FE-2645-05
Distribution Categories UC-90 and UC-90d

DEASPHALTING, DEASHING AND UPGRADING OF COAL LIQUIDS

Quarterly Technical Progress Report
for
The Period October-December, 1979

Fredrick J. Riedl and Armand J. deRosset

UOP Inc.
Corporate Research Center
Ten UOP Plaza
Des Plaines, IL 60016

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ABSTRACT

Initial work on deashing of the SRC-I filter feed has yielded deashed oil recoveries of 73.2-75.5 wt-% with an ash content of <0.001 wt-%. The reject bottoms yield ran from 24.5-26.8 wt-%.

The first of three deashed oils derived from UOP coal liquefaction has been catalytically cracked. Conversions of 49 and 56 vol-% were obtained.

Work Accomplished

Task 1.3

A "High Resolution Mass Spectral Characterization" of deashed oil 3777-8 has been completed and is shown in Table 1 and Appendix Table A-1. This product comprised 85% aromatic and polar compounds. Oxygen was the predominant hetero atom. Polycyclics with up to three oxygen atoms per molecule were identified. This stock was hydrotreated and used as a coal liquefaction solvent, as reported in FE-2645-03.

Task 2.0

The deashing of the Wilsonville SRC-I filter feed (sample 3777-3, Table 2) via UOP Demex technology was started on UOP Research Plant 633.

UOP deashing proceeds as follows: preheated SRC-I filter feed is combined with preheated solvent upstream of the deasher. The combined feed is passed downflow through the in-line mixer into the deasher (Figure 1). Phase separation takes place in the deasher. The oil rich upper phase flows to the stripper for removal of solvent. The solid rich bottom phase, containing the ash, is removed through a lock hopper system, which is controlled by a capacitance sensing interface detector. Both deashed oil and deasher bottoms are weighed and analyzed. The percent deashed oil and percent reject bottoms are calculated on the basis of the total solvent free effluent.

Two runs, 113 and 116, were made (1) to determine range of attainable rejection levels; (2) to demonstrate the mechanical operability of the plant; and (3) to obtain sufficient deashed oil and reject bottoms for analysis.

Plant 633, Run 113

A summary of the deashing Run 113 is presented in Table 3. During the initial 16 hours of operation, level control problems were encountered which resulted in a buildup of reject material in the vessel. The operation was lined out during the next 8 hours. The ash content of the deashed oil rose slightly due to the upset, but came back down to less than 10 ppm during the last 12 hours of operation. The C_7^- insoluble content of the deashed oil was 6.74 wt-%, at 73.3 wt-% recovery. The rejection was 26.7 wt-%, and the bottoms contained 15.52 wt-% ash.

Plant 633, Run 116

This run, also described in Table 3, was a repeat of Run 113 except for the slightly higher operating temperature. No operational problems were encountered. Following the initial line out period from 0-12 hours, sufficient material was collected during the remaining 17 hours, to obtain the necessary detailed analysis on the deashed oil and reject bottoms. Operating stream samples show the deashed oil contained 10 ppm of ash and 10.1 wt-% C_7 insolubles, while the reject bottoms contained 19.8 wt-% ash.

The rejection decreased in Run 116 to 24.5 wt-% from 26.7 wt-% in Run 113 due to the 4°C higher operating temperature. This is due to the increased solvency at the higher temperature.

Inspections of the deashed oil are presented in Table 4. Approximately 48% of the sulfur and 25-30% of the oxygen and nitrogen were removed by deashing. Approximately 60% of the C_7 insoluble and essentially all the toluene insoluble material reported to the rejected bottoms.

Inspections of the composite deasher bottoms, 3810-75, are shown in Table 5. Essentially all of the material appears to be C_7 insoluble. A high portion of this material (43.7 wt-%) is soluble in a dimethylformamide(DMF)-xylene solvent mixture.

A sample of the deasher bottoms 3810-75, designated as sample 3810-77, was Soxhlet extracted with toluene. Inspections of the soluble and insoluble portions of the Soxhlet extraction are shown in Table 5. The soluble portion, containing 6.39 wt-% hydrogen, appears to be of the same quality as a raw Illinois No. 6 coal. The insoluble portion contains all of the original coal ash and roughly half of the sulfur, nitrogen and oxygen present in the original filter feed.

Product recoveries indicated in Table 3 were acceptable. However, ash recoveries were high, 120-140 wt-%. This suggests a feed ash content of around 4.5 wt-%, rather than the analyzed value of 3.42 wt-% (Table 2). Segregation of ash by settling may be responsible for the inconsistency.

Continuing deashing work will be directed to reduce the rejection to below 15%. The work plan and progress, shown in Figure 2, has been adjusted to coincide with completion of the fluid catalytic cracking (FCC) studies by the middle of May, 1980.

Task 3.0

The hydrotreatment of deashed oil derived from UOP coal liquefaction is continuing. The object is to add sufficient hydrogen to make a suitable FCC feedstock. Table 15, "Product Hydrogen Content Hydrotreating Deashed Oil 3777-44; Plant 532, Run 1134", shown in the July-September Quarterly Technical Progress Report FE-2645-04, is revised and shown as Table 6 in this report. Neither the reduction in space velocity nor the increase in temperature during the run resulted in any marked increase in hydrogen content of this product. The lack of response was unexpected, and requires further investigation.

The product distributions, hydrogen consumption and hydrogen distributions for the hydrotreated deashed oil products, derived from UOP coal liquefaction, obtained from Plant 532 hydrotreating, Runs 1133, 1134 and 1135, reported in FE-2645-04 are presented in Tables 7 through 14.

The three times hydrotreated deashed oil 3777-46 (Table 18 in Report FE-2645-04) was sent for a "High Resolution Mass Spectral Types Analysis", as shown in Table 15 and Appendix Table A-2. Also included is an elemental analysis by MS. The latter verifies chemical analyses previously reported. The high aromatic content (68.9 wt-%) reflects the low hydrogen consumption (809 SCF/bbl) during the three successive hydrotreating runs. More severe hydrotreating conditions will be required to produce a higher hydrogen content FCC feedstock.

Task 5.0

FCC feedstock 3777-43 (Table 12, FE-2645-04) is the first of three deashed and hydrotreated oils prepared for FCC studies. It was cracked in UOP Research Pilot Plant 593. Results are shown in Tables 16 and 17. Cracking conditions were as follows:

P-P(base)	= -10 psi
T-T(base)	= 3 and 31°C
$\frac{\text{Cat/Oil}}{\text{Cat/Oil(base)}}$	= 1 and 1.4

Four tests were made at each temperature condition, but only the acceptable tests are listed in the tables.

The volume-% conversion for this feedstock is abstracted from the tables and shown below.

Feed No.	3777-43
Hydrogen, Wt-%	10.19
	Vol-% Conversion
T-T(base), °C	
3	49.4
31	55.7

The remaining two feedstocks will be processed in January and the results reported in the January-March quarterly report.

Table 1

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

Sample Analysis Summary

Compound Type C_nH_{2n-z}	Wt.%	Avg. C No.	Avg. M.W.	Avg. z No.
Saturated Hydrocarbons (P+N)	15.1	23.0	307	2.4
Aromatic Hydrocarbons	65.0	18.8	246	17.4
Aromatic Nitrogens	7.2	17.7	244	18.0
Aromatic Oxygens	5.3	16.2	227	16.0
Aromatic Sulfurs	0.1	15.6	234	16.3
Aromatic Dioxygenates	7.0	18.1	267	17.9
Aromatic Trioxygenates	0.3	18.8	295	16.5

Elemental Analysis by M.S.

	Wt.%
Atomic Carbon	89.51
Atomic Hydrogen	8.80
Atomic Nitrogen	0.41
Atomic Oxygen	1.25
Atomic Sulfur	0.03
	100.00

Table 2

Inspections of SRC-I Filter Feed

Sample No.	3777-3
°API @ 60°F	-4.4
Sp. Gr. @ 60°F	1.1133
Distillation ASTM D-86	
IBP°F	445
5%	490
10%	515
20%	551
30%	586
40%	622
50%	675
60%	741
70%	830
80%	
90%	
95%	
EP	
% Over	70.0
% Bottoms	30.0
Hydrogen, Wt-%	7.55
Carbon, Wt-%	83.85
Sulfur, Wt-ppm	8300
Nitrogen, Wt-ppm	12670
Oxygen, Wt-ppm	22700
Ash ASTM, Wt-%	3.42
C_7 Insoluble, Wt-%	25.4
Toluene Insoluble, Wt-%	14.9
Pour Point, °F	+50
Viscosity SUS @ 210°F sec	125.1
Furol @ 122°F sec	230.0

Table 3

Solvent Deashing of SRC-I Filter Feed 3777-3

Plant 633

Run	113	113	116
Hours on Stream	16-24	24-36	12-29
Conditions			
P-P(base), psi	480	480	480
T-T(base), °C	43	44	48
Solvent/Feed Ratio	base	base	base
Feed Total, gms	3612	5488	7806
Product Recovered			
Deashed Oil, gm	2584	3890	5741[a]
Reject Bottoms, gm	948	1416	1864[b]
Total, gm	3532	5306	7605
Recovery, Wt-%	97.8	96.7	97.4
Deashed Oil			
Recovered, Wt-%	73.2	73.3	75.5
C_7 Insol., Wt-%	6.43	6.74	10.1
Ash, Wt-%	0.002	<0.001	0.001
Reject Bottoms			
Recovered, Wt-%	26.8	26.7	24.5
Ash, Wt-%	17.86	15.52	19.80

[a]Designated as Deashed Oil 3810-73

[b]Designated as Deasher Bottoms 3910-75

Table 4

Inspections of Deashed Oil 3810-73

Plant 633, Run 116

°API @ 60°F	3.5
Sp. Gr. @ 60°F	1.0481
Distillation ASTM D-1160	
IBP°F	465
5%	495
10%	520
20%	552
30%	580
40%	615
50%	658
60%	701
70%	755
80%	822
87%	963
95%	
EP	
% Over	87.0
% Bottoms	13.0
Hydrogen, Wt-%	8.45
Carbon, Wt-%	86.15
Sulfur, Wt-ppm	4300
Nitrogen, Wt-ppm	10400
Oxygen, Wt-ppm	17400
ASTM Ash, Wt-%	0.001
C_7 Insoluble, Wt-%	10.1
Toluene Insoluble, Wt-%	0.04
Viscosity cSt @ 210°F	4.923
SUS @ 210°F	42.4
Molecular Wt.	251

Table 5

Inspections of Deasher Bottoms

Plant 633, Run 116

Composite Sample	3810-75
	Wt-%
Carbon	69.06
Hydrogen	5.79
Sulfur	2.19
C_7 Insoluble	99.52
Toluene Insoluble	94.28
DMF/Xylene Insoluble	43.70
Ash	19.80

Soxhlet Extraction with Toluene (Liquid Phase)

Sample	3810-77
Soluble Oil	Wt-%
Carbon	88.73
Hydrogen	6.39
C_7 Insoluble	67.50
Yield	29.00
Insoluble Portion	
Carbon	59.02
Hydrogen	4.32
Sulfur	2.61
Oxygen	6.00
Nitrogen	1.74
Ash	26.70
H_2O	1.0
Yield	70.00

Table 6[a]

Product Hydrogen Content
Hydrotreating Deashed Oil 3777-44
Plant 532, Run 1134

P-P(base), psi = -300

Period No.	Hrs on Stream	T-T(base) °C	LHSV / LHSV base	Product Analysis, Wt-% H	C
1	22-30	-39	2.0	10.77	88.52
4	46-54	-40	2.0	10.64	88.97
8	78-86	-40	2.0	10.53	88.80
10	94-102	-39	2.0	10.59	88.60
12	110-118	-39	1.2	10.65	88.81
14	126-134		1.2	10.66	88.83
16	142-150	-28	1.2	10.72	89.11
19	166-174	-28	1.2	10.87	88.89

[a]Corrects Table 15, FE-2645-04

Table 7

Hydrotreating Deashed Oil 3777-42
Overall Product Distribution
Plant 532, Run 1133, Periods 1-19

Product Distribution	Wt-%
C_1-C_4	0.20
C_5-C_6 (in Plant Gas)	0.51
Stripper Bottoms[a]	99.16
H_2O	0.43
NH_3	0.21
H_2S	0.08
Total	100.59
Hydrogen Consumption, Wt-% of Feed	0.59
Hydrogen Consumption SCF/bbl	390

[a]Designated as Hydrotreated Deashed Oil 3777-43.

Table 8

Hydrotreating Deashed Oil 3777-42
Distribution of Hydrogen Consumption
Plant 532, Run 1133, Periods 1-19

	Wt-%
C_1-C_4	7.3
C_5-C_6 (in Plant Gas)	6.9
Stripper Bottoms[a]	63.9
H_2O	8.7
NH_3	12.1
H_2S	1.1
Total	100.0
Total Hydrogen Consumption SCF/bbl	390

[a]Designated as Hydrogenated Deashed Oil 3777-43.

Table 9

Hydrotreating Deashed Oil 3777-42
Overall Product Distribution
Plant 532, Run 1133, Periods 20-55

Product Distribution	Wt-%
C_1-C_4	0.40
C_5-C_6 (in Plant Gas)	0.87
Stripper Bottoms[a]	99.00
H_2O	0.31
NH_3	0.06
H_2S	0.10
Total	100.74
Hydrogen Consumption, Wt-% of Feed	0.74
Hydrogen Consumption SCF/bbl	497

[a]Designated as Hydrotreated Deashed Oil 3777-44.

Table 10

Hydrotreating Deashed Oil 3777-42
Distribution of Hydrogen Consumption
Plant 532, Run 1133, Periods 20-55

	Wt-%
C_1-C_4	8.5
C_5-C_6 (in Plant Gas)	11.2
Stripper Bottoms[a]	67.2
H_2O	1.3
NH_3	10.6
H_2S	1.2
Total	100.0
Total Hydrogen Consumption SCF/bbl	497

[a]Designated as Hydrotreated Deashed Oil 3777-44.

Table 11

Hydrotreating Deashed Oil 3777-44[a]
Overall Product Distribution
Plant 532, Run 1134

Product Distribution	Wt-%
C_1-C_4	0.14
C_5-C_6 (in Plant Gas)	0.39
Stripper Bottoms[b]	99.56
H_2O	0.21
NH_3	0.06
H_2S	0.06
Total	100.52
Hydrogen Consumption, Wt-% of Feed	0.52
Hydrogen Consumption SCF/bbl	280

[a]Second Hydrotreatment of Deashed Oil 3777-42.

[b]Designated as Hydrotreated Deashed Oil 3777-45.

Table 12

Hydrotreating Deashed Oil 3777-44[a]
Distribution of Hydrogen Consumption
Plant 532, Run 1134

Product Distribution	Wt-%
C_1-C_4	3.5
C_5-C_6 (in Plant Gas)	5.9
Stripper Bottoms[b]	84.4
H_2O	5.1
NH_3	0.2
H_2S	0.9
Total	100.0
Total Hydrogen Consumption	280

[a]Second Hydrotreatment of Deashed Oil 3777-42.

[b]Designated as Hydrotreated Deashed Oil 3777-45.

Table 13

Hydrotreating Deashed Oil 3777-45[a]

Overall Product Distribution

Plant 532, Run 1135

Product Distribution	Wt-%
C_1-C_4	0.36
C_5-C_6 (in Plant Gas)	0.29
Stripper Bottoms[b]	99.37
H_2O	<0.01
NH_3	0.02
H_2S	0.00
Total	100.04
Hydrogen Consumption, Wt-% of Feed	0.04
Hydrogen Consumption SCF/bbl	32

[a]Third Hydrotreatment of Deashed Oil 3777-42.

[b]Designated as Hydrotreated Deashed Oil 3777-46.

Table 14

Hydrotreating Deashed Oil 3777-45[a]
Distribution of Hydrogen Consumption
Plant 532, Run 1135

Product Distribution	Wt-%
C_1-C_4	63.5
C_5-C_6 (in Plant Gas)	30.2
Stripper Bottoms[b]	0.0
H_2O	0.0
NH_3	6.3
H_2S	0.0
Total	100.0
Total Hydrogen Consumption SCF/bbl	32

[a]Third Hydrotreatment of Deashed Oil 3777-42.

[b]Designated as Hydrotreated Deashed Oil 3777-46.

Table 15

High Resolution Mass Spectral Types Analysis
of Three Time Hydrotreated Deashed Oil 3777-46

Compound Types $C_nH_{2n-z}(x)$	Wt-%	Ave. C No.	Ave. Mol. Wt.	Ave. z No.
Saturated Hydrocarbons (P&N)	26.7	15.1	209	2.5
Aromatic Hydrocarbons	68.9	17.9	237	13.8
Aromatic Nitrogens	2.4	18.0	249	16.2
Aromatic Oxygens	2.0	16.8	235	16.3
Aromatic Sulfurs	T	15.9	239	15.3

T <0.05%

Elemental Analysis by M.S., Wt-%

Atomic Carbon	89.39
Atomic Hydrogen	10.35
Atomic Nitrogen	0.13
Atomic Oxygen	0.13
Atomic Sulfur	0.0

Table 16

Fluid Catalytic Cracking of Hydrotreated Deashed Oil 3777-43

Plant 593, Run 302

Test No.	1	2	3
Operating Conditions			
P-P(base), psig	-10	-9	-10
T-T(base), °C	-1	4	4
$\frac{\text{Cat./Oil}}{\text{Cat./Oil(base)}}$	1.05	1.07	1.03
Conversion, Vol-%	50.1	50.7	47.5
Product Distribution, Wt-%			
C_3^-	7.1	5.4	5.1
C_4	3.2	2.6	2.4
C_5	1.9	1.5	1.9
C_6-EP Gasoline	25.1	24.8	24.0
Cycle Oil	52.6	51.8	54.8
Carbon	8.4	9.4	10.1
Wt. Recovery	98.3	95.6	98.2
Products, Vol-%			
C_5-EP Gasoline	32.8	31.9	31.6
Cycle Oil	49.9	49.3	52.5
Inspections of C_5-EP Gasoline			
°API @ 60°F	0.8137	0.8170	0.8090
Sp. Gr. @ 60°F	42.4	41.7	43.4
Distillation, ASTM D-86			
IBP, °F	118	127	107
5%	148	159	135
10%	166	175	153
50%	266	263	261
90%	390	374	384
95%	410	388	398
EP	435	410	418
RON, Clear	←	95.5	→
RON, 3 ml TEL/Gallon	←	100.1	→
MON, Clear	←	80.6	→
FIA, Vol-%			
A	46.6	47.8	44.1
O	21.1	18.3	25.2
P&N	32.3	33.9	30.7

Table 16 (Cont'd.)

Test No.	1	2	3
Properties of Cycle Oil			
°API @ 60°F	4.3	4.8	5.6
Sp. Gr. @ 60°F	1.0420	1.0382	1.0321
Distillation, UOP No. 1			
IBP, °F	450	462	454
5%	480	480	482
10%	491	492	492
15%	504	501	503
% Over at 650°F	65.0	67.0	65.0
°API of 650°F$^-$ @ 60°F	11.8	11.7	13.0
Sp. Gr. of 650°F$^-$ @ 60°F	0.9874	0.9881	0.9792
°API of 650°F$^+$ @ 60°F	-7.3	-7.2	-5.9
Sp. Gr. of 650°F$^+$ @ 60°F	1.1393	1.1384	1.1266
C_3^-, Mole %			
H_2	45.4	54.1	59.7
C_1	20.0	17.0	15.1
C_2 (Total)	15.5	13.1	11.8
C_3 Olefins	14.3	12.5	10.7
C_3	4.7	3.3	2.8
Total	100.0	100.0	100.0
C_4, Vol-%			
C_4 Olefins	63.7	60.9	64.3
i-C_4	26.6	27.1	24.4
n-C_4	9.7	12.0	11.3
Total	100.0	100.0	100.0
C_5, Vol-%			
C_5 Olefins	59.0	59.9	71.1
i-C_5	36.4	34.9	24.6
n-C_5	4.6	5.2	4.2
Total	100.0	100.0	100.0

Table 17

Fluid Catalytic Cracking of Hydrotreated Deashed Oil 3777-43

Plant 593, Run 302

Test No.	4	5	6	7
Operating Conditions				
P-P(base), psig	-9	-10	-9	-10
T-T(base), °C	29	29	32	32
Cat./Oil / Cat./Oil(base)	1.42	1.28	1.46	1.53
Conversion, Vol-%	54.7	56.4	56.6	55.2
Product Distribution, Wt-%				
C_3-	7.7	9.9	7.7	14.0
C_4	3.9	4.1	3.5	5.0
C_5	2.6	2.2	2.1	2.6
C_6-EP Gasoline	25.1	25.8	24.7	23.4
Cycle Oil	48.4	47.1	46.5	48.3
Carbon	10.5	9.7	13.1	9.6
Wt. Recovery	98.2	98.8	97.6	102.8
Products, Vol-%				
C_5-EP Gasoline	34.0	33.6	32.5	31.4
Cycle Oil	45.3	43.6	43.4	44.8
Inspections of C_5-EP Gasoline				
°API @ 60°F	43.7	41.1	43.6	41.8
Sp. Gr. @ 60°F	0.8076	0.8198	0.8081	0.8165
Distillation, ASTM D-86				
IBP, °F	110	108	95	104
5%	137	137	123	133
10%	153	155	143	152
50%	252	271	258	265
90%	376	390	384	378
95%	392	406	404	393
EP	415	424	416	411
RON, Clear	← 97.7 →			
RON, 3 ml TEL/Gallon	← 101.8 →			
MON, Clear	← 82.8 →			
MON, 3 ml TEL/Gallon	← 87.7 →			
FIA, Vol-%				
A	49.5	55.7	50.9	54.8
O	19.2	16.3	18.9	20.4
P&N	31.3	28.0	30.2	24.8

Table 17 (Cont'd.)

Test No.	4	5	6	7
Properties of Cycle Oil				
°API @ 60°F	2.5	0.8	2.2	1.2
Sp. Gr. @ 60°F	1.0560	1.0695	1.0583	1.0663
Distillation, UOP No. 1				
IBP, °F	460	476	460	455
5%	474	494	479	475
10%	485	508	493	488
15%	498	516	500	495
% Over at 650°F	65.0	59.0	64.0	63.0
°API of 650°F$^-$ @ 60°F	9.8	8.9	9.7	9.9
Sp. Gr. of 650°F$^-$ @ 60°F	1.0014	1.0078	1.0021	1.0007
°API of 650°F$^+$ @ 60°F	-8.6	-9.7	-9.4	-8.9
Sp. Gr. of 650°F$^+$ @ 60°F	1.1513	1.1617	1.1589	1.1542
C_3^-, Mole %				
H_2	51.0	47.6	55.8	52.9
C_1	19.0	22.8	18.2	20.6
C_2 (Total)	13.4	15.1	12.7	13.8
C_3 Olefins	13.0	11.0	10.2	10.1
C_3	3.6	3.5	3.2	2.6
Total	100.0	100.0	100.0	100.0
C_4, Vol-%				
C_4 Olefins	64.4	64.7	66.0	71.0
$\underline{i}$-C_4	24.1	23.5	22.2	20.0
$\underline{n}$-C_4	11.5	11.8	11.8	9.0
Total	100.0	100.0	100.0	100.0
C_5, Vol-%				
C_5 Olefins	60.5	60.0	64.9	73.1
$\underline{i}$-C_5	35.2	34.5	29.9	23.6
$\underline{n}$-C_5	4.3	5.4	5.2	3.3
Total	100.0	100.0	100.0	100.0

Errata: Report FE-2645-04:

Table 12 add Plant 532, Run 1133, Periods 1-19 below table heading.

Table 14 add Plant 532, Run 1133, Periods 20-55 below table heading.

Table 16 add Plant 532, Run 1134, Periods 1-19 below table heading.

Table 18 add Plant 532, Run 1135, Periods 1-16 below table heading.

Figure 1

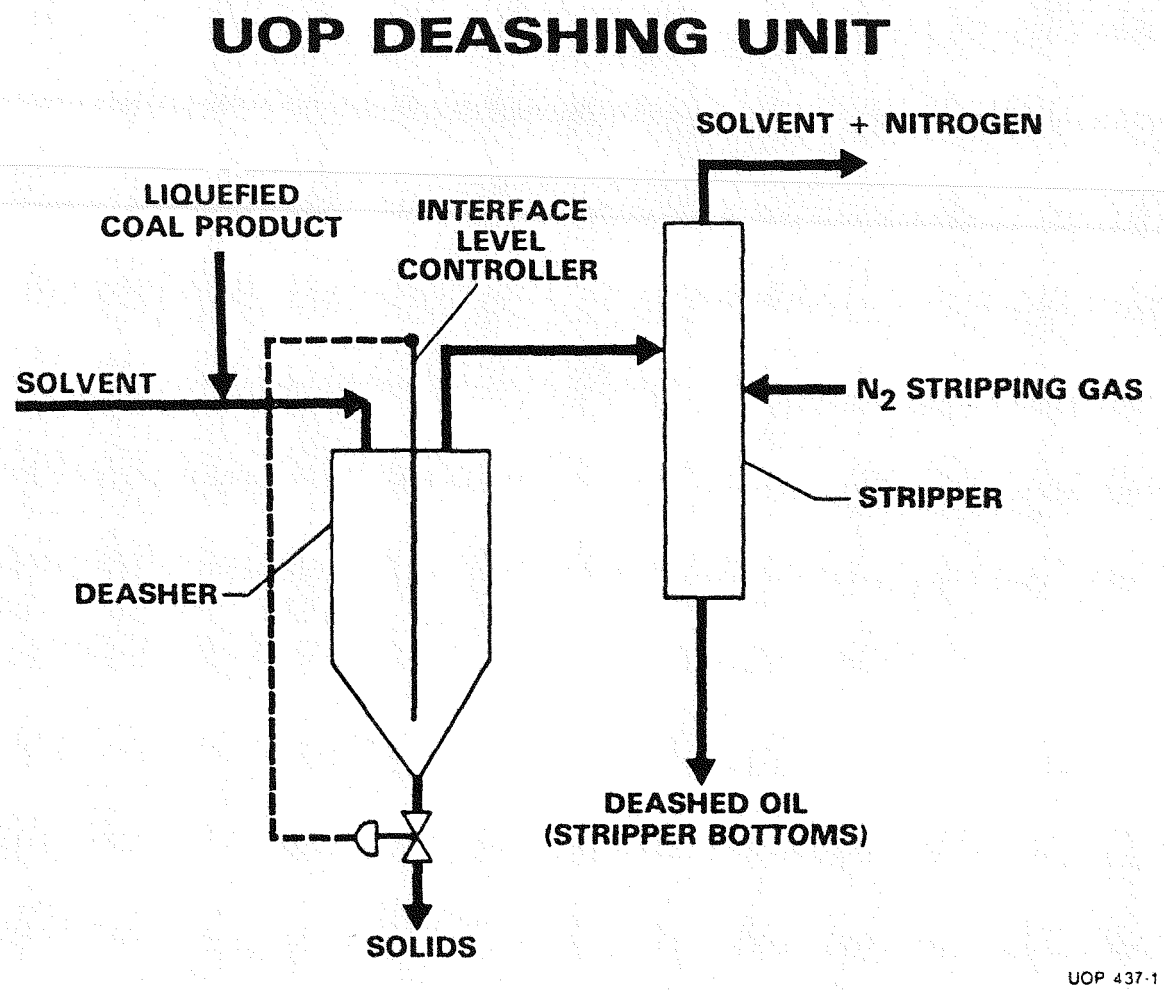
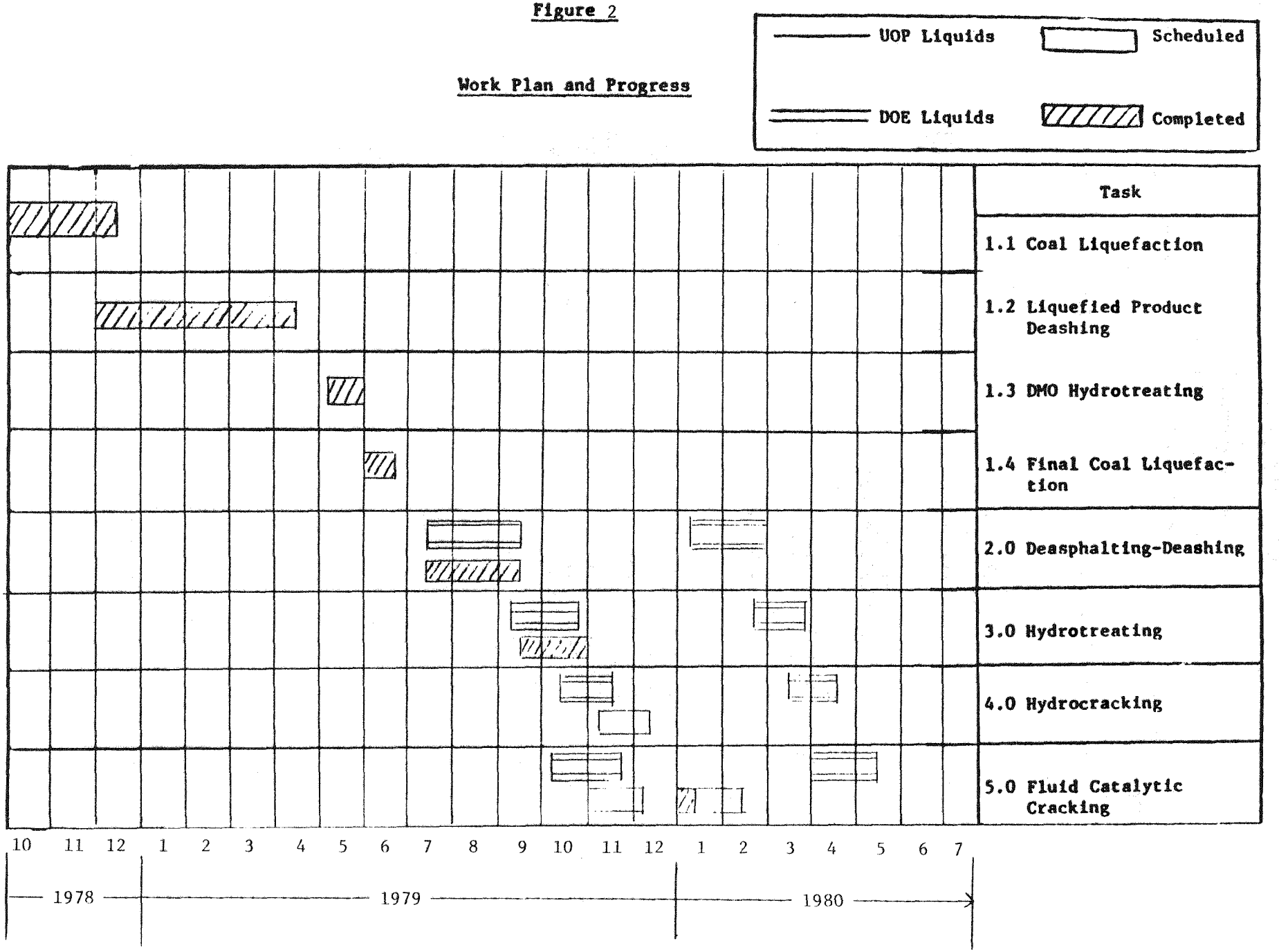

UOP DEASHING UNIT
SOLVENT + NITROGEN
LIQUEFIED COAL PRODUCT
INTERFACE LEVEL CONTROLLER
SOLVENT
N_2 STRIPPING GAS
STRIPPER
DEASHER
DEASHED OIL (STRIPPER BOTTOMS)
SOLIDS
UOP 437-1

Figure 2

Work Plan and Progress



APPENDIX

Table A-1

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

Hydrocarbon Types Analysis

(C_nH_{2n-z}) z No.	Compound Types**	Wt.%	Avg. MW
z=-2	Paraffins	2.2	324
z=0	1 Ring Naphthenes	2.8	322
z=2	2 Ring Naphthenes	3.6	306
z=4	3 Ring Naphthenes	3.5	304
z=6	4 Ring Naphthenes	2.2	288
z=8	5 Ring Naphthenes	0.8	286
		15.1	307
	Aromatic Hydrocarbons		
z No.	Compound Types, C_nH_{2n-z}**		
z=6	Benzenes	0.6	166
z=8	Indans/Tetralins	8.2	182
z=10	Dinaphthene Benzenes	8.0	212
z=12	Naphthalenes	4.5	219
z=14	Acenaphthenes/Biphenyls	7.1	220
z=16	Fluorenes	7.4	245
z=18	Phenanthrenes	5.2	258
z=20	Aceanthrenes	4.5	263
z=22	Pyrenes	5.8	259
z=24	Chrysenes	3.8	290
z=26	Benzofluoranthenes	2.3	308
z=28	Benzopyrenes	1.8	323
z=30	Dibenzanthracenes	1.3	328
z=32	Benzoperylenes	2.3	327
z=34	Dibenzopyrenes	0.9	345
z=36	Coronenes	0.7	348
z=38	Naphthcoronenes	0.6	355
		65.0	246
	Aromatic Oxygens		
z No.	Compound Types, $C_nH_{2n-z}O$**		
$z=6^O$	Phenols	0.8	136
$z=8^O$	Naphthenophenols	0.8	167
$z=10^O$	Benzofurans	0.4	211
$z=12^O$	Naphthols	0.2	203
$z=14^O$	Naphthenonaphthols	0.2	211
$z=16^O$	Dibenzofurans	0.5	222
$z=18^O$	Hydroxyanthracenes	0.5	246
$z=20^O$	Hydroxynaphthenoanthracenes	0.2	263
$z=22^O$	Hydroxypyrenes	0.8	264
$z=24^O$	Hydroxychrysenes	0.3	296
$z=26^O$	Hydroxycholanthrenes	0.2	288
$z=28^O$	Hydroxybenzopyrenes	0.2	318
$z=30^O$	Hydroxydibenzanthracenes	0.2	337
$z=32^O$	Hydroxybenzoperylenes	0.2	348
$z=34^O$	Hydroxybenzopyrenes	0.1	363
$z=36^O$	Hydroxycoronenes	T	
		5.6	227

** Suggested compound types
T ≤ 0.05%
*Estimates due to lack of calibration coefficients

Table A-1 (Cont'd.)

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

z No.	Aromatic Dioxygenates Compound Types, $C_nH_{2n-z}O_2$**	Wt.%***	Avg. MW
$z=6^{O}2$	Hydroxyphenols	0.3*	144
$z=8^{O}2$	Hydroxynaphthenophenols	<0.1*	169
$z=10^{O}2$	Hydroxybenzofurans	T *	
$z=12^{O}2$	Hydroxynaphthols	T *	
$z=14^{O}2$	Hydroxynaphthenonaphthols	0.8*	233
$z=16^{O}2$	Hydroxydibenzofurans	1.5*	238
$z=18^{O}2$	Dihydroxyanthracenes	2.0*	275
$z=20^{O}2$	Dihydroxynaphthenoanthracenes	0.7*	289
$z=22^{O}2$	Dihydroxypyrenes	0.3*	298
$z=24^{O}2$	Dihydroxychrysenes	0.5*	316
$z=26^{O}2$	Dihydroxycholanthrenes	0.3*	358
$z=28^{O}2$	Dihydroxybenzopyrenes	T *	
$z=30^{O}2$	Dihydroxydibenzanthracenes	T *	
$z=32^{O}2$	Dihydroxybenzoperylenes	0.2*	360
$z=36^{O}2$	Dihydroxycoronenes	T *	
		6.7*	267

z No.	Aromatic Trioxygenates Compound Types, $C_nH_{2n-z}O_3$**		
$z=8^{O}3$	Dihydroxynaphthenophenols	T *	
$z=12^{O}3$	Dihydroxynaphthols	T *	
$z=14^{O}3$	Dihydroxynaphthenonaphthols	T *	
$z=16^{O}3$	Dihydroxydibenzofurans	<0.1*	256
$z=18^{O}3$	Trihydroxyanthracenes	<0.1*	355
$z=20^{O}3$	Trihydroxynaphthenoanthracenes	T *	
		0.3*	295

z No.	Aromatic Nitrogens Compound Types, $C_nH_{2n-z}N$**		
$z=5^{N}$	Pyridines	0.1	144
$z=7^{N}$	Naphthenopyridines	0.3	180
$z=9^{N}$	Indoles	0.5	176
$z=11^{N}$	Quinolines	0.9	195
$z=13^{N}$	Naphthenoquinolines	0.6	209
$z=15^{N}$	Carbazoles	0.8	226
$z=17^{N}$	Acridines	0.6	234
$z=19^{N}$	Naphthenobenzoquinolines	0.7	251
$z=21^{N}$	Benzocarbazoles	0.8	260
$z=23^{N}$	Benzacridines	0.4	285
$z=25^{N}$	Naphthenobenzacridines	0.2	303
$z=27^{N}$	Dibenzocarbazoles	0.4	316
$z=29^{N}$	Dibenzacridines	0.2	333
$z=31^{N}$	Tribenzocarbazoles	0.2	319
$z=33^{N}$	Acenaphthacridines	0.1	357
$z=35^{N}$	Benzonaphthacridines	0.2	350
$z=37^{N}$	Diindenoacridines	T	
$z=39^{N}$	Dinaphthocarbazoles	0.1	392
		7.1	244

Table A-1 (Cont'd.)

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

z No.	Aromatic Sulfurs Compound Types, $C_nH_{2n-z}S$**	Wt.%	Avg. MW
$z=8^S$	Dihydrothionaphthenes	T	
$z=12^S$	Naphthenobenzothiophenes	T	
$z=14^S$	Indenothiophenes	T	
$z=16^S$	Dibenzothiophenes	<0.1	204
$z=24^S$	Acephenanthrylenethiophenes	T	
		0.2	214

Table A-1 (Cont'd.)

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

Carbon Number Distribution for Aromatic Hydrocarbons on a 100% Basis

C#	z#	6	8	10	12	14	16	18	20	22	24	26	28	30	32	34	36	38
8			.09															
9		.09	.18	.02														
10		.11	.81	.26	.03													
11		.18	1.76	.29	.38													
12		.15	1.71	.37	.44	.11												
13		.13	1.74	1.21	.49	.98	.09											
14		.15	2.09	2.00	.50	1.50	.21	.15										
15		.08	1.50	1.97	.61	1.51	.61	.34	.02									
16		.08	1.07	1.53	.73	1.56	1.21	.60	.55	1.16								
17			.58	1.57	1.13	1.41	1.86	.96	.63	1.37								
18			.81	1.31	.82	1.50	2.06	.93	1.05	.78	.06							
19			.21	.69	.63	.92	1.57	.89	.92	.83	.96							
20				.53	.57	.70	1.22	1.10	.99	1.16	.87	.08						
21			.06	.41	.26	.53	1.18	.92	.70	1.07	.54	.41	.26					
22				.26	.17	.17	.53	.66	.66	.86	.58	.70	.27	.22	.58			
23						.17	.37	.52	.47	.46	.78	.46	.21	.11	.57			
24					.09	.09	.23	.40	.41	.38	.55	.49	.50	.41	.26	.02	.14	
25					.08		.21	.18	.21	.21	.58	.69	.29	.40	.18	.29	.09	
26							.05	.17	.14	.34	.50	.26	.41	.38	.53	.20	.15	.11
27								.17	.06	.12	.34	.21	.17	.17	.29	.47	.12	.21
28									.03	.09	.05	.11	.21	.15	.40	.23	.14	.29
29									.11	.14		.09	.18	.03	.26	.09	.14	
30											.06		.11		.35	.09	.20	.23
31													.06	.15	.06	.03	.02	
		.97	12.62	12.42	6.93	11.14	11.41	7.97	6.95	8.97	5.87	3.50	2.69	1.97	3.35	1.41	.99	.84

$\Sigma = 100$

Numbers are shown to two decimal places for normalization purposes only.

Table A-1 (Cont'd.)

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

Carbon Number Distribution for Aromatic Nitrogenates on a 100% Basis

C#	z#	5^N	7^N	9^N	11^N	13^N	15^N	17^N	19^N	21^N	23^N	25^N	27^N	29^N	31^N	33^N	35^N	37^N	39^N
7		.11																	
8		.22	.55																
9		.11	.22	.11	.88														
10		.22	.55	1.64	.33														
11		.11	.44	1.32	.99														
12		.11	.44	1.21	2.41	.44	.44												
13		.11	.77	1.21	2.30	1.54	1.43												
14			.11	.88	1.64	.77	1.43	.66											
15			.66	.66	1.64	2.30	2.08	1.43	.66	.77									
16			.66		1.64	1.75	1.75	1.43	2.08	.66									
17				.11	.55	.77	1.21	2.19	.77	1.10									
18				.22	.22	.11	.99	.77	2.08	1.75	.55								
19					.11		.22	.44	2.74	3.51	.77	.22							
20					.11	.11	.77	.99	.88	2.08	1.10	.22	.22						
21					.44		.66	.22	.33	.44	.99	.33	.66		.11				
22							.11			.11	.44	.44	1.10	.22	.66				
23							.44			.99	.55	.77	.44	.77	.55				
24									.22		.44	.33	.66	.22	1.10	.33	.44		
25									.44		.33	.55	1.10	.44			.33		
26										.33			.11	1.21	.11	.22	.44	.33	.11
27													.55	.11	.66	.33	.33	.11	
28													.11	.11	.11	.33	.22	.22	
29																.33	.22		.33
30																			.11
32																	.11		.44
		.99	4.39	7.35	13.37	7.79	11.51	8.11	10.20	11.73	5.15	2.85	4.93	3.07	3.29	1.54	2.08	.66	.99

$\Sigma = 100$

Numbers are shown to two decimal places for normalization purposes only.

Table A-1 (Cont'd.)

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

Carbon Number Distribution for Aromatic Oxygenates on a 100% Basis

C#	z#	6^0	8^0	10^0	12^0	14^0	16^0	18^0	20^0	22^0	24^0	26^0	28^0	30^0	32^0	34^0	36^0
6		.19															
7		1.98															
8		3.88	.09														
9		3.69	1.51	.09													
10		2.65	3.88	.19	.19												
11		1.23	3.59	.09	.47												
12		.76	2.46	.76	.47												
13		.19	1.42	1.51	.28	.38	.09										
14		.09	1.13	1.89	.38	.85	2.55	.28									
15			.47	1.42	.38	.85	1.13	.57									
16			.38	.66	.28	.57	2.36	1.61	.19								
17				.57	.95	.66	1.61	1.42	1.04	.95							
18				.76	.38	.19	1.80	1.70	1.23	1.51							
19				.47	.28	.09		1.80	.48	1.61	.85						
20								1.61		1.42	.85	.47					
21									.95	1.51	1.89	.57					
22							.09		.66	1.32		.76	.85				
23									.09		.47	.85	.95	.28	.57		
24											.28	1.04	.85	.85	.28	.19	
25											1.13			.85	.38		
26												.38		.57	1.13	.66	
27												.09		.28	.47	.47	
28													.38	.09	.38	.85	
29															.28	.38	
30															.38	.09	.66
		14.65	14.93	8.41	4.06	3.59	9.64	8.98	4.64	8.32	5.48	4.16	3.02	2.93	3.88	2.65	.66

$\Sigma = 100$

Numbers are shown to two decimal places for normalization purposes only.

Table A-1 (Cont'd.)

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

Carbon Number Distribution for Aromatic Dioxygenates on a 100% Basis

C#	z#	6^02	8^02	10^02	12^02	14^02	16^02	18^02	20^02	22^02	24^02	26^02	28^02	30^02	32^02	36^02
6		.12														
7		1.17														
8		1.42														
9		1.29	.18													
10		.43	.74	.06												
11				.18												
12			.31		.31	.74	.06									
13		.25				2.52	1.66									
14							2.22									
15				.68		4.68	4.86	.37								
16							5.23	2.52								
17						1.85	6.03	3.45	1.23	.55						
18						1.97		8.68			.31					
19						.55		7.20	1.72							
20							.49	4.56	5.48	2.09						
21							.74		.43	.74						
22								.74	.74	1.05	5.54	.92				
23								1.48			1.42					
24								.43	.37							
25										.31					.55	.25
26												3.45	.55		1.54	
28														.55		
		4.68	1.23	.92	.31	12.32	21.31	29.43	9.98	4.74	7.27	4.37	.55	.55	2.09	.25

$\Sigma = 100$

Numbers are shown to two decimal places for normalization purposes only.

Table A-1 (Cont'd.)

High Resolution Mass Spectral
Characterization of Deashed Oil, 3776-8

Carbon Number Distribution for Aromatic Trioxygenates on a 100% Basis

C#	z#	$8O_3$	$12O_3$	$14O_3$	$16O_3$	$18O_3$	$20O_3$
11		4.48					
12			5.97				
13				2.99			
15				8.96			
16					29.85		
20							20.89
23						20.89	
25						5.97	
		4.48	5.97	11.95	29.85	26.86	20.89

$\Sigma = 100$

Numbers are shown to two decimal places for normalization purposes only.

Table A-2

High Resolution Mass Spectral Types Analysis
of Three Time Hydrotreated Deashed Oil 3777-46

Hydrocarbon Types Analysis

z No.	Compound Types, C_nH_{2n-z}	Wt.%	Avg. MW
z=-2	Paraffins	2.71	226
z=0	1 Ring Naphthenes	5.04	224
z=2	2 Ring Naphthenes	6.85	208
z=4	3 Ring Naphthenes	7.48	206
z=6	4 Ring Naphthenes	4.65	190
z=8	5 Ring Naphthenes	0.0	0
z=10	6 Ring Naphthenes	0.0	0
		26.73	209
	Aromatic Hydrocarbons		
z No.	Compound Types, C_nH_{2n-z}*		
z=6	Benzenes	0.65	171
z=8	Indans/Tetralins	11.19	186
z=10	Dinaphthene Benzenes	14.59	217
z=12	Naphthalenes	8.09	249
z=14	Acenaphthenes/Biphenyls	7.22	246
z=16	Fluorenes	10.09	251
z=18	Phenanthrenes	5.74	274
z=20	Aceanthrenes	4.18	271
z=22	Pyrenes	3.95	260
z=24	Chrysenes	1.97	276
z=26	Benzofluoranthenes	0.63	302
z=28	Benzopyrenes	0.13	299
z=30	Dibenzanthracenes	0.06	299
z=32	Benzoperylenes	0.09	286
z=34	Dibenzopyrenes	0.00	316
z=36	Coronenes	0.00	317
z=38	Naphthcoronenes	0.00	0
		68.57	237
	Aromatic Oxygens		
z No.	Compound Types, $C_nH_{2n-z}O$*		
z=60	Phenols	0.09	143
z=80	Naphthenophenols	0.07	190
$z=10^0$	Benzofurans	0.04	213
$z=12^0$	Naphthols	0.02	247
$z=14^0$	Naphthenonaphthols	0.06	228
$z=16^0$	Dibenzofurans	0.98	223
$z=18^0$	Hydroxyanthracenes	0.49	256
$z=20^0$	Hydroxynaphthenoanthracenes	0.12	287
$z=22^0$	Hydroxypyrenes	0.02	273
$z=24^0$	Hydroxychrysenes	0.03	289
$z=26^0$	Hydroxycholanthrenes	0.03	319
$z=28^0$	Hydroxybenzopyrenes	0.02	284
$z=30^0$	Hydroxydibenzanthracenes	0.00	294
$z=32^0$	Hydroxybenzoperylenes	0.00	292
$z=34^0$	Hydroxybenzopyrenes	0.00	0
$z=36^0$	Hydroxycoronenes	0.00	0
		1.97	235

*Suggested Compound Types

Table A-2 (Cont'd.)

High Resolution Mass Spectral Types Analysis
of Three Time Hydrotreated Deashed Oil 3777-46

z No.	Aromatic Nitrogens Compound Types, $C_nH_{2n-z}N$*	Wt.%	Avg. MW
$z=5^N$	Pyridines	0.05	176
$z=7^N$	Naphthenopyridines	0.09	224
$z=9^N$	Indoles	0.07	204
$z=11^N$	Quinolines	0.11	235
$z=13^N$	Naphthenoquinolines	0.13	235
$z=15^N$	Carbazoles	0.60	241
$z=17^N$	Acridines	0.72	254
$z=19^N$	Naphthenobenzoquinolines	0.29	276
$z=21^N$	Benzocarbazoles	0.11	259
$z=23^N$	Benzacridines	0.10	273
$z=25^N$	Naphthenobenzacridines	0.06	274
$z=27^N$	Dibenzocarbazoles	0.01	301
$z=29^N$	Dibenzacridines	0.00	303
$z=31^N$	Tribenzocarbazoles	0.02	283
$z=33^N$	Acenaphthacridines	0.00	345
$z=35^N$	Benzonaphthacridines	0.00	301
$z=37^N$	Diindenoacridines	0.00	0
$z=39^N$	Dinaphthocarbazoles	0.00	0
		2.36	249

z No.	Aromatic Sulfurs Compound Types, $C_nH_{2n-z}S$*		
$z=6^S$	Benzenethiols	0.00	334
$z=8^S$	Dihydrothionaphthenes	0.00	164
$z=10^S$	Benzothiophenes	0.00	176
$z=12^S$	Naphthenobenzothiophenes	0.00	0
$z=14^S$	Indenothiophenes	0.00	0
$z=16^S$	Dibenzothiophenes	0.01	249
$z=18^S$	Acenaphthenothiophenes	0.00	0
$z=20^S$	Fluorenothiophenes	0.00	0
$z=22^S$	Tribenzothiophenes	0.00	0
$z=24^S$	Acephenanthrylenethiophenes	0.00	0
$z=26^S$	Pyrenothiophenes	0.00	0
$z=28^S$	Dinaphthothiophenes	0.00	0
$z=30^S$	Perylenothiophenes	0.00	0
$z=32^S$	Indenophenanthrothiophenes	0.00	0
$z=34^S$	Benzopyrenothiophenes	0.00	0
$z=36^S$	Diacenaphthothiophenes	0.00	0
		0.01	253

*Suggested Compound Types

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