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REFINING AND UPGRADING OF SYNFUELS FROM COAL AND
OIL SHALES BY ADVANCED CATALYTIC PROCESSES

Quarterly Report for the Period October—December 1983

By
R. F. Sullivan

February 1984
Date Published

Work Performed Under Contract No. AC22-76ET10532

Chevron Research Company
Richmond, California

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FROM COAL AND OIL SHALES
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PREPARED FOR THE UNITED STATES
DEPARTMENT OF ENERGY

Under Contract No. DE-AC22-76ET10532
(Formerly EF-76-C-01-2315)

I. Abstract

A second-stage hydrocracker feed was prepared by blending hydro-treated 350°F+ Integrated Two-Stage Liquefaction (ITSL) product from Pilot Plant Run 86-75. A second-stage hydrocracking run has been in progress for about 800 hours with this feed and Chevron's commercial ICR 202 catalyst. This report gives the inspections of the second-stage hydrocracker feed; additional yield data and product properties from hydrotreating tests; and inspections of heavy ITSL distillate before and after filtration and distillation. It also includes, as an appendix, a recent paper summarizing results of the ITSL study to date.

II. Contract Objective and Status

The objective of this program is to determine the feasibility and to estimate the costs of hydroprocessing synthetic crude feedstocks to distillate fuels using modern commercial petroleum processing technology. Tests are conducted only to the extent needed to enable making reasonable estimates of commercial plant performance and only to the extent a commercial plant is feasible using presently existing technology, subject to the mutual agreement of DOE and Chevron Research. Tests are made for each whole synthetic oil and, if appropriate, for the fractions derived therefrom. Tests will not be carried out for processes which can be reliably estimated.

The experimental work on all of the feedstocks is now complete except for that now in progress under Task 12 of this contract, upgrading of ITSL oil. The Interim Report describing the study of EDS oil is now being prepared. Interim Reports to date are as follows:

Interim Report No.	DOE Report No.	Subject	Date of Issue
1	FE-2315-25	Paraho Shale Oil	April 1978
2	FE-2315-45	SRC-I	November 1979
3	FE-2315-47	SRC-II	March 1980
3 (Reissued)	DOE/ET/10532-T10	SRC-II	November 1982
4	FE-2315-50	Paraho Shale Oil (Update)	June 1980
5	DOE/ET/10532-T3	H-Coal	September 1981
5 (Addendum)	FE-2315-77	H-Coal	May 1982
6	DOE/ET/10532-T5	SRC-II (For Health-Related Studies)	April 1982
7	DOE/ET/10532-T11	H-Coal, EDS (For Health-Related Studies)	January 1983
8	DOE/ET/10532-Txx (FE-2315-93)	H-Coal (For Health Related Studies)	September 1983
9	DOE/ET-10532-Txx	EDS	In Preparation

III. Task 12: Upgrading of ITSL Product

A. Feeds

The object of Task 12 is to upgrade ITSL product to distillate fuels using modern petroleum processing technology.

The ITSL process development unit at Lummus has been operated to produce either a product boiling below 650°F or product boiling below 850°F. ITSL light oil and middle distillate from Illinois No. 6 coal (Burning Star Mine) were blended in the ratio recommended by Lummus to represent whole liquid product when operating at 650°F cut point. The inspections of the blend (see Appendix) indicate that the boiling range was closer to "Start-700°F" than "Start-650°F" and that the actual end point was about 750°F. Most of our work to date in this task has been carried out using this feed.

One drum of the "Start-700°F" ITSL oil was distilled to produce a 650°F end point oil for additional testing. Unfortunately, due to a laboratory error, this feed was contaminated with methylene chloride during the distillation. Some of the methylene chloride reacted with nitrogen compounds in the ITSL oil and reduced the nitrogen content from an expected 500 ppm for this fraction to 225 ppm. Therefore, even if the methylene chloride could be removed from the 650°F- fraction, the heteroatom content would no longer be representative of 650°F- ITSL, and the sample is not suitable for further pilot plant tests.

Lummus also sent us two partial drums (about 65 gal. total) of heavy heavy distillate to represent additional product obtained when the ITSL process is operating at 850°F cut point. Table I shows that this material contained a considerable amount of 850°F+ residuum and over 1000 ppm of metals including 470 ppm of iron. Table I also shows that even after filtration through a 3-micron filter, the blend contained over 600 ppm of metals. Therefore, an attempt was made to redistill the heavy distillate in a continuous vacuum column to remove the 850°F+ residuum. However, after the column lined out and about 40 lb of overhead material had been collected, the column suddenly plugged with a solid, cokelike material. Presumably, the plugging was due to thermal degradation in the distillation column. It was also noted that the interior walls of the drums containing the undistilled material were coated with a tarlike deposit and some solid particles which also suggests that the oil is unstable. Apparently, some polymerization had also occurred in the drums prior to the attempted distillation. Properties of the overhead fraction, also shown in Table I, indicate that virtually all of the metals, 99% of the hot hexane insolubles, and 90% of the Ramsbottom carbon were removed by distillation. Because only a

small quantity of the 850°F- fraction is available, only a limited experimental program will be possible.

B. Pilot Plant Run 86-75:
Preparation of Second-
Stage Hydrocracker Feed

A large fraction of hydrotreated "Start-700°F" ITSL oil boils in the middle distillate boiling range. Further cracking to naphtha is necessary if this middle distillate fraction is to be reformed to high octane gasoline.

A 500-hr hydrotreating pilot plant run (Run 86-75) was made to prepare a sufficient quantity of 350°F+ hydrocracker feed for subsequent second-stage hydrocracking to naphtha. Pilot Plant 86 operates with three reactors in series, and contained a total of 750 ml of ICR 106 catalyst (whole extrudate) in this run. The target product nitrogen in this run was 0.5 ppm; run conditions were 1.0 LHSV, 2300 psia hydrogen partial pressure (2500 psig total pressure), and 8000 SCF/bbl. Specification product was made at an average catalyst temperature of about 720°F after about 250 hr onstream. (During a 250-hr transient period at the start of the run, the required catalyst temperature gradually increased from 700°F to 720°F before the catalyst activity for the desired product quality stabilized at 720°F.)

Table II gives the properties of the product blend collected from 261 to 505 hr to be used as second-stage hydrocracker feed. Pilot Plant Run 62-281, described in "C" below, is being made using this feed.

Table III gives two yield periods obtained in Run 86-75 during the lined-out period when on-specification product was being made. Hydrogen consumption was between about 1150 and 1200 SCF/bbl for 350°F end point product containing 0.25-0.5 ppm nitrogen and 32-35% aromatics.

Table IV gives inspections of the naphtha product and the 350°F+ product as the run progressed. The first two sets of samples were taken early in the run during the initial transient period before the activity lined out. The second two sets of analyses were obtained after lining out.

C. Pilot Plant Run 62-281:
Hydrocracking of Hydrotreated
ITSL Oil

Pilot Plant Run 62-281 is currently in progress using the hydro-treated 350°F+ ITSL oil, WOW 5251 (see Table II), and Chevron's ICR 202 catalyst.

The following conditions were selected:

Hydrogen Partial Pressure, psia	2100
Total Pressure, psig	2300
Recycle Gas Rate, SCF/bbl	5600
Recycle Cut Point, °F	350
Per Pass Conversion, LV%	60

After 800 hours onstream, the catalyst operating temperature is about 577°F and the catalyst appears to be stable. Yield data is being collected, and we expect to give initial results in our next report.

D. Pilot Plant Run 90-167;
Additional Yields and
Product Properties

Tables V through VIII give additional yields and product properties obtained during Run 90-167 in which ITSL oil was hydro-treated at several different severities with ICR 106 catalyst. The run has been discussed in detail in other reports and in the Appendix. The results shown in these tables were obtained at 1.5 LHSV and pressures of 1800 and 1500 psia hydrogen partial pressure.

E. Technical Presentation

A paper, "Refining of Syncrudes from Direct Coal Liquefaction Processes," was presented at the 1983 Direct Liquefaction Contractors' Conference in Pittsburgh, Pennsylvania, November 16-17, 1983. This paper summarizes our work with ITSL oil to the date of the conference and is given in the Appendix.

F. Program

The second-stage hydrocracking pilot plant run is expected to continue through February. We are also planning brief pilot plant tests with higher end point ITSL oils for comparison with lower end point feedstocks. Following completion of these tests, we will begin Process Engineering studies for ITSL oil. Meanwhile, Process Engineering estimates for the other coal-derived liquids previously studied are being updated for comparisons on a common basis.

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REFINING AND UPGRADING OF SYNFUELS
FROM COAL AND OIL SHALES
BY ADVANCED CATALYTIC PROCESSES
DOE CONTRACT DE-AC22-76ET10532

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TABLE I
DOE CONTRACT DE-AC22-76ET10532
EFFECT OF FILTRATION AND DISTILLATION
ON COMPOSITION OF ITSL HEAVY DISTILLATE

Description Identification	As-Received Heavy Distillate*	Filtered Heavy Distillate**	Redistilled Heavy Distillate***
	WOW 4967/WOW 4968	WOW 5218	WOW 5162
Gravity, °API	-0.5	1.4	4.3
Sulfur, Wt %	0.34	0.21	0.13
Total Nitrogen, Wt %	0.38	0.27	0.19
Basic Nitrogen, Wt %	0.16	N/A	0.08
Oxygen, Wt %	1.14	0.80	0.46
Hydrogen, Wt %	8.16	N/A	8.92
Carbon, Wt %	89.98	N/A	90.30
Chlorine, ppm	21	N/A	33
Water, ppm	478	N/A	230
Hot Heptane Insolubles, Wt %	7.76	4.70	0.06
Ramsbottom Carbon, %	6.4	4.5	0.47
ASTM D 2887 Distillation (TBP by GC)			
ST/5	458/571	(122)/560	465/562
10/30	594/662	583/649	585/649
50	696	686	684
70/90	738/808	728/798	719/769
96/99	858/989	840/976	798/859
ASTM D 1160 Distillation, °F			
St/5	520/606	N/A	590/621
10/30	638/687		637/676
50	720		703
70/90	763/883		732/781
95/EP	-/926(92.5%)		812/865
% Overhead	92.5		99
Metals by Atomic Adsorption			
Iron	470	288	0.15
Aluminum	332	200	<0.3
Calcium	113	64	0.12
Potassium	47	34	<0.5
Titanium	18	14	<0.03
Magnesium	17	12	<0.09
Silicon	13	(440)(?)	0.15
Sodium	8	8	0.25
Boron	8	N/A	0.14

*Average of two drums.

**Filtered through a 3-micron filter.

***Approximately 95% overhead.

N/A = Not Analyzed

TABLE II

DOE CONTRACT DE-AC22-76ET10532
 PROPERTIES OF 350°F+ HYDROTREATED ITSL OIL
 HYDROCRACKER FEED
PREPARED IN PILOT PLANT 86-75 AT 261-505 HR

Conditions: 1.0 LHSV
 721°F
 ~2300 psia Hydrogen
 ~1200 SCF/Bbl Hydrogen Consumption

Blend Identification	WOW 5251
Inspections	
Gravity, °API	21.7
Aniline Point, °F	105.3
Sulfur, ppm	0.58
Nitrogen, ppm	0.25
Oxygen, ppm	80
Hydrogen, Wt %	12.11
Carbon, Wt %	87.89
Group Type, LV %	
Paraffins	0.0
Naphthenes	67.8
Aromatics	32.2
ASTM D 2887 Distillation, °F	
(TBP by GC)	
St/5	298/359
10/30	384/483
50	543
70/90	591/654
95/99	683/747
ASTM D 86 Distillation, °F	
St/5	368/401
10/30	425/496
50	550
70/90	590/637
95/EP	664/667
% Overhead	97

TABLE III

DOE CONTRACT DE-AC22-76ET10532
 YIELDS FROM HYDROTREATING OF ITSL OIL, WOW 5104
 WITH ICR 106 CATALYST AT 1.0 LHSV
 AND 2300 PSIA HYDROGEN PRESSURE
 PILOT PLANT RUN 86-75

Run Hr	261-285		333-357	
Average Catalyst Temp., °F	722		722	
LHSV	1.01		1.00	
Total Pressure, psig	2504		2487	
H ₂ Mean Pressure, psia	2311		2292	
Total Gas, SCF/Bbl	9769		9499	
Recycle Gas, SCF/Bbl	8517		8234	
No Loss Product Yields	Wt %	Vol %	Wt %	Vol %
C ₁	0.06		0.05	
C ₂	0.12		0.09	
C ₃	0.17		0.13	
iC ₄	0.02	0.04	0.02	0.03
nC ₄	0.21	0.34	0.16	0.26
C ₅ -150°F	0.30	0.44	0.22	0.34
150-350°F	9.36	11.41	8.72	10.61
350°F+	91.24	93.88	92.16	94.82
Total C ₅ +	100.90	105.72	101.10	105.77
Actual/No Loss Recovery	99.14/101.82		100.59/101.89	
H ₂ S Consumption (Gross), SCF/Bbl	1252		1265	
H ₂ Consumption (Chem.), SCF/Bbl	1141		1180	
Nitrogen in 350°F+ Product	0.45		0.29	

Note: See Table IV for inspections for product blends from 261-357 hr.

TABLE IV

DOE CONTRACT DE-AC22-76ET10532
 PRODUCT PROPERTIES FROM HYDROTREATING ITSL OIL, WOW 5104
 WITH ICR 106 CATALYST AT 1.0 LHSV AND 2300 PSIA HYDROGEN PRESSURE
 PILOT PLANT RUN 86-75

Run Hr	30-78*	78-114*	261-357	357-381
Average Catalyst Temperature, °F	703	713	722	720
150-350°F Product				
Gravity, °API	46.9	47.6	50.0	50.0
Aniline Point, °F	93.7	92.0	92.1	90.9
Sulfur, ppm		5.8		
Total Nitrogen, ppm	0.24	0.32	0.30	0.69
Oxygen, ppm		<50		
Group Type (Low Mass), LV %				
Paraffins		7.7	7.3	
Naphthenes		83.0	85.1	
Aromatics		9.3	7.6	
ASTM D 2887 Distillation, °F (TBP by GC)				
St/5		159/177	164/180	165/184
10/30		182/214	184/193	187/195
50		227	220	221
70/90		277/332	242/276	243/275
95/99		342/362	295/330	284/290
350°F+ Product				
Gravity, °API	22.0	21.5	21.7	21.6
Aniline Point, °F	114.4	107.5	103.4	102.2
Sulfur, ppm		0.6	0.6	0.5
Total Nitrogen, ppm	0.20	0.32	0.43	0.33
Oxygen, ppm		140	100	100
Group Type (22-Component), LV %				
Paraffins		0.5	0.0	
Naphthenes		65.6	65.4	
Aromatics		33.7	34.2	
ASTM D 2887 Distillation, °F (TBP by GC)				
St/5	342/376	333/370	270/356	
10/30	396/490	394/488	380/479	
50	540	546	540	
70/90	589/649	593/653	589/651	
95/99	678/739	682/747	680/737	

*Samples taken during initial transient period before the catalyst activity was stable.

TABLE V
DOE CONTRACT DE-AC22-76ET10532
YIELDS FROM HYDROTREATING OF ITSL OIL, WOW 5104
WITH ICR 106 CATALYST AT 1.5 LHSV;
1800 AND 1500 PSIA HYDROGEN PARTIAL PRESSURES;
PILOT PLANT RUN 90-167

Run Hr	4371-4395	4851-4875	4923-4947	5067-5091
Average Catalyst Temperature, °F	761	761	760	761
LHSV	1.50	1.50	1.48	1.49
Total Pressure, psig	2010	1997	2001	1703
H ₂ Mean Pressure, psia	1843	1823	1819	1495
Total Gas in, SCF/Bbl	8227	8490	8621	8281
Recycle Gas, SCF/Bbl	7582	7884	7997	7886
No Loss Product Yields	Wt % LV %	Wt % Vol %	Wt % LV %	Wt % LV %
C ₁	0.05	0.04	0.05	0.03
C ₂	0.08	0.05	0.06	0.04
C ₃	0.06	0.05	0.05	0.01
iC ₄	0.01 0.01	0.01 0.01	0.01 0.01	0.00 0.00
nC ₄	0.05 0.08	0.04 0.06	0.04 0.06	0.02 0.04
C ₅ -150°F	0.07 0.10	0.15 0.23	0.06 0.08	0.02 0.02
150-250°F	6.93 8.58	6.12 7.65	6.22 7.69	5.60 6.92
250-350°F	5.51 6.42	{94.10} {95.04}	4.02 4.73	5.40 6.30
350°F+	87.86 87.56		90.07 90.01	89.10 88.80
Total C ₅ +	100.36 102.67	100.37 102.92	100.36 102.52	100.12 102.04
Actual/No Loss Recovery	99.2/101.0	99.2/100.9	99.0/100.9	98.7/100.6
H ₂ Consumption (Gross), SCF/Bbl	644	606	624	394
H ₂ Consumption (Chem.), SCF/Bbl	594	560	575	378
Whole Liquid Product Properties				
Gravity, °API	21.1	20.6	20.5	19.4
Aniline Point, °F	61.1	59.2	59.0	48.1
Sulfur, ppm	11.1	Incomplete	5.6	13.8
Total Nitrogen, ppm	6.0	6.0	6.1	23.1
Oxygen, ppm	300	400	400	500
Hydrogen, %	11.33	11.23	11.14	10.88
Carbon, %	88.64	88.73	88.82	89.06
Group Type Analysis, LV % (22-Component)				
Paraffins	1.2	1.2	1.2	1.6
Naphthenes	40.7	40.7	40.9	34.98
Aromatics	58.0	58.1	57.9	63.56
Group Type Analysis, LV % (Calculated from Weighted Average of Components)				
Paraffins	1.5	1.2	1.4	1.4
Naphthenes	44.1	41.4	41.6	37.3
Aromatics	54.4	57.4	57.0	61.3
TPB Distillation, °F (Simulated by Chromatography)				
St/5	92/212	127/215	128/216	118/230
10/30	297/451	312/454	320/456	331/465
50	538	540	542	549
70/90	596/667	597/667	599/670	604/674
95/99	695/762	696/763	699/771	704/767

TABLE VI

DOE CONTRACT DE-AC22-76ET10532
 HYDROTREATING OF ITSL OIL AT 1.5 LHSV;
 1800 AND 1500 PSIA HYDROGEN PRESSURES
 WITH ICR 106 CATALYST
PROPERTIES OF 150-250°F PRODUCT FRACTIONS

Run Hr	4371-4395	4851-4875	4923-4947	5055-5067
Average Catalyst Temp., °F	761	761	760	761
Hydrogen Partial Pressure, psia	1843	1823	1819	1495
150-250°F Product Inspections				
Gravity, °API	53.0	54.6	52.6	52.5
Aniline Point, °F	91.1	89.1	89.3	90.2
Octane Number				
F-1 Clear	77.4	N/A	76.7	N/A
Group Type (Low Mass), LV %				
Paraffins	11.6	12.1	12.5	13.5
Naphthenes	81.9	79.4	79.1	77.9
Aromatics	6.5	8.5	8.4	8.6
Aromatics Distribution				
C ₆	1.8	1.9	2.0	2.3
C ₇	4.6	5.2	5.2	5.9
C ₈	0.0	1.4	1.3	1.5
Hydrogen, Wt %				
Analysis	N/A	13.88	N/A	N/A
Calc. from Mass Spec.	14.1	14.0	14.0	14.0
Carbon, Wt % (Analysis)	N/A	86.12	N/A	N/A
TBP Distillation, °F				
(Simulated by Chromatography)				
30/5	63/154	66/164	N/A	55/159
10/30	168/187	180/189		180/189
50	199	216		216
70/90	221/237	224/249		224/247
95/99	248/283	268/296		267/287

N/A = Not Analyzed

TABLE VII

DOE CONTRACT DE-AC22-76ET10532
 HYDROTREATING OF ITSL OIL AT 1.5 LHSV;
 1800 AND 1500 PSIA HYDROGEN PRESSURES WITH ICR 106 CATALYST
 PROPERTIES OF 250-350°F PRODUCT FRACTION

Run Hr	4371-4395	4923-4947	5055-5067
Average Catalyst Temperature, °F	761	760	761
Hydrogen Partial Pressure, psia	1843	1819	1495
250-350°F Product Inspections			
Gravity, °API	42.2	44.0	42.5
Aniline Pont, °F	87.9	87.5	84.9
Octane Number F-1 Clear	58.7	60.0	N/A
Group Type (Low Mass), LV %			
Paraffins	7.5	7.0	7.6
Naphthenes	74.3	75.1	73.4
Aromatics	18.2	17.9	19.0
Naphthene Distribution			
Cycloparaffins	59.7	63.4	58.4
Cicycloparaffins	14.6	11.7	15.0
Alkylbenzene Distribution			
C6	0.1	0.1	0.1
C7	0.8	1.3	1.4
C8	7.5	8.8	6.7
C9	7.0	6.3	6.8
C10	1.6	0.9	2.2
Bicycle Aromatics			
Benzonaphthenes	1.2	0.5	1.8
Naphthalenes	0.0	0.0	0.0
Hydrogen, Wt %			
Analysis	N/A	N/A	13.12
Calc. from Mass Spec.	13.3	13.4	13.2
Carbon, Wt % (Analysis)	N/A	N/A	86.88
TBP Distillation, °F (Simulated by Chromatography)			
St/5	N/A	192/237	181/236
10.30		248/275	252/282
50		296	312
70/90		318/340	332/357
95/99		351/383	364/376

N/A = Not Analyzed

TABLE VIII

DOE CONTRACT DE-AC22-76ET10532
 HYDROTREATING OF ITSL OIL AT 1.5 LHSV; 1800 AND 1500 PSIA
 HYDROGEN PRESSURES WITH ICR 106 CATALYST
 PROPERTIES OF 250°F+ AND 350°F+ PRODUCT FRACTIONS

Run Hr	4851-4875	4371-4395	4923-4947	5067-5091
Average Catalyst Temp., °F				
Hydrogen Partial Pressure, psia	1823	1843	1819	1495
Boiling Range, °F	250+	350+	350+	350+
Product Inspections				
Gravity, °API	18.9	16.9	17.3	17.1
Aniline Point, °F	57.4	57.1	57.6	44.7
Group Type (22-Component), LV %				
Paraffins	0.0	0.0	0.0	0.0
Naphthenes	38.4	38.2	36.7	31.6
Aromatics	61.5	61.7	63.3	68.4
Naphthene Distribution				
Cycloparaffins	13.7	15.4	13.2	12.5
Dicycloparaffins	14.4	13.4	13.8	11.0
Tricycloparaffins	10.2	9.6	9.8	8.2
Aromatics Distribution				
Monoaromatics				
Alkylbenzenes	11.4	12.0	11.8	13.4
Benzocycloparaffins	15.3	14.6	15.0	13.9
Benzodicycloparaffins	9.0	8.4	9.3	8.4
Diaromatics				
C(N)H(2N-12) Naphthalenes	10.0	10.2	10.5	10.0
C(N)H(2N-14)	5.1	5.0	4.9	5.8
C(N)H(2N-16)	4.5	4.3	4.5	6.1
Triaromatics				
C(N)H(2N-18)	1.8	1.8	2.1	3.6
C(N)H(2N-22)	4.6	5.2	5.2	7.1
Hydrogen Wt %				
Analysis	11.03	N/A	N/A	10.55
Calc. from Mass Spec.	11.3	11.3	11.2	10.9
Carbon, Wt % (Analysis)	88.93	N/A	N/A	88.40
ASTM D 2887 Distillation, °F (TBP by GC)				
St/5	256/361	346/388	327/381	351/396
10/30	394/490	411/501	403/499	424/510
50	561	565	564	571
70/90	608/672	610/676	610/676	617/681
95/99	700/764	706/785	706/784	711/774
ASTM D 86 Distillation, °F				
St/5	354/397	418/442	391/421	N/A
10/30	427/504	456/512	443/508	
50	558	563	560	
70/90	601/652	603/654	603/655	
95/EP	679/710	681/708	686/710	
% Overhead	98	98	98	
Viscosity, cSt at 122°F	3.823	3.856	3.764	N/A

N/A = Not Analyzed

A P P E N D I X

REFINING OF SYNCRUDES FROM
DIRECT COAL LIQUEFACTION PROCESSES

By

R. F. Sullivan

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REFINING OF SYNCRUDES FROM
DIRECT COAL LIQUEFACTION PROCESSES

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A B S T R A C T

Syncrudes produced in direct coal liquefaction processes can be converted to transportation fuels using modern commercial petroleum hydroprocessing technology. Upgrading routes typically consist of hydrogen addition and removal of heteroatom and inorganic impurities. The upgraded liquids are low in paraffin content and consist mainly of cyclic hydrocarbons. As a result, these liquids have some unusual and desirable properties for transportation fuels. Chevron Research Company, under DOE contract, has conducted pilot plant studies on the refining of product from the Solvent Refined Coal-2 (SRC-II), H-Coal, and Exxon Donor Solvent (EDS) processes and is currently studying the upgrading of liquids from the Integrated Two-Stage Liquefaction (ITSL) Process. This paper is a progress report on the ITSL study and compares and contrasts results with ITSL oil to those obtained with other coal-derived liquids.

Encl. - See Index of Enclosures

I. Introduction

Synthetic oils derived from direct coal liquefaction processes are typically too low in hydrogen content and too high in heteroatom and inorganic impurities to be acceptable as present day transportation fuels. Therefore, upgrading is required to convert these oils to specification fuels. Upgrading must include steps to: (1) increase the hydrogen content, or in some cases decrease the carbon content (as in a coking process); (2) remove nitrogen, sulfur, oxygen, and inorganic impurities; and (3) convert high boiling compounds into compounds boiling in an acceptable range.

Fortunately, the petroleum industry has developed high pressure hydroprocessing technology to remove nitrogen, sulfur, and metals from vacuum gas oils and residual stocks and to convert heavy oils to distillate fuels. Much of this petroleum processing technology is directly applicable to the refining of synthetic crudes.

Chevron Research Company, under a contract sponsored by the U.S. Department of Energy (DOE), has been conducting a program since 1976 to determine the feasibility of converting synthetic crudes to distillate fuels using hydroprocessing and other modern petroleum processing technologies. Oils derived from shale and coal have been studied. In this program pilot plant tests for the key processing steps were conducted to the extent needed to make reasonable estimates of commercial catalyst performance to produce specification products. Detailed results of these studies are presented in a series of DOE reports (Reference 1).

As a part of the contract, we developed refining schemes for processing each of the syncrudes in a "grass roots" refinery to produce fuels meeting current specifications. The ground rules called for finished products rather than blending stocks. In reality, it is likely that the first commercial syncrudes will be processed in existing petroleum refineries. The resulting products could then be used as blending stocks. The latter option will provide additional refinery flexibility for the optimum utilization of the products. However, studies of blends of products derived from syncrudes are beyond the scope of the present study.

Coal liquids studied under this contract include liquids from the following liquefaction processes: SRC-II, H-Coal, EDS, and ITSL. Much of the information on the first three studies has been reported in other papers. This is our first paper describing results from the upgrading of ITSL liquid. This work is still in progress; therefore, this paper serves as a progress report and some of the conclusions are tentative. Comparisons are made to previously reported results for the other coal liquids.

II. Feeds

The feeds used in this study are listed below:

Liquefaction	Source of Coal	Type of Coal	Supplier Process
SRC-II	Pittsburgh Seam (West Virginia)	Bituminous	Pittsburg and Midway Coal Mining Co.
H-Coal	Illinois No. 6 (Burning Star)	Bituminous	Hydrocarbon Research, Inc.
H-Coal	Wyodak	Sub-Bituminous	Hydrocarbon Research, Inc.
EDS	Big Brown (Texas)	Lignite	Exxon Research and Engineering Co.
ITSL	Illinois No. 6 (Burning Star)	Bituminous	Lummus Co.

Differences observed between the results for the different feedstocks are believed due to a combination of the following factors: (1) differences in the liquefaction processes; (2) differences among the coals; (3) differences in the distillation procedures used in separating the syncrude from the recycle material and residue; and (4) differences in storage and handling of the syncrudes.

Previously, we compared two syncrudes prepared in a single process (the H-Coal process). The results for H-Coal oils from Illinois No. 6 and Wyodak coals were reported previously (References 1-4, included). In the current study, we are able to compare syncrudes from two different liquefaction processes (H-Coal and ITSL) prepared from the same coal (Illinois No. 6, Burning Star Mine).

It will be recognized that, although each syncrude was selected as being representative of the net whole liquid product that the liquefaction process was expected to produce from a given coal at the time it was selected, all of the products were prepared on a pilot scale, and none of the processes are yet fully optimized. The boiling ranges of the syncrudes and the quantities of impurities that they contain are likely to vary considerably as the processes evolve.

According to Lummus, the ITSL process development unit has been operated to produce either a product boiling below 650°F or a product boiling below 850°F. At DOE's request, our program has been directed toward processing the lower boiling product.

Some of the interrelated factors which we believe contribute to the relative ease or difficulty of processing coal liquids are:

(1) amount and types of heteroatoms (nitrogen- and oxygen-containing compounds in particular); (2) amount of hot heptane insolubles; (3) amount of Ramsbottom carbon; (4) boiling range of the coal liquid (in general, the higher the average boiling point, the more difficult a feed is to process); (5) hydrogen content (the greater the hydrogen content, the easier a feed is to process); (6) the amount of high end point "tail" (that is, the sharpness of the end point); (7) the amount and types of polynuclear aromatics present; and (8) age of the sample (coal liquids are notoriously unstable before extensive hydroprocessing).

Table I summarizes the properties of the syncrudes. The ITSL process product differs from the other liquids in several respects:

1. The ITSL oil is much lower in heteroatom content than any of the other liquids.
2. The ITSL oil is considerably higher in average boiling range than the other oils, as illustrated in Figures 1 and 2. The mid-point of the ITSL liquid is 560°F, those of the other coal liquids range from about 350-425°F. The ITSL oil contains only 12% 350°F-naphtha; the other coal oils contain quantities of 350°F-naphtha ranging from 25% for SRC-II to more than 60% for Wyodak H-Coal. (Note that the end point of the ITSL oil is over 700°F rather than the target of 650°F.)
3. The ITSL oil has considerably fewer hot heptane insolubles than the other oils. However, it has a Ramsbottom carbon content similar to that of the H-Coal liquids.
4. In spite of the low heteroatom content of the ITSL oil compared to the other oils, it has a lower hydrogen content than any of the other oils except SRC-II oil.

The low hydrogen content of a given coal-oil is not necessarily a disadvantage in the overall processing scheme. The downstream processing steps generally utilize hydrogen more efficiently than the liquefaction process itself. As will be shown, virtually no light gases are formed in the hydrotreating unit. Therefore, less hydrogen will be required for the combination of upstream and downstream

processes to make comparable end product if the downstream hydro-treating unit does more of the hydrogenation. However, catalyst deactivation rates would be expected to be higher in the hydro-treating unit with the feed containing less hydrogen (other feed properties being equivalent).

Figure 3 shows the hydrogen content of narrow boiling fractions of the ITSL oil plotted versus the mid-boiling point of the fraction. Results are compared to those for Illinois H-Coal. Note that, although the H-Coal oil has a higher total hydrogen content, the hydrogen content of most of the fractions of a given boiling range fraction are appreciably higher for the ITSL oil. However, because the ITSL oil contains much larger quantities of the higher boiling fractions, the average for the whole ITSL oil is lower.

Figure 4 shows the distribution of nitrogen and oxygen heteroatom containing compounds in the ITSL. Nitrogen content increases as the boiling range increases. The oxygen content reaches a maximum in the 300-350°F fraction and is also high in the 350-400°F fraction. The high concentration of oxygen-containing compounds in the 300-400°F range is typical for coal-derived oils and was previously observed for SRC-II, H-Coal, and EDS oils.

All of the coal-derived oils contained traces of chlorine containing compounds. Upon hydrotreating, these compounds are converted to HCl, which can cause corrosion of the equipment. Also, in the presence of ammonia (another product of hydroprocessing), ammonium chloride is formed which can plug the reactor exit lines. These

chlorine-containing compounds can be removed to about 1 ppm by water washing the oils at ambient temperature. The ITSL oil was water washed prior to processing; the significant changes in product properties were as follows:

	ITSL Oil Properties	
	Before Water Wash	After Water Wash
Chlorine, ppm	19	1.2
Oxygen, ppm	6000	1800
Iron, ppm	2.5	1.3

The above table shows that in addition to the removal of chlorine, water washing causes a significant decrease in the oxygen content and some decrease in soluble iron impurities. Any other changes are masked by the normal scatter of the data.

III. Pilot Plant Test

A 5200-hr pilot plant test was made in which the ITSL oil was hydrotreated using Chevron's ICR 106 catalyst. The conditions were chosen so that the results could be compared directly to those obtained in tests made with other coal-derived oils using the same catalyst. Severity was varied by changing the pressure and the liquid hourly space velocity (LHSV). Temperature was adjusted to vary product quality.

The tests were as follows:

Summary of Pilot Plant Run 90-167 with ITSL Oil

Test No.	1	2	3	4	5
Length of Test, Hr	1590	1660	770	810	370
Total Pressure, psig	2500	2500	2500	2000	1700
Hydrogen Partial Pressure, psia	2300	2300	2300	1800	1500
LHSV, Volumes of Feed per Volume Catalyst per Hr	0.5	1.0	1.5	1.5	1.5

All of the tests were made with a target recycle gas rate of 8000 standard cubic feet per barrel (SCF/B) of feed.

Figure 5 summarizes the first four periods of the run (5000 hr). Product nitrogen, product aromatics content, and the average catalyst temperature are plotted versus time onstream. (Nitrogen and aromatics contents after 5000 hr would be offscale, so Period 5 is not shown.)

The first 170 hr were made with a petroleum-derived feed to line out the catalyst and conditions. At 170 hr, the ITSL feed was introduced.

Period 1 (170-1760 hr). The first test with ITSL oil was made at a low LHSV (0.5) and high hydrogen partial pressure (about 2300 psia) with the purpose of making a maximum amount of mid-distillate product meeting either jet fuel or diesel specifications.

Our past experience has shown that it is necessary to remove virtually all of the heteroatoms and to saturate most of the aromatic

compounds to make acceptable jet and diesel fuels. The target was achieved at a lined-out catalyst temperature of 710°F. At 710°F, the nitrogen in the whole liquid product was less than 0.2 ppm and the aromatics were about 10 LV %. Hydrogen consumption was 1600-1700 SCF/B.

Period 2 (1760-3420 hr). The purpose of the second test was to simulate the first stage of a two-stage hydrocracker. In the first stage the oil is hydrotreated to remove almost all of the hetero-atoms. The feed to the second stage should contain less than 1-ppm nitrogen. In the second stage, the 350°F+ hydrotreated oil will be cracked to extinction; that is, it will be converted entirely to 350°F- product. The naphtha product from the second stage will then be converted to high octane gasoline in a catalytic reformer. To keep the nitrogen in the hydrotreated product below 1 ppm, the catalyst temperature was increased to 730°F during Period 2. Product aromatics increased to about 26 LV %. Hydrogen consumption was about 1400 SCF/B.

Two upsets occurred during the 1660-hr Period 2 operation. Both of these upsets were associated with changing to a new feed barrel on the pilot plant. We speculate that some contaminant [such as: (1) heavy residue or (2) liquid water that had not completely separated at the time the feed was water washed] was introduced into the pilot plant from the bottom of the new feed barrel. (Feed to the pilot plant comes through a tube that reaches to the bottom of the feed barrel.) The first upset resulted in about 10°F loss

in catalytic activity, the second in about 5°F activity loss. The combined total activity loss for the two upsets was a loss of about 15°F of catalyst activity. However, there appears to have been no measurable gradual catalyst fouling during the 1660 hr at 1.0 LHSV in Period 2.

Period 3 (3420-4190 hr). The LHSV was increased to 1.5 for the next test. The purpose of this test was again to make a second-stage hydrocracker feed, but at a higher feed throughput than in Period 2. It was necessary to raise the temperature to 760°F to keep the product nitrogen below the target of 1 ppm. No catalyst fouling was observed Period 3. Aromatics in the whole liquid product increased to about 38 LV %. Hydrogen consumption was about 950 SCF/B.

Period 4 (4190-5000 hr). To study catalyst performance at a lower severity, the hydrogen partial pressure was decreased to 1800 psia. Other conditions were the same; LHSV was 1.5 and catalyst temperature was 760 °F. Product nitrogen lined out at 6 ppm and product aromatics at 58%. This nitrogen content is too high for the product to be a premium second-stage hydrocracker feed, but it could be used as a fuel oil blending component. Hydrogen consumption was about 600 SCF/B. Catalyst deactivation rate was still too low to be measured.

Period 5 (5000-5370 hr). A short test was made at even lower severity. The pressure was dropped further to 1500 psia hydrogen. LHSV was held at 1.5 and the temperature at 760°F. Product

nitrogen increased to 24 ppm., the product aromatics increased to 64%, and the hydrogen consumption decreased to 375 SCF/B. (The test was terminated when it was discovered that the remaining feed had been contaminated with a chlorine-containing compound which decomposed to form HCl during the hydrotreating process. The HCl reacted with ammonia product to form ammonium chloride which plugged the reactor exit lines.)

IV. Results

A. Activity

Table II summarizes results of previous tests we have made with other coal-derived oils with ICR 106 catalyst. All of these tests were made at 750°F and with relatively fresh catalyst. The results show that the EDS oil is the most difficult to hydroprocess and the Wyodak H-Coal oil is the easiest.

The EDS oil was particularly hard to process. Although its average boiling range was low, this particular sample of EDS oil had a very high end point tail (Figure 1) and contained heavy material boiling up to 1000°F. However, when the heaviest fraction (12 vol %) was removed by distillation, the redistilled 600°F- overhead was relatively easy to process. Similar studies with Illinois H-Coal showed that redistilled H-Coal oil was also much easier to process than the full boiling range oil. These results emphasize the need for a highly efficient distillation system at the liquefaction

facility to separate the product oil from the recycle oil and residue; small amounts of heavy contaminants make hydroprocessing of coal-derived syncrudes much more difficult.

The Wyodak H-Coal oil was high in hydrogen content, low in boiling range, and contained fewer heteroatom containing compounds and hot heptane insolubles than any of the other oils tested except ITSL oil. Therefore, it is not surprising that Wyodak H-Coal oil was relatively easy to hydrotreat.

Table III summarizes the results with ITSL oil, and results can be compared to those for the other oils shown in Table II. There are two significant differences between these tests and the tests on the previous oils. First, the ITSL oil is easier to process than most of the other whole oils; therefore, the first tests were made at temperatures lower than 750°F. Second, all the tests were made on the same catalyst sample. The tests at 1.5 LHSV were made after the catalyst had lost about 15°F activity due to earlier pilot plant upsets.

The best comparison of results is that made at 1.5 LHSV and 2300 psia hydrogen pressure. All of the oils except ITSL were tested at these conditions and at 750°F. The ITSL oil was tested at the same conditions but at 760°F. However, the catalyst in the ITSL test had been deactivated about 15°F; the other oils were tested with fresh catalyst. If corrected for the 15°F of catalyst deactivation, the starting temperature with ITSL would be 745°F, within 5°F of the temperature of the other tests. The results show that the

only full boiling range oils to achieve complete nitrogen removal at these conditions were Wyodak H-Coal and ITSL oils. However, both redistilled oils (EDS and Illinois H-Coal oils) were completely denitrogenated at these conditions, also. The product aromatics content of the Wyodak H-Coal oil and the redistilled feeds were lower than that obtained with the ITSL oil, suggesting that these oils are somewhat easier to hydroprocess than the full boiling range ITSL oil.

Two other comparisons are worth noting, although all of the oils were not tested at the same conditions:

1. The amount of aromatics saturation obtained with ITSL oil at 710°F, 0.5 LHSV, and 2300 psia hydrogen pressure were better than that achieved with the EDS oil at a 40°F higher temperature (750°F). (The SRC-II and Illinois H-Coal oils were also tested at these conditions and 750°F, but more saturation was obtained than for the ITSL oil at 710°F.)
2. At 1.0 LHSV, the ITSL oil showed at least a 20°F advantage over Illinois H-Coal and SRC-II. This can be inferred because product properties were roughly the same from the tests and the temperature for ITSL testing was lower by 20°F. (The Wyodak H-Coal oil was tested at the higher temperature, but more aromatics saturation was achieved. The EDS oil was not tested at 1.0 LHSV.)

B. Stability

The test at 1800 psia and 1.5 LHSV provides the best comparison of stability of ICR 106 catalyst for the processing of the coal-derived

oils. In an 810-hr test, the ITSL caused little or no catalyst deactivation. (There was an equilibration period of about 250 hr prior to lining out.) The EDS, SRC-II, and Illinois H-Coal oil all caused about 20°F catalyst deactivation in a comparable length of time at the same conditions. The Wyodak H-Coal was not tested at these conditions but was tested with an alternate catalyst (ICR 113). Performance of Wyodak H-Coal oil with ICR 113 was about the same as that with ITSL oil and ICR 106. With most feeds, ICR 106 is somewhat more stable than ICR 113. Therefore, based on the ICR 113 results, ICR 106 catalyst would be expected to be at least as stable and probably more stable with Wyodak H-Coal oil than with ITSL oil.

C. Yields

Typical yields obtained during the tests with ITSL oil are given in Tables IV-VI. For comparison, yields obtained with Illinois H-Coal are also given.

Table IV gives results during Period 1 at 0.5 LHSV. As expected, because of the ITSL feed boiling range, yields of mid-distillate are very high. A comparison of product boiling ranges between H-Coal and ITSL oils is given below:

	Illinois H-Coal Oil	ITSL Oil
Product Yield, LV % of Fresh Feed		
C ₅ -350°F	47	14
350°F+	<u>64</u>	<u>94</u>
Total C ₅ +	111	108
C ₅ -250°F	21	7
250-550°F	84	60
550°F+	6	41

The H-Coal liquid contains a large amount of naphtha; the amount of naphtha produced by ITSL is relatively small. Almost all of the mid-distillate produced from the H-Coal oil is in the jet fuel boiling range; much of that produced from the ITSL oil boils above 550°F. The higher boiling material from the ITSL oil would have to be further cracked to maximize jet fuel production. However, it could be marketed as diesel without further conversion.

Table V compares yields from Illinois H-Coal and ITSL at 1.0 LHSV and 2300 psia hydrogen pressure. In previous papers these conditions were referred to as "gasoline mode" operation because the purpose was to prepare a feed that could be hydrocracked to naphtha in the second stage of a hydrocracker and subsequently be reformed to gasoline. (In the case of ITSL oil, hydrocracking could also serve to make jet fuel if the recycle cut point were increased.) The product distribution comparison again reflects the higher boiling range of the ITSL oil compared to H-Coal oil. Also included in Table V is a yield period for ITSL oil at 1.5 LHSV and 2300 psia hydrogen pressure. The product at this higher space velocity is

more aromatic than at 1.0 LHSV but would still be a suitable feed to the second stage of a hydrocracker because of its low nitrogen content.

Table VI compares yields obtained at 1800 psia from Illinois H-Coal and ITSL oils. This test has been previously referred to as "fuel oil mode" and reflects a lower severity operation feasible if the major product is to be used as fuel oil rather than a transportation fuel. Product from ITSL oil at these conditions is much lower in heteroatom content than that from the H-Coal. However, because of the ITSL product has a much higher boiling range than that from H-Coal oil, the ITSL gravity is considerably lower, far below the current 30°API specification for home heating oil. However, product prepared at these conditions could be used as a blending stock if higher gravity petroleum-derived oils were available for blending also.

D. Hydrogen Consumption

Figure 6 compares the hydrogen consumption for ITSL oil with that for the other coal-derived feeds as a function of aromatics content of the whole liquid product. Hydrogen consumptions for ITSL oil are in the range of that for Illinois H-Coal and EDS oils. Although the ITSL hydrogen content is somewhat lower than in those oils, less hydrogen is required to remove heteroatoms. Also, there is somewhat less hydrocracking of the ITSL oil; the hydrogen is used somewhat more efficiently. The more efficient use of the

hydrogen in saturation reactions is also shown by the steeper slope of the ITSL curve compared to that for the other oils.

Hydrogen consumption is plotted versus nitrogen in the product for a number of synthetic crudes in Figure 7. [EDS oil (not shown) falls close to the curve for Illinois H-Coal.] Paraho shale oil, an extremely high nitrogen (2.2%) feed, is included. The shape of the ITSL curve is different from the curves for the other oils; with ITSL, a large fraction of the heteroatoms are removed at a low hydrogen consumption. For example, the last yield period shown in Table VI shows that product nitrogen is reduced to 24 ppm (97% removal) by a hydrogen consumption of about 375 SCF/B.

E. Product Properties

Our work to date shows that specification transportation fuels can be produced by refining coal-derived oils using modern commercial hydroprocessing technology. Products from coal oils have very unusual properties because of the high content of cyclic compounds and low paraffin content. Many of the unusual properties make them more valuable than their petroleum counterparts. Other properties make them less desirable. Hydrotreated naphthas from coal are easy to reform and give excellent yields of very high octane gasoline. Jet and diesel fuels from coal oils have high volumetric heating values and unusually good cold climate properties. A disadvantage of middle distillates from coal oils is that a large hydrogen input is required for the production of jet fuel with an acceptable smoke point or diesel fuel with specification cetane number.

Some of the key product properties for fractions of ITSL prepared at the highest severity (0.5 LHSV) are summarized in Table VII. These can be compared to those from Illinois H-Coal given in Table VIII.

As indicated above, the paraffin contents of products from coal-derived oils are typically low; with ITSL oil they are lower than with the other coal oils. The lower severity conditions of the upstream, two-stage liquefaction process apparently result in less cracking of cyclics. Some typical paraffin contents of 180-350°F naphthas of a number of coal-derived oils are given in the following table:

Feed Source	Paraffin Content of 180-350°F Hydrotreated Product
EDS	21
Wyodak H-Coal	18
Illinois H-Coal	9
SRC-II	9
ITSL	5

Composition of the 150-180°F naphthas from hydrotreated Illinois H-Coal and ITSL oils are compared in Table IX. H-Coal naphtha contains 25% paraffins; ITSL naphtha contains 13% paraffins. ITSL naphtha contains 72% of a single component, cyclohexane. Cyclohexane is converted to benzene upon reforming; therefore, this would be an excellent feed source for benzene production.

All of the hydrotreated coal-naphthas make excellent reformer feeds because of the high content of cyclic hydrocarbons. In a recent

paper (Reference 5), we discuss the reforming of H-Coal, SRC-II, and EDS naphthas to high octane gasoline and aromatics. ITSL naphthas are expected to be exceptionally good reformer feeds because of their unusually low paraffin contents.

The ASTM specification for jet fuel smoke point is 20 (minimum). We previously concluded that the 250-600°F coal-derived jet fuels studied must contain no more than 10 LV % aromatics if the 20-mm specification is to be met. However, higher smoke points can be achieved if the jet end point is lowered, as will be shown below.

Figure 8 shows that the 20-mm smoke point target can just be met with the 250-550°F fraction of ITSL oil at about 10 LV % aromatics. However, Figure 9 shows that the smoke point depends very strongly on the boiling range of the fraction. For example, the 500-550°F fraction has a lower smoke point (17) than the lower boiling fractions. If the the end point of the jet fuel is lowered from 550°F to 500°F, the smoke point of the jet will be higher and the jet yield will be lower. (With the other coal-derived oils, the target smoke point was met at 600°F end point with 10% aromatic content in the jet. However, because the ITSL oil contains fewer paraffins than the other oils, the 550°F end point appears to be about the maximum unless the aromatics are reduced still further.)

The effect of changing end point of the jet upon smoke point is also illustrated by some previously unpublished results obtained

with EDS oil. The smoke point of the 250-600°F fraction of hydro-treated EDS oil met the specification of 20 mm at about 10% aromatics. However, when EDS oil feed was first redistilled to a 600°F end point and then hydrotreated, the smoke point of the resulting jet was considerably higher than expected at a given aromatics content. This result is illustrated in Figure 10. The reason for the apparent discrepancy is that aromatics boil at a higher temperature than the corresponding hydrogenated cyclic. An effect of hydro-treating is also to lower the end point. (If, on the other hand, the distillation is performed after hydrotreating, the 600°F end point includes hydrogenated species of aromatics that boiled considerably above 600°F before hydrogenation.)

Figure 11 shows the cetane number of the diesel fraction of coal liquids as a function of the aromatics content. A typical cetane number specification is 40. We previously showed an aromatics content of about 10% or less is necessary for the 250°F+, 300°F+, or 350°F+ fractions of hydrotreated coal oils to meet the 40 cetane number specification. The cetane number for the ITSL diesel fraction is about 44 at 10% aromatics, somewhat higher than for the other hydrotreated oils. Therefore, the hydroprocessing severity could be lowered somewhat and the 40 specification still met. Also, as shown in a previous paper (Reference 4), commercially available cetane extenders can be used to improve the cetane numbers of coal-derived diesels. It may be cost-effective to reduce the hydroprocessing severity and add cetane extenders to make specification product.

V. Conclusions

Coals oils derived from different processes (SRC-II, H-Coal, EDS, and ITSL) and from coals of different rank (bituminous, bituminous, and lignite) yield products of any given boiling range that are surprisingly similar. However, there are some important differences in products from ITSL oil and the other coal-derived oils.

ITSL oil has a higher boiling range than the other liquid test. It contains a relatively small fraction of naphtha and consists mainly of mid-distillate. In particular, the ITSL product has a large fraction boiling between 550°F and 700°F. This fraction can be hydrotreated to diesel fuel or hydrocracked to lower boiling products. (Our hydrocracking studies with this feed are still in progress.) Also, products from the ITSL oil contain even fewer paraffins than the other oils, making the naphthas excellent reformer feeds.

The ITSL oil is much easier to upgrade than H-Coal oil made from the same coal (Illinois No. 6, Burning Star Mine). Presumably, this is the result of its low heteroatoms content and because it contains few hot heptane insolubles. The only full boiling range coal oil that we have studied that appears to be easier to process than the ITSL oil is Wyodak H-Coal oil which had a much higher hydrogen content and much lower boiling range than the ITSL oil.

For all of the coal-derived oils studied, the hydrogen input required for upgrading to specification products can be directly related to the hydrogen content and heteroatom impurity content.

VI. References

1. Chevron Research Company, "Refining and Upgrading of Synfuels from Coal and Oil Shales by Advanced Catalytic Processes," DOE Interim Reports:

Report No.	Subject	Date
FE 2315-25	Paraho Shale Oil	April 1978
FE 2315-45	SRC-I	November 1979
DOE/ET/10532-T3	H-Coal	September 1981
DOE/ET/10532-T10 (Formerly FE-2315-47)	SRC-II	November 1982 (Reissued)
FE 2315-50	Shale Oil (Update)	June 1980
FE 2315-77	H-Coal (Addendum)	May 1982
DOE/ET10532-T5	SRC-II (for Biological Tests)	April 1982
DOE/ET/10532-T11	H-Coal, EDS (for Biological Tests)	January 1983
DOE/ET/10532-Txx	H-Coal (for Biological Tests)	September 1983
DOE/ET/10532-Txx	EDS	In Preparation

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REFINING OF SYNCRUDES FROM
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FIGURE 1

SIMULATED TBP DISTILLATIONS OF
ILLINOIS ITSL OIL, SRC-II OIL, AND
EDS (TEXAS LIGNITE) OIL

FIGURE 2

SIMULATED TBP DISTILLATIONS OF
ILLINOIS ITSL OIL AND TWO H-COAL OILS

FIGURE 3

HYDROGEN CONTENT OF ITSL OIL AND
H-COAL OIL FRACTIONS VERSUS BOILING RANGE

Coal Source — Illinois No. 6 (Burning Star)

FIGURE 4

NITROGEN AND OXYGEN DISTRIBUTION IN
ITSL OIL FRACTIONS BOILING RANGE

FIGURE 5

HYDROTREATING OF ITSL OIL WITH ICR 106 CATALYST

FIGURE 6

PRODUCT AROMATIC CONTENT VERSUS HYDROGEN CONSUMPTION FOR
ITSL OIL COMPARED TO FOUR OTHER COAL-DERIVED OILS

FIGURE 7

PRODUCT NITROGEN VERSUS
HYDROGEN CONSUMPTION FOR FIVE SYNCRUDES

FIGURE 8

EFFECT OF AROMATICS ON THE
SMOKE POINT OF KEROSENE JET FUELS
DERIVED FROM FIVE COAL-DERIVED OILS

FIGURE 9

SMOKE POINT AND AROMATIC CONTENT OF
NARROW BOILING FRACTIONS OF SEVERELY HYDROTREATED ITSL OIL AS A
FUNCTION OF BOILING RANGE

Whole Liquid Composition, LV %:
Paraffins, 1.3; Naphthenes, 87.7; Aromatics, 11

FIGURE 10

SMOKE POINT OF JET FUELS FROM WHOLE AND
REDISTILLED (600°F-) EDS SYNCRUDES VERSUS
AROMATIC CONTENT

FIGURE 11
EFFECT OF AROMATICS ON THE
CETANE NUMBER OF DIESEL FUELS
DERIVED FROM FOUR COAL-DERIVED OILS

TABLE I
PROPERTIES OF COAL-DERIVED PILOT PLANT FEEDS

Liquefaction Process	ITSL	H-Coal	H-Coal	SRC-II	EDS
Type of Coal	Illinois No. 6	Illinois No. 6	Wyodak	Pittsburgh Seam	Texas Lignite
Inspections					
Gravity, °API	17.9	25.8	35.1	18.6	29.0
Sulfur, ppm	700	2,000	4,100	2,900	1,180
Nitrogen, ppm	770	4,600	1,700	8,500	3,000
Basic Nitrogen, ppm	483	3,000	1,300	7,000	1,500
Oxygen, ppm	6,000	18,000	8,500	37,900	19,200
Hydrogen, Wt %	10.62	11.29	12.74	10.46	11.25
Carbon, Wt %	88.65	86.25	86.20	84.61	86.41
Chlorine, ppm	19	32	3	50	10
Iron, ppm	2.5	20	3	3	6
Water, ppm	337	2,200	<500	6,000	1,580
Hot Heptane Insolubles, ppm	310	3,500	680	469	1,300
Ramsbottom Carbon, Wt %	0.30	0.29	0.23	0.70	0.57
ASTM D-2887 (Distillation, °F TBP by GC)					
St/5	97/214	56/177	53/156	56/189	53/164
10/30	314/471	213/333	173/261	241/379	203/317
50	560	404	354	424	370
70/90	609/676	476/588	429/535	473/562	452/662
95/99	703/763	654/765	602/785	642/820	799/(950+)

TABLE II
HYDROTREATING PILOT PLANT TESTS FOR
COAL-DERIVED OILS AT 750°F CATALYST
TEMPERATURE WITH FRESH ICR 106 CATALYST

LHSV	0.5	1.0	1.5	1.5
Hydrogen Pressure, psia (Approximate)	2300	2300	2300	1800
SRC-II				
Hydrogen Consumption, SCF/Bbl	3100	2500	2000	1725
Product Nitrogen, ppm	<0.3	0.4	20	150
Product Aromatics, LV %	4	20	40	47
Illinois H-Coal				
Hydrogen Consumption, SCF/Bbl	2150	1600	1275	825
Product Nitrogen, ppm	<0.3	0.3	10	50
Product Aromatics, LV %	2	20	35	45
Wyodak H-Coal				
Hydrogen Consumption, SCF/Bbl		1225	950	
Product Nitrogen, ppm		<0.3	<0.3	
Product Aromatics, LV %		3	13	
Rerun Illinois H-Coal				
Hydrogen Consumption, SCF/Bbl		2000	1950	
Product Nitrogen, ppm		<0.3	<0.3	
Product Aromatics, LV %		2	5	
Lignite EDS				
Hydrogen Consumption, SCF/Bbl	1550		825	725
Product Nitrogen, ppm	<0.3		170	350
Product Aromatics, LV %	16		38	40
Rerun Lignite EDS				
Hydrogen Consumption, SCF/Bbl			1600	1500
Product Nitrogen, ppm			<0.3	<0.3
Product Aromatics, LV %			6	10

TABLE III
HYDROTREATING PILOT PLANT TESTS
FOR ITSL OIL WITH ICR 106 CATALYST

LHSV	0.5	1.0	1.5	1.5	1.5
Hydrogen Pressure, psia Approximate	2300	2300	2300	1800	1500
Average Catalyst Temperature, °F	710	730	760	760	760
Catalyst Activity Relative to Fresh Catalyst, Δ°F	Fresh	Fresh	-15	-15	-15
Hydrogen Consumption, SCF/Bbl	1600	1400	950	600	375
Product Nitrogen, ppm	<0.2	<0.2	0.4	6	24
Product Aromatics, LV %	10	26	38	58	64

TABLE IV

YIELDS FROM "JET MODE" HYDROTREATING OF H-COAL
OIL AND ITSL OIL (FROM ILLINOIS
NO. 6 COAL) WITH ICR 106 CATALYST

Feed Source	H-Coal		ITSL	
Run No.	76-171		90-167	
Run Hours	222-246		1673-1697	
Catalyst Temperature, °F	750		710	
LHSV	0.5		0.5	
Total Pressure, psig	2,495		2,498	
H ₂ Pressure, psia	2,232		2,319	
Recycle Gas, SCF/Bbl	7,921		7,878	
No Loss Yields	Wt %	Vol %	Wt %	Vol %
C ₁	0.05		0.04	
C ₂	0.08		0.05	
C ₃	0.13		0.05	
iC ₄	0.02	0.03	0.01	0.02
nC ₄	0.06	0.09	0.03	0.05
C ₅ -150°F	{3.64}	{4.55}	0.06	0.09
150-180°F			1.60	2.05
180-250°F	13.39	15.84	3.98	4.87
250-350°F	23.15	26.30	5.77	6.78
350-550°F	{61.28}	{64.10}	50.36	53.64
550°F+			40.29	40.59
350°F+	61.28	64.10	90.65	94.23
250°F+	84.43	90.40	96.42	101.01
Total C ₅ +	101.48	110.80	102.07	108.03
H ₂ Cons. (Gross), SCF/Bbl	2,206		1,720	
H ₂ Cons. (Chem.), SCF/Bbl	2,146		1,617	
Whole Liquid Product Properties				
Gravity, °API	39.1		26.7	
Aniline Point, °F	123		126	
Sulfur, ppm			2	
Nitrogen, ppm	0.2		0.2	
Oxygen, ppm	160		<100	
Hydrogen, Wt %	13.45		12.78	
Carbon, Wt %	86.55		87.22	
Group Type, LV %				
Paraffins	5.3		0.8	
Naphthenes	92.5		86.8	
Aromatics	2.2		12.4	
ASTM D 2887 Distillation, °F (TBP by GC)				
ST/5	39/177		158/222	
10/30	215/298		321/442	
50	367		516	
70/90	428/515		575/634	
95/99	563/650		662/712	

TABLE V

YIELDS FROM "GASOLINE MODE" HYDROTREATING OF
H-COAL OIL AND ITSL OIL (FROM ILLINOIS
NO. 6 COAL) WITH ICR 106 CATALYST

Condition of Catalyst	"Fresh"	"Fresh"	Aged (~15°F)
Feed Source	H-Coal	ITSL	ITSL
Run No.	76-171	90-167	90-167
Run Hours	342-366	1961-1985	3747-3771
Catalyst Temperature	750	732	761
LHSV	1.0	1.0	1.5
Total Pressure, psig	2,497	2,497	2,492
Hydrogen Pressure, psia	2,250	2,300	2,294
Recycle Gas, SCF/Bbl	8,050	7,411	7,464
No Loss Yields	Wt % Vol %	Wt % Vol %	Wt % Vol %
C ₁	0.03	0.04	0.04
C ₂	0.04	0.05	0.07
C ₃	0.06	0.06	0.08
iC ₄	0.01 0.01	0.01 0.01	0.01 0.01
nC ₄	0.02 0.04	0.03 0.05	0.05 0.08
C ₅ -150°F	{4.01} {4.95}	0.04 0.06	{7.03} {8.71}
150-180°F		1.63 2.05	
180-250°F	12.29 14.39	3.66 4.48	
250-350°F	22.41 25.02	5.78 6.78	5.76 6.73
350-550°F	{62.22} {63.49}	46.25 49.32	42.20 44.40
550°F+		44.36 44.51	46.01 45.17
350°F+	62.22 63.49	90.61 93.83	88.21 89.57
Total C ₅ +	100.9 107.8	101.7 107.2	101.0 105.0
Hydrogen Consumption (Gross), SCF/Bbl	1,644	1,488	1,053
Hydrogen Consumption (Chemical), SCF/Bbl	1,613	1,414	989
Whole Liquid Product Properties			
Gravity, °API	30.6	25.3	23.6
Aniline Point, °F	99	111	83
Sulfur, ppm	5.4	2.6	3.2
Nitrogen, ppm	0.15	0.16	0.45
Oxygen, ppm	160	80	130
Hydrogen, Wt %	12.86	12.41	11.76
Group Type, LV %			
Paraffins	5.6	0.9	1.5
Naphthenes	74.9	73.5	60.4
Aromatics	19.5	25.5	38.0
D 2887 Distillation, °F (TBP by GC)			
ST/5	48/177	89/225	90/214
10/30	216/311	326/447	292/439
50	380	519	523
70/90	447/534	580/642	583/652
95/99	584/690	671/730	681/744

TABLE VI

YIELDS FROM "FUEL OIL MODE" HYDROTREATING OF
H-COAL OIL AND ITSL OIL (FROM ILLINOIS
NO. 6 COAL) WITH ICR 106 CATALYST

Condition of Catalyst	Fresh		Aged (~15°F)		Aged (~15°F)	
Feed Source	H-Coal		ITSL		ITSL	
Run No.	76-171		90-167		90-167	
Run Hours	1535-1559		4923-4947		5067-5091	
Catalyst Temperature	750		760		760	
LHSV	1.5		1.5		1.5	
Total Pressure, psig	2,001		2,001		1,703	
Hydrogen Pressure, psia	1,778		1,819		1,495	
Recycle Gas, SCF/Bbl	7,213		7,997		7,886	
No Loss Yields	Wt %	Vol %	Wt %	Vol %	Wt %	Vol %
C ₁	0.07		0.05		0.03	
C ₂	0.07		0.06		0.04	
C ₃	0.07		0.05		0.04	
iC ₄	0.03	0.04	0.01	0.01	0.00	0.00
nC ₄	0.04	0.07	0.04	0.06	0.02	0.04
C ₅ -150°F	{4.85}	{5.99}	0.06	0.08	0.02	0.02
150-180°F			{6.22}	{7.69}	{5.60}	{6.92}
180-250°F	11.13	13.00				
250-350°F	19.07	21.15	4.02	4.73	5.40	6.30
350°F+	64.43	63.11	90.07	90.01	89.10	88.80
Total C ₅ +	99.48	103.25	100.36	102.52	100.12	102.04
Hydrogen Consumption (Gross), SCF/Bbl	909		624		394	
Hydrogen Consumption (Chemical), SCF/Bbl	824		575		378	
Whole Liquid Product Properties						
Gravity, °API	30.6		20.5		19.4	
Aniline Point, °F	49		59		48	
Sulfur, ppm	6.7		5.6		14	
Nitrogen, ppm	140		6.1		23.1	
Oxygen, ppm	870		400		500	
Hydrogen, Wt %	11.8		11.4		11.0	
Group Type, LV %						
Paraffins	7.1		1.2		1.6	
Naphthenes	47.5		40.9		34.9	
Aromatics	45.4		57.9		63.5	
D 2887 Distillation, °F (TBP by GC)						
ST/5	70/179		128/216		118/230	
10/30	212/231		320/456		331/465	
50	398		542		549	
70/90	460/566		599/670		604/674	
95/99	621/727		699/771		704/767	

TABLE VII

REPRESENTATIVE PROPERTIES OF PRODUCT FRACTIONS
OF HYDROTREATED ITSL OIL ("JET/DIESEL MODE")

ICR 106 Catalyst - 710°F
2300 psia Hydrogen Pressure
0.5 LHSV

Boiling Range of Fraction, °F	180-250	250-350	350-550	550+	250+	350+
Inspections						
Gravity, °API	51.3	44.6	27.9	19.4	25.8	23.4
Aniline Point, °F	99	111	121	144	132	129
Hydrogen, Wt %	14.3	13.8	13.1	12.4	13.2	12.6
Group Type, LV %						
Paraffins	5	5	0	0	1	0
Naphthenes	92	90	90	83	89	88
Aromatics	3	5	10	17	10	12
Smoke Point, mm		29	19			
Freeze Point, °F			Below -70		Below -80	-80
Pour Point, °F				-65	Below -80	
Cetane Number					43	45
TBP 95% Point, °F				681	670	672

TABLE VIII
 REPRESENTATIVE PROPERTIES OF PRODUCT
 FRACTIONS OF HYDROTREATED ILLINOIS H-COAL
 OIL ("JET/DIESEL MODE")

ICR 106 Catalyst - 750°F
 2300 psia Hydrogen Pressure
 0.5 LHSV

Boiling Range of Fraction, °F	180-250	250-350	250+	350+
Inspections				
Gravity, °API	53.9	46.4	36.3	32.4
Aniline Point, °F	*	*	128	132
Hydrogen, Wt %	14.4	14.0	13.5	13.4
Group Type, LV %				
Paraffins	11	8	3	4
Naphthenes	87	90	95	94
Aromatics	2	2	2	2
Smoke Point, mm			23	21
Freeze Point, °F			-53	-41
Pour Point, °F				-60
Cetane Number				42
TBP 95% Point, °F			580	584

*Aniline point of 180-350°F blend is 115.

TABLE IX

DISTRIBUTION OF PRODUCT FROM H-COAL OIL
AND ITSL OIL (FROM ILLINOIS NO. 6 COAL)
AT 0.5 LHSV WITH ISR 106 CATALYST

Feed Source	H-Coal	ITSL
Composition, LV % of 150-180°F (by Chromatography)		
C ₅ -	4.1	4.1
2,3-Dimethylbutane	0.1	0.1
2-Methylpentane	1.9	0.9
3-Methylpentane	1.3	0.8
n-Hexane	14.1	4.1
Isoheptanes	3.2	2.3
n-Heptane	0.2	0.2
C ₈ Isoparaffins	-	0.1
Total Paraffins	24.9	12.6
Cyclopentane	5.3	1.2
Methylcyclopentane	22.3	8.8
Cyclohexane	42.5	71.8
Dimethylcyclopentanes,		
Ethylcyclopentane	1.3	0.2
Methylcyclohexane	1.2	3.4
Total Naphthenes	72.6	85.4
Benzene	2.3	1.9
Toluene	0.1	0.1
Total Aromatics	2.4	2.0