	300-350 (SRC)	0.089266	0.0	0.089266
50	350-400 (SRC)	0.488928	0.0	0.488928
51	400-450 (SRC)	0.563841	0.0	0.563841
52	450-500 (SRC)	1.042562	0.0	1.042562
53	500-550 (SRC)	0.891624	0.0	0.891624
54	550-600 (SRC)	0.755040	0.0	0.755040
55	600-650 (SRC)	0.358596	0.0	0.358596
56	650-700 (SRC)	0.364184	0.0	0.364184
57	700-750 (SRC)	0.127130	0.0	0.127130

750-800(SRC)	0.056394	0.056394	0.0
800-850(SRC)	0.002013	0.002013	0.0
850-900(SRC)	0.026147	0.026147	0.0
* FLOW RATES LBS/HR			
HYDROGEN	23.524940	23.524940	0.0
HYDROGEN	353.681641	353.681641	0.0
ARGON	22.959991	22.959991	0.0
ETHANE	4.078276	4.078276	0.0
ETHANE	3.788545	3.788545	0.0
PROPANE	2.761324	2.761324	0.0
BUTANE	0.817994	0.817994	0.0
PENTANE	0.161863	0.161863	0.0
CARBON MONOXIDE	0.870719	0.870719	0.0
CARBON DIOXIDE	4.124559	4.124559	0.0
HYDROGEN SULFIDE	8.088556	8.088556	0.0
WATER	42.989166	42.989166	0.0
CS-150(SRC)	0.003540	0.003540	0.0
150-200(SRC)	0.221447	0.221447	0.0
200-250(SRC)	0.517253	0.517253	0.0
250-300(SRC)	0.808465	0.808465	0.0
300-350(SRC)	3.439279	3.439279	0.0
350-400(SRC)	19.541031	19.541031	0.0
400-450(SRC)	23.941254	23.941254	0.0
450-500(SRC)	50.152054	50.152054	0.0
500-550(SRC)	46.607315	46.607315	0.0
550-600(SRC)	42.061234	42.061234	0.0
600-650(SRC)	51.018690	51.018690	0.0
650-700(SRC)	23.364594	23.364594	0.0
700-750(SRC)	8.903020	8.903020	0.0
750-800(SRC)	4.305579	4.305579	0.0
800-850(SRC)	0.166679	0.166679	0.0
850-900(SRC)	2.951798	2.951798	0.0
* TOTAL VELOC LBS/HR			
	29.659943	29.659943	0.0
* TOTAL VELOC LBS/HR			
	745.927734	745.927734	0.0
* ACTUAL CPU			
	3.350550	3.350550	0.0

* INDICATES INPUT STREAM

UNIT 871-117

0.06 CPU SECONDS,

0.93 ELAPSED SECONDS,

0.43 SIGMA SECONDS

STREAM SUMMARY
VERSION 84.262-A

AIR PRODUCTS & CHEMICALS, INC -- CYCLE SYNTHESIS

KANG
87-7-1540

24SEP.84 PAGE 7
8:57:15

STREAM SUMMARY -- THID = DEFAULT , THERMO = CAPP , ITHRMO = 17, TRANS = NBS

T D A L	STREAM NUMBER	117	118	119
	PRESSURE PSIA	2014.70	2014.70	2014.70
	TEMPERATURE DEG.F	760.00	760.00	760.00
	OPEN FLOW DEG.F	1150.20	760.00	
	MUDGUE PT DEG.F			760.00
	ENTHALPY BTU/LB	690063.50	395879.19	294204.31
	AVE. MOL WT	54.136261	75.149338	194.361115
	FLOW RATES MOLES/HR			
	HYDROGEN	12.104221	11.674023	0.429222
	NITROGEN	13.026813	12.625632	0.401097
	ARGON	0.801247	0.574762	0.026481
	METHANE	0.267423	0.254225	0.013196
	ETHANE	0.136020	0.125095	0.010024
	PROPANE	0.069167	0.062621	0.006546
	BUTANE	0.016001	0.014073	0.001927
	PENTANE	0.002633	0.002243	0.000390
	CARBON MONOXIDE	0.032131	0.031066	0.001045
	CARBON DIOXIDE	0.099071	0.093721	0.005349
	HYDROGEN SULFIDE	0.259428	0.237375	0.022051
	WATER	2.513933	2.346259	0.227616
	CS-150 (SFC)	0.001278	0.001063	0.000215
	150-200 (SFC)	0.003070	0.002144	0.000626
	200-250 (SFC)	0.006579	0.004955	0.001624
	250-300 (SFC)	0.009827	0.006866	0.002941
	300-350 (SFC)	0.041461	0.026476	0.014984
	350-400 (SFC)	0.252043	0.145015	0.107625
	400-450 (SFC)	0.330217	0.167235	0.163010
	450-500 (SFC)	0.755015	0.309224	0.425787
	500-550 (SFC)	0.763963	0.264455	0.499502
	550-600 (SFC)	0.820620	0.223944	0.546676
	600-650 (SFC)	1.224955	0.254659	0.970288
	650-700 (SFC)	0.709090	0.108017	0.601069
	700-750 (SFC)	0.347450	0.031707	0.309748
	750-800 (SFC)	0.223324	0.016727	0.206597
	800-850 (SFC)	0.011872	0.000597	0.011275
	850-880 (SFC)	1.062663	0.007755	1.074901
	TOTAL FLOW MOLES/HR	35.791336	24.659943	6.131206
	COEFF	1937.608697	745.927734	1191.667725
I O U T	ENTHALPY BTU/LB	294204.31	0.0	294204.31
	AVE. MOL WT	43.963013	0.0	43.963013
	FLOW RATES MOLES/HR	194.361115	0.0	194.361115
	HYDROGEN	0.429222	0.0	0.429222
	NITROGEN	0.401097	0.0	0.401097
	ARGON	0.026481	0.0	0.026481
	METHANE	0.013196	0.0	0.013196
	ETHANE	0.010024	0.0	0.010024
	PROPANE	0.006546	0.0	0.006546
	BUTANE	0.001927	0.0	0.001927
	PENTANE	0.000390	0.0	0.000390

^	CARBON MONOXIDE	0.001045	0.0	0.001045
^	CARBON DIOXIDE	0.005349	0.0	0.005349
^	HYDROGEN SULFIDE	0.022051	0.0	0.022051
^	WATER	0.227616	0.0	0.227616
^	C5-150(SPC)	0.000215	0.0	0.000215
^	150-200(SPC)	0.000626	0.0	0.000626
^	200-250(SPC)	0.001624	0.0	0.001624
^	250-300(SPC)	0.002941	0.0	0.002941
^	300-350(SPC)	0.014984	0.0	0.014984
^	350-400(SPC)	0.107025	0.0	0.107025
^	400-450(SPC)	0.163010	0.0	0.163010
^	450-500(SPC)	0.425787	0.0	0.425787
^	500-550(SPC)	0.499502	0.0	0.499502
^	550-600(SPC)	0.596676	0.0	0.596676
^	600-650(SPC)	0.970288	0.0	0.970288
^	650-700(SPC)	0.601069	0.0	0.601069
^	700-750(SPC)	0.309748	0.0	0.309748
^	750-800(SPC)	0.206597	0.0	0.206597
^	800-850(SPC)	0.011275	0.0	0.011275
^	850-900(SPC)	1.074901	0.0	1.074901
^	TOTAL LTR. SOL/LR	6.131206	0.0	6.131206
^		1191.667725	0.0	1191.667725
V	ENTHALPY BTU/LR	395879.19	395879.19	0.0
A	VEP. DEVIATION/COEFF	3.710474	3.710474	0.0
P	Avg. ZUL, M	25.149338	25.149338	0.0
U	FLOR DATA: SOLID/LR			
R	HYDROGEN	11.674923	11.674923	0.0
	CHLORINE	12.625632	12.625632	0.0
	ARGON	0.574762	0.574762	0.0
	METHANE	0.254225	0.254225	0.0
	ETHANE	0.125995	0.125995	0.0
	PROPANE	0.062621	0.062621	0.0
	BUTANE	0.014073	0.014073	0.0
	PENTANE	0.002243	0.002243	0.0
	CARBON MONOXIDE	0.031086	0.031086	0.0
	CARBON DIOXIDE	0.093721	0.093721	0.0
	HYDROGEN SULFIDE	0.237375	0.237375	0.0
	WATER	2.386299	2.386299	0.0
	C5-150(SPC)	0.001063	0.001063	0.0
	150-200(SPC)	0.002444	0.002444	0.0
	200-250(SPC)	0.004955	0.004955	0.0
	250-300(SPC)	0.008886	0.008886	0.0
	300-350(SPC)	0.026476	0.026476	0.0
	350-400(SPC)	0.145016	0.145016	0.0
	400-450(SPC)	0.167235	0.167235	0.0
	450-500(SPC)	0.309224	0.309224	0.0
	500-550(SPC)	0.264455	0.264455	0.0
	550-600(SPC)	0.223944	0.223944	0.0
	600-650(SPC)	0.254653	0.254653	0.0
	650-700(SPC)	0.108017	0.108017	0.0
	700-750(SPC)	0.037707	0.037707	0.0
	750-800(SPC)	0.015727	0.015727	0.0
	800-850(SPC)	0.000597	0.000597	0.0
	850-900(SPC)	0.007755	0.007755	0.0
^	TOTAL VAPOR SOLID/LR	29.659943	29.659943	0.0
^		749.927734	749.927734	0.0

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ACTUAL CFM	3.350550	3.350550	0.0
HYDROGEN	5.622730	0.0	0.0
NITROGEN	6.506969	0.0	0.0
ARGON	4.486710	0.0	0.0
METHANE	3.982350	0.0	0.0
Ethane	2.594161	0.0	0.0
PROPANE	1.977500	0.0	0.0
BUTANE	1.509760	0.0	0.0
PENTANE	1.189207	0.0	0.0
CARBON MONOXIDE	6.148293	0.0	0.0
CARBON DIOXIDE	3.521840	0.0	0.0
HYDROGEN SULFIDE	2.225281	0.0	0.0
WATER	2.167190	0.0	0.0
CS-150(SPC)	1.023137	0.0	0.0
150-200(SPC)	0.807327	0.0	0.0
200-250(SPC)	0.630064	0.0	0.0
250-300(SPC)	0.483957	0.0	0.0
300-350(SPC)	0.365251	0.0	0.0
350-400(SPC)	0.280095	0.0	0.0
400-450(SPC)	0.212074	0.0	0.0
450-500(SPC)	0.150120	0.0	0.0
500-550(SPC)	0.109443	0.0	0.0
550-600(SPC)	0.077585	0.0	0.0
600-650(SPC)	0.054254	0.0	0.0
650-700(SPC)	0.037149	0.0	0.0
700-750(SPC)	0.025164	0.0	0.0
750-800(SPC)	0.016730	0.0	0.0
800-850(SPC)	0.010919	0.0	0.0
850-900(SPC)	0.001491	0.0	0.0

CYCLE SYNTHESIS RUN TIME :

4.63 CPU SECONDS

19.48 SIGMA SECONDS