Appendix D

Catalytic Condensation Pilot Plant Study

Three feedstocks were oligomerized over proprietary UOP catalysts. A C_6 olefin feed, a C_3/C_4 feed with the same olefin/paraffin ratio expected from a commercial Arge reactor, and a primarily C_5/C_6 feed were tested in the program. Only the C_5/C_6 feed was coal derived (Arge Rectisol Condensate).

Results of the pilot plant program were used to generate a yield estimate for a Catalytic Condensation unit processing Fischer-Tropsch reactor products presented in Section 6.

Initial attempts to oligomerize the C_5/C_6 fraction of the Arge Rectisol Condensate were not successful because of extremely rapid catalyst deactivation caused by high concentrations of oxygenates. The C_5/C_6 material was water washed to remove oxygenates before a second attempt to oligomerize this material. This water treatment resulted in improved catalyst stability, however, deactivation remained rapid indicating the need for more severe treating prior to oligomerization. Accordingly, the C_5/C_6 material was treated with a high temperature alumina process and drying step. After this procedure, the C_5/C_6 material was successfully oligomerized and fractionated into the appropriate boiling range fractions for subsequent blending studies (Table D-1).

The results of this oligomerization work indicate that treating of Arge condensate materials will be required before successful oligomerization can be accomplished in a commercial upgrading facility.

Table D-1

Fischer-Tropsch C_5/C_6 Oligomerized Products

Fraction	IBP-356°F	356°-EP
API	79.5	44.6
Distillation, °F		
IBP		392
5%		405
10%		414
30%		441
50%		491
70%		555
90%		676
95%		712
EP		723
Flash Pt., °F		160
Pour Pt., °F		-60
Viscosity, cSt,		
@ 100°F		3.50
@ 122°F		2.70
Weight Fraction	0.65	0.35

Appendix E

Development of Blending Correlations

ASTM 50% Point

Predicted ASTM 50% points were determined by taking a weighted average of the individual component ASTM 50% points.

Cetane Index Blending

Cetane number or index is an indication of the ignition quality of the fuel. It is similar in concept to the octane rating of gasoline. A cetane number is the numerical result of an engine test.

A cetane index is an estimate of the cetane number for a specific fuel. The cetane index is convenient because it is based on physical properties (API gravity and ASTM mid-boiling point) and does not require an engine test.

Cetane indices were calculated using the equation provided in ASTM Method D-976. The blend cetane index is determined by a volumetric average of the component cetane indices.

The correction factor for LCO content in this study is shown below:

$$BCICF = 4 - 0.12*LCO$$

where:

BCICF = Blend Cetane Index LCO Correction Factor
LCO = Diesel Blend LCO Content, Wt-%

Flash Point Blending

Flash point measures the response of a sample to heat and flame under controlled laboratory conditions. It is important primarily from a fuel handling safety standpoint. Flash points of blends are determined using the volume fraction and flash point index of each component in the blend. The flash point index for a component is simply a function of the component flash point. A table of flash point indices is attached (Table E.1).

The equations shown below were developed from the data in the table. They are reasonably accurate over the range of 20-300°F.

1. CFPI = A * exp{[ln(CFP) - B]^2 / C}

2. BFP = exp{[C * ln(BFPI/A)]^0.5 + B}

3. BFPCF = 12 - 0.1*LCO

where:

CFP = Component Flash Point
CFPI = Component Flash Point Index

BFP = Blend Flash Point
BFPI = Blend Flash Point Index

BFPCF = Blend Flash Point LCO Correction Factor
LCO = Diesel Blend LCO Content, Wt-%

A = 51708
B = 2.6287
C = -0.91725

Method of Use:

1. Calculate flash point indices (CFPI) for all components in the blend using Equation 1 and the component flash point (CFP).

2. Calculate a blend flash point index (BFPI) by volume averaging the component flash point indices.

3. Calculate the blend flash point (BFP) using Equation 2 and the blend flash point index.

4. Correct for LCO content using Equation 3.

<u>Pour Point Blending</u>

Pour point is the lowest temperature at which oil is observed to flow. It is an especially important consideration when ambient temperatures are low (cold starting) and the danger is posed that the fuel may set up. Pour points of blends are determined using the weight fraction and pour point <u>index</u> of each component in the blend. The pour point index for a component is a function of the component pour point and the ASTM 50% point. A table of pour point indices is attached (Table E.2).

The equations shown below were developed from the data in the table. They are reasonably accurate over the range of pour points from -70 to 70°F and ASTM 50% points from 300 to 700°F.

1. CPPI = M * N^K

2. BPP = [log(BPPI/M) / log(N)] - 100

3. BPPCF = -8 - 0.083*LCO

where:

M = A + B*(50%PT) + C/(50%PT)

N = 1/[D*(50%PT - E)^2+F]

K = CPP + 100

CPP = Component Pour Point

CPPI = Component Pour Point Index

BPP = Blend Pour Point

BPPI = Blend Pour Point Index

BPPCF = Blend Pour Point LCO Correction Factor

LCO = Diesel Blend LCO Content, Wt-%

A = -1.0226

B = 0.00061317

C = 422.73

D = -5.7232E-08

E = 67.965

F = 0.97125

Method of Use:

1. Calculate pour point indices (CPPI) for all components in the blend using Equation 1, the component pour points (CPP) and the component ASTM 50% points.

2. Calculate a blend pour point index (BPPI) by weight averaging the component pour point indices.

3. Calculate a blend ASTM 50% point by weight averaging the component ASTM 50% points.

4. Calculate the blend pour point (BPP) using Equation 2, the blend pour point index, and the blend ASTM 50% point.

5. Correct for LCO content using Equation 3.

Viscosity Blending

The viscosity of a fluid is a measure of its resistance to flow. The viscosity of a fuel has a large impact on atomization and shape of fuel spray which are important combustion characteristics. Viscosities of blends are determined using the weight fraction and viscosity index of each component in the blend. The viscosity index for a component is a function of the component viscosity.

The equations shown below were developed from the viscosity data. They are reasonably accurate over the range of viscosities from 0.8 to 14 cSt.

1. $CVI = A + B*CV + C/CV$

2. $BV = \{-(A - BVI) + [(A - BVI)^2 - (4*B*C)]^{0.5}\} / (2*B)$

3. $BVCF = 0.6 - 0.01*LCO$

where:

CV = Component Viscosity
CVI = Component Viscosity Index

BV = Blend Viscosity
BVI = Blend Viscosity Index

BVCF = Blend Viscosity LCO Correction Factor
LCO = Diesel Blend LCO Content, Wt-%

A = 18.892
B = 0.60727
C = -16.297

Method of Use:

1. Calculate viscosity indices (CVI) for all components in the blend using Equation 1 and the component viscosities (CV).

2. Calculate a blend viscosity index (BVI) by weight averaging the component viscosity indices.

3. Calculate the blend viscosity (BV) using Equation 2 and the blend viscosity index.

4. Correct for LCO content using Equation 3.

TABLE E.1
FLASH POINT BLENDING INDEX NUMBERS

May be used to blend flash temperatures determined in any apparatus but, preferably, not to blend closed cup with open cup determinations.

Flash Point, °F	0	1	2	3	4	5	6	7	8	9
0	168,000	157,000	147,000	137,000	128,000	120,000	112,000	105,000	98,600	92,400
10	86,600	81,200	76,100	71,400	67,000	62,900	59,000	55,400	52,100	49,000
20	46,000	43,300	40,700	38,300	36,100	34,000	32,000	30,100	28,400	26,800
30	25,200	23,800	22,400	21,200	20,000	18,900	17,800	16,800	15,900	15,000
40	14,200	13,500	12,700	12,000	11,400	10,800	10,200	9,680	9,170	8,690
50	8,240	7,810	7,410	7,030	6,670	6,330	6,010	5,700	5,420	5,150
60	4,890	4,650	4,420	4,200	4,000	3,800	3,620	3,441	3,280	3,120
70	2,970	2,830	2,700	2,570	2,450	2,330	2,230	2,120	2,020	1,930
80	1,840	1,760	1,680	1,600	1,530	1,460	1,400	1,340	1,280	1,220
90	1,170	1,120	1,070	1,020	978	935	896	857	821	786
100	753	722	692	662	635	609	584	560	537	515
110	495	475	456	438	420	404	388	372	358	344
120	331	318	305	294	283	272	261	252	242	233
130	224	216	208	200	193	186	179	172	166	160
140	154	149	144	138	134	129	124	120	116	112
150	108	104	101	97.1	93.8	90.6	87.5	84.6	81.7	79.0
160	76.3	73.8	71.4	69.0	66.7	64.5	62.4	60.4	58.4	56.5
170	54.7	52.9	51.3	49.6	48.0	46.5	45.1	43.6	42.3	40.9
180	39.7	38.4	37.3	36.1	35.0	33.9	32.9	31.9	30.9	30.0
190	29.1	28.2	27.4	26.6	25.8	25.0	24.3	23.6	22.9	22.2
200	21.6	20.9	20.3	19.7	19.2	18.6	18.1	17.6	17.1	16.6
210	16.1	15.7	15.2	14.8	14.4	14.0	13.6	13.3	12.9	12.5
220	12.2	11.9	11.6	11.2	10.9	10.6	10.4	10.1	9.82	9.56
230	9.31	9.07	8.83	8.60	8.37	8.16	7.95	7.74	7.55	7.35
240	7.16	6.98	6.80	6.63	6.47	6.30	6.15	5.99	5.84	5.70
250	5.56	5.42	5.29	5.16	5.03	4.91	4.79	4.68	4.56	4.45
260	4.35	4.24	4.14	4.04	3.95	3.86	3.76	3.68	3.59	3.51
270	3.43	3.35	3.27	3.19	3.12	3.05	2.98	2.91	2.85	2.78
280	2.72	2.66	2.60	2.54	2.48	2.43	2.37	2.32	2.27	2.22
290	2.17	2.12	2.08	2.03	1.99	1.95	1.90	1.86	1.82	1.79

Flash Point, °F	0	10	20	30	40	50	60	70	80	90
300	1.75	1.41	1.15	0.943	0.777	0.643	0.535	0.448	0.376	0.317
400	0.269	0.229	0.196	0.168	0.145	0.125	0.108	0.094	0.082	0.072
500	0.063	0.056	0.049	0.044	0.039	0.035	0.031	0.028	0.025	0.022

Example: Component	Volume	Flash Point, °F	Blending Index	Volume X Blending Index
A	0.30	100	753	226
B	0.10	90	1,170	117
C	0.60	130	224	134
Total	1.00	111	477	477

Reference: Wickey, R.O., and Chittenden, D.H., "Flash Points of Blends Correlated," Petroleum Refiner, 42, No. 6, pp 157-8 (June 1963).

Table E.2

Pour Point Indices*

Pour Point °F	ASTM 50% Point °F				
	300	400	500	600	700
70	133	123	120	110	100
50	72	63	54	44	35
30	37	31	24	18	13
10	20	15	11	7.1	4.5
-10	10	7.3	4.7	2.8	1.6
-30	5.5	3.6	2.1	1.1	0.56
-50	2.8	1.7	0.93	0.47	0.20
-70	1.5	0.84	0.42	0.20	0.05

* This is not the complete table.