IX. Analytical Procedures and Supporting Tests

A. Introduction

The streams that require analysis include carbon monoxide, hydrogen, the combined feed gas, the first-stage F T products (gaseous, aqueous, liquid hydrocarbon, and reactor wax phases), and the second-stage products (gaseous, aqueous, and liquid hydrocarbon phases). The analytical procedures and supporting tests for these streams are summarized in this section.

B. Carbon Monoxide, Hydrogen, and Combined Feed-Gas

These streams are analyzed on-line using a Mobil-developed automated gas chromatographic (GC) system. The same system is used for on-line analysis of the gaseous product streams from both the first-stage and the second-stage reactors.

C. First-Stage Fischer-Tropsch Products

The analysis of the F-T products are very complicated because of the wide boiling range and the diversity of the product components. Figure 57 summarizes the analytical scheme.

The combined gas stream from the cold and chilled condenser is analyzed on-line using the on-line GC system. The stream contains N_2, H_2, CO, CO_2, H_2O, and hydrocarbons. The amount of hydrocarbons heavier than C_8 is insignificant in this stream. A typical GC plot for such a sample is given in (A) of Figure 58.

Non-acidic oxygenates in the aqueous phase are determined by fused silica capillary column GC (FS-GC) as indicated in Figure 59. Acids are determined by ion chromatography. The major oxygenates in the aqueous phase identified by gas chromatography-mass spectrometry (GC-MS) are summarized in Table 40. Normally, the C_1-C_8 linear alcohols are the major components with smaller amounts of ketones, acids, and mixed esters.

The C_5^+ oxygenates present in the liquid-hydrocarbon phase are determined as previously reported by Di Sanzo (1981). Recently the gas chromatographic analysis has been improved by employing fused silica capillary columns and cool on column splitless injections. Figures 60 and 61 represent typical gas chromatograms of C_6^+ alcohols and acids, and $C_5^{'}$ ketones and esters, respectively, isolated from the hydrocarbon phase by liquid chromatography (LC). Normally, linear alcohols are the major oxygenates, followed by methylketones. Mixed esters as a result of secondary reactions between the various acids (acetic, propanoic, butyric, etc.) and alcohols are also present. The $C_5^{'}$ acid content has been determined to be generally low ($^-0.1\%$ wt of

FIGURE 57

ANALTYICAL SCHEME
OF FISCHER-TROPSCH PRODUCTS

FIGURE 58

GC PLOT OF TYPICAL COMBINED GAS SAMPLES

(A) FIRST-STAGE REACTOR GAS SAMPLE

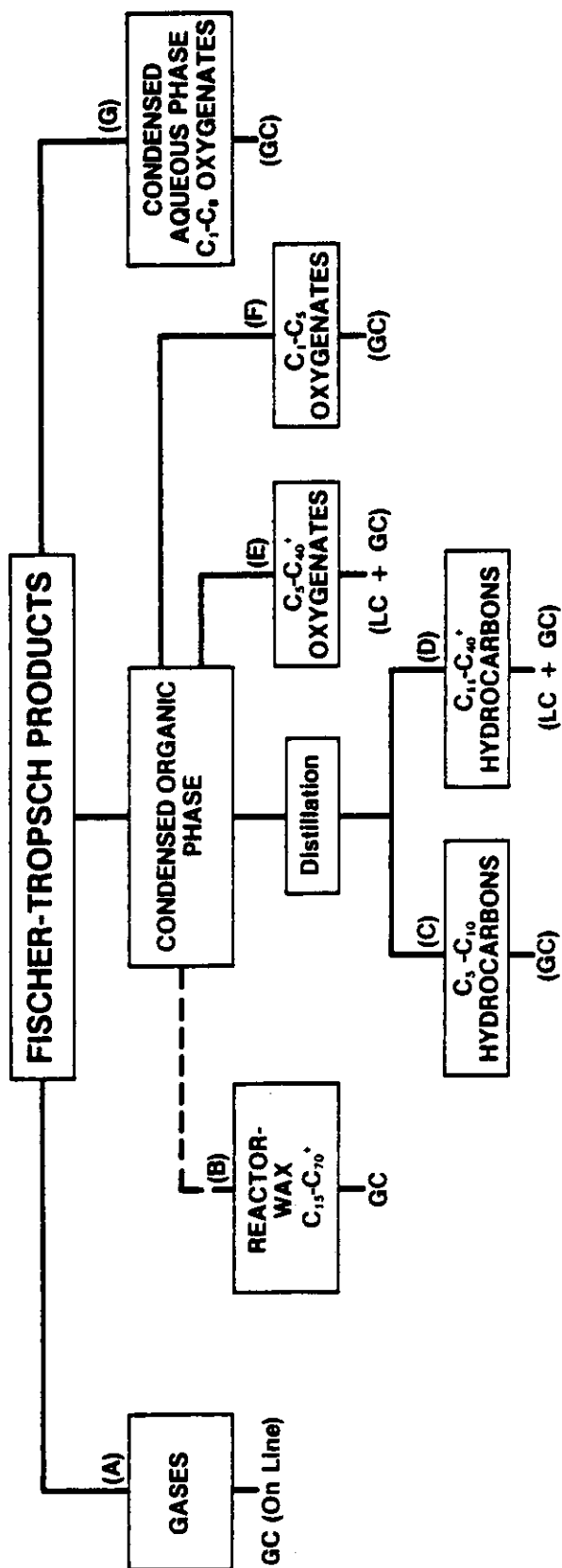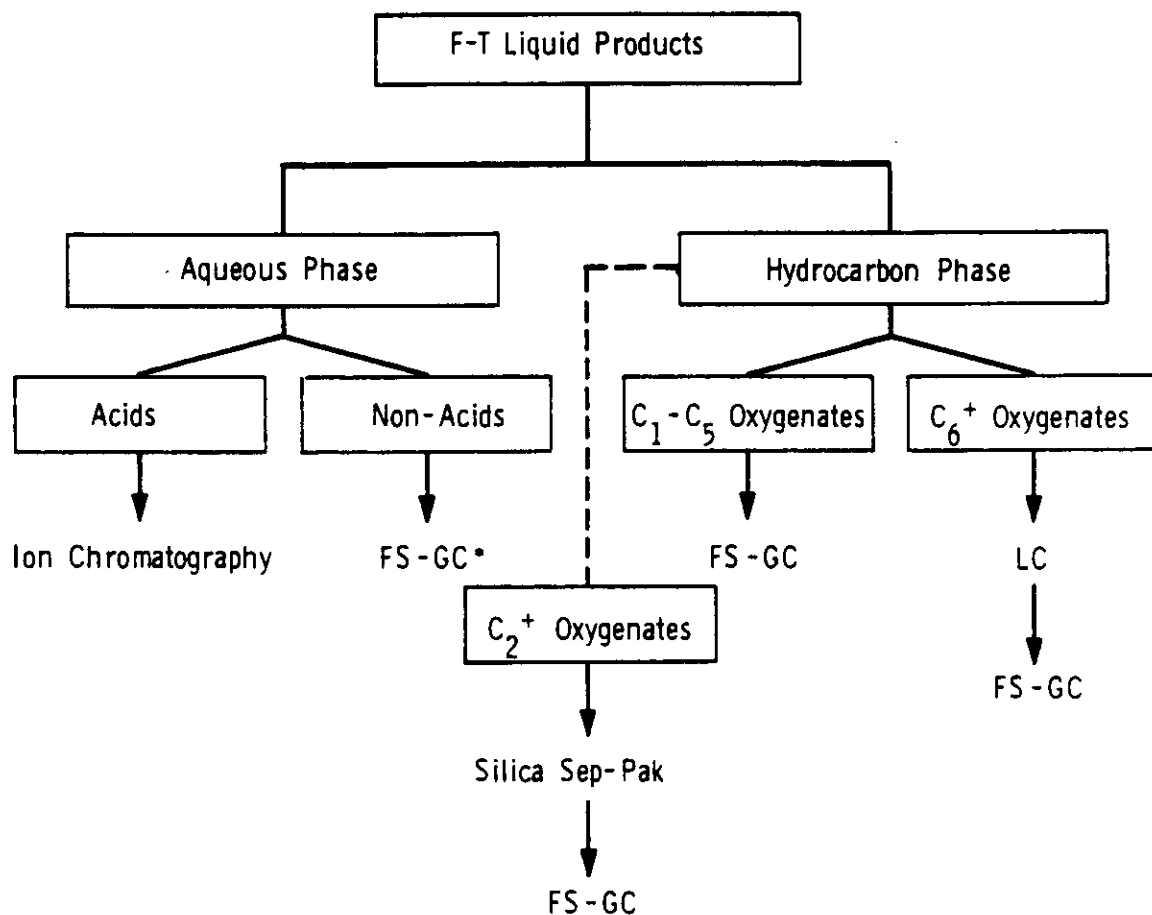## (B) SECOND-STAGE REACTOR GAS SAMPLE

FIGURE 59

ANALYTICAL SCHEME OF
FISCHER-TROPSCH OXYGENATES

* FS-GC = Fused Silica Capillary Gas Chromatography.

Table 40

Identities of Major Aqueous Phase Oxygenates

Peak No. [1]	Oxygenates
1	methanol
2	ethanol
3	acetone
4	isopropanol
5	t-butyl alcohol
6	1-propanol
7	butanal
8	methylethyl ketone
9	2-butanol
10	ethyl acetate
11	isobutanol
12	2-methyl-2-butanone
13	acetic acid
14	1-butanol
15	2-pentanone
16	pentanal+3-pentanone
17	2-pentanol
18	ethyl propanoate
19	propyl acetate
20	methyl butanoate
21	propanoic acid
22	3-methyl-1-butanol
24	1-pentanol
25	2-hexanone
26	butyric acid
27	other C_6 oxygenates
28	1-hexanol
29	other C_7 oxygenates
30	1-heptanol
31	other C_8 oxygenates
32	1-octanol

[1] Identified by gas chromatography-mass spectrometry.

FIGURE 60

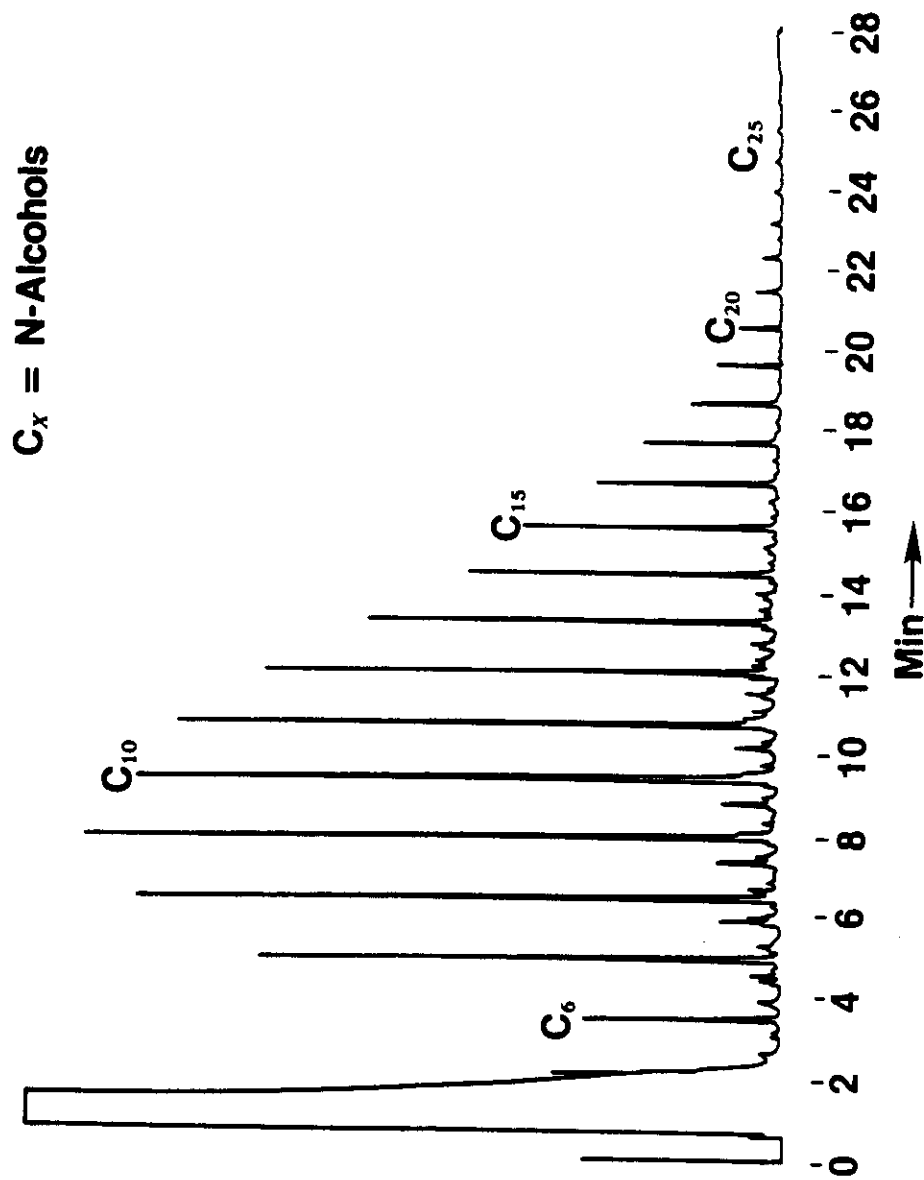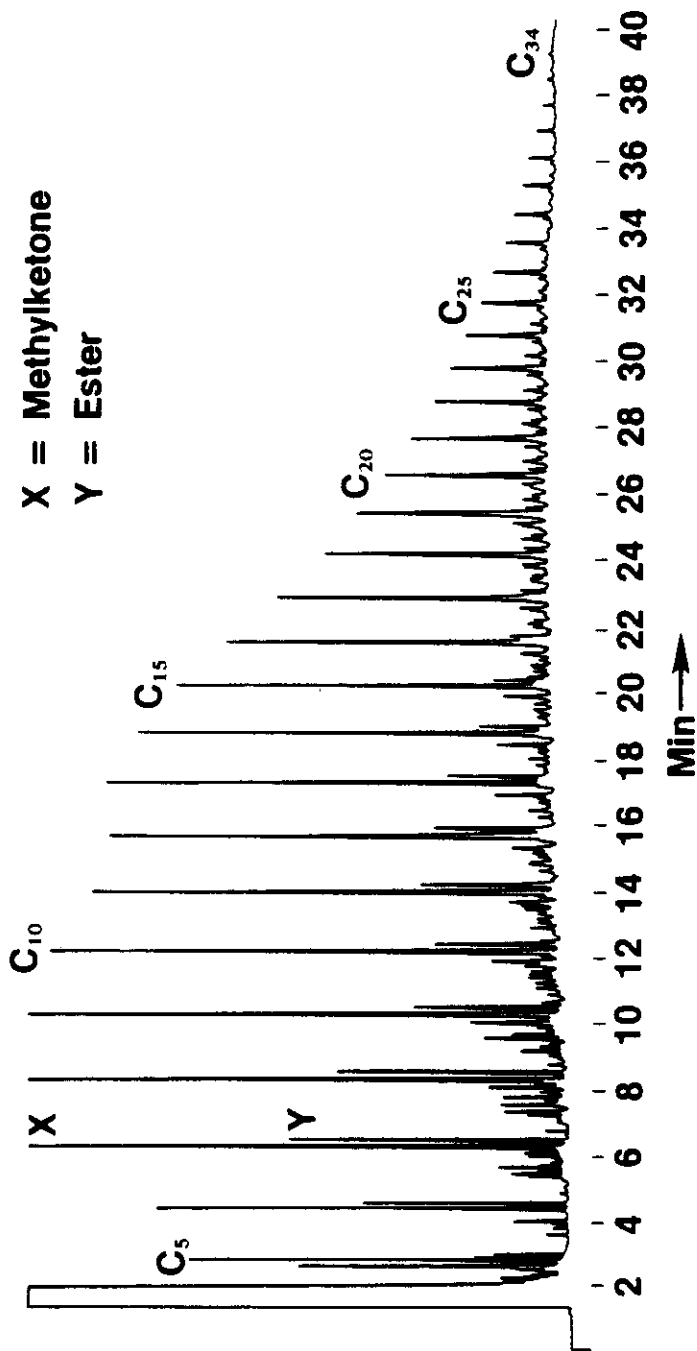## GAS CHROMATOGRAM OF C_6^+ ORGANIC PHASE ALCOHOLS AND ACIDS

C_x = N-Alcohols

FIGURE 61

GAS CHROMATOGRAM OF C₅⁺ ORGANIC
PHASE KETONES AND ESTERS

X = Methylketone

Y = Ester

hydrocarbon phase). With these methods, oxygenates up to C_{40} can readily be determined.

The C_1 to C_5 oxygenates present in hydrocarbon phase are determined by aqueous extraction of the hydrocarbon phase followed by gas chromatographic analysis of the aqueous extract.

An optional analysis for the aqueous F-T product is Acid Number.

The liquid hydrocarbon phase contains mainly olefins and paraffins. The olefinic and paraffinic compositional analysis is carried out by various GC and LC techniques. Carbon number distribution is readily obtained (<1 hour) by a single injection onto an FS-GC capillary column. A typical chromatogram is given in Figure 62. This simple technique will indicate how the major olefins, i.e., linear α-olefins and cis, trans-2 linear olefins, vary with respect to the normal paraffins. Significant changes in the reactor hydrocarbon composition is thus readily detected.

A more detailed analysis is also performed on selected material balances. A liquid hydrocarbon sample is separated into two fractions distilled at 196°C B.P. (about C_{11}) by distillation. The C_{11}^- fraction after removing the oxygenates by passage through a silica gel SepPak (Waters Associates, Milford, Mass.) is injected into a gas chromatograph equipped with an olefin scrubber and two flame ionization detectors. By comparing detector signals total olefins/paraffins can be determined. In addition, major components are identified. Figure 63 shows typical chromatograms of these analyses. The $C_{12}^{'}$ olefins/paraffins are determined as described by Di Sanzo (1981).

Other analyses for the first-stage liquid hydrocarbon product include Acid Number, Bromine Number, Hydroxyl Number, and Simulated Distillation.

The reactor-wax withdrawn from the slurry reactor consists of components with a carbon number distribution from about C_8 to C_{70}^+. A gas chromatographic technique has been developed employing a short (8 m) fused silica capillary column. The reactor-wax (catalyst-free) after being dissolved in hot toluene is injected into the capillary column by the cool on-column injection technique. The latter injection technique minimizes discrimination for the high boiling components. A sample chromatogram is given in Figure 64 for a F-T wax sample employed as a start-up medium in the operation of the two-stage bench-scale pilot plant.

A LC method has also been developed for the determination of oxygenates in the reactor-wax. Total oxygenates is obtained by weighing the isolated oxygenate fraction after solvent evaporation. Carbon number distribution of the oxygenates is

FIGURE 62

TYPICAL GAS CHROMATOGRAM OF
TOTAL LIQUID HYDROCARBON PHASE
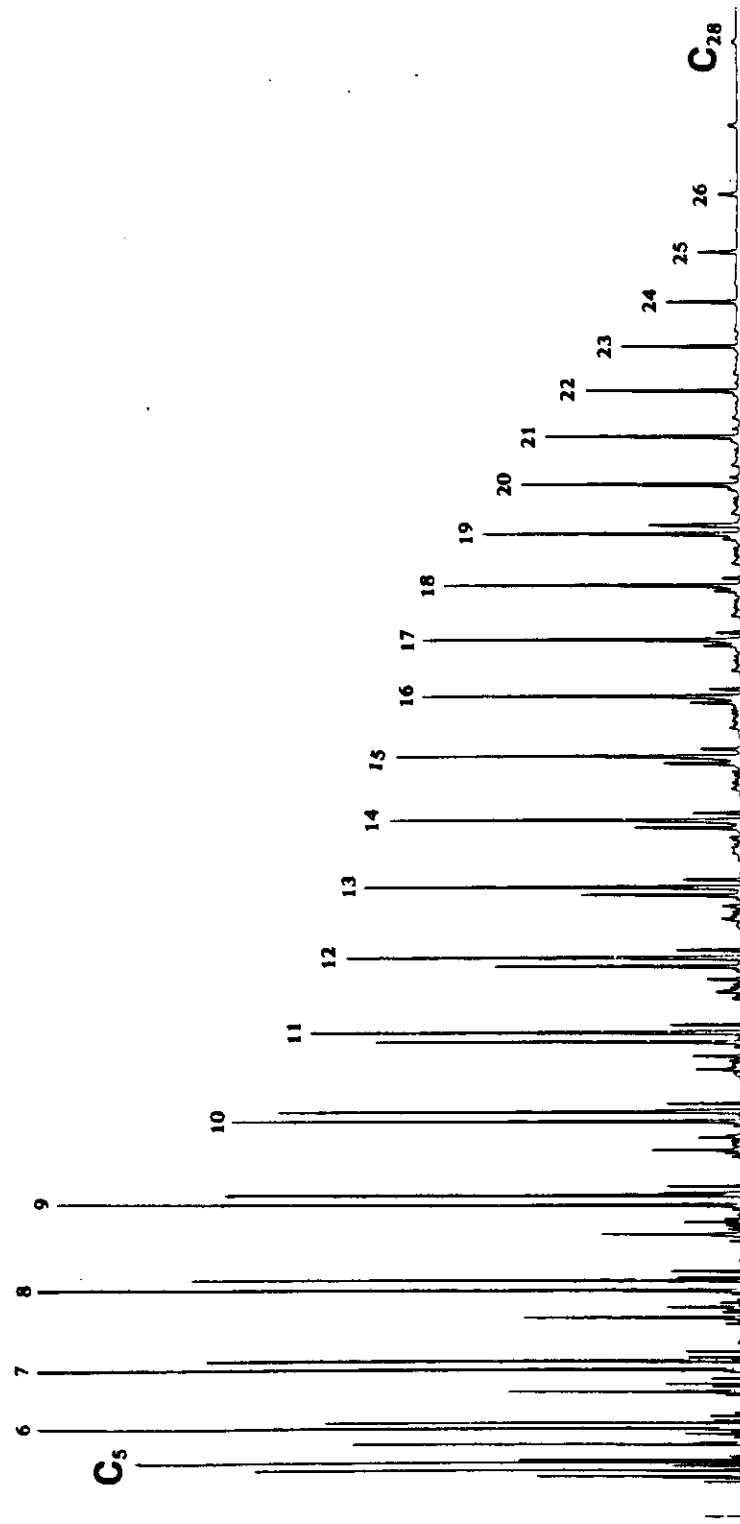
FIGURE 63

TYPICAL CHROMAGRAMS OF C_{11}^- FROM LIQUID HYDROCARBON PHASE

(A) OLEFINS + PARAFFINS
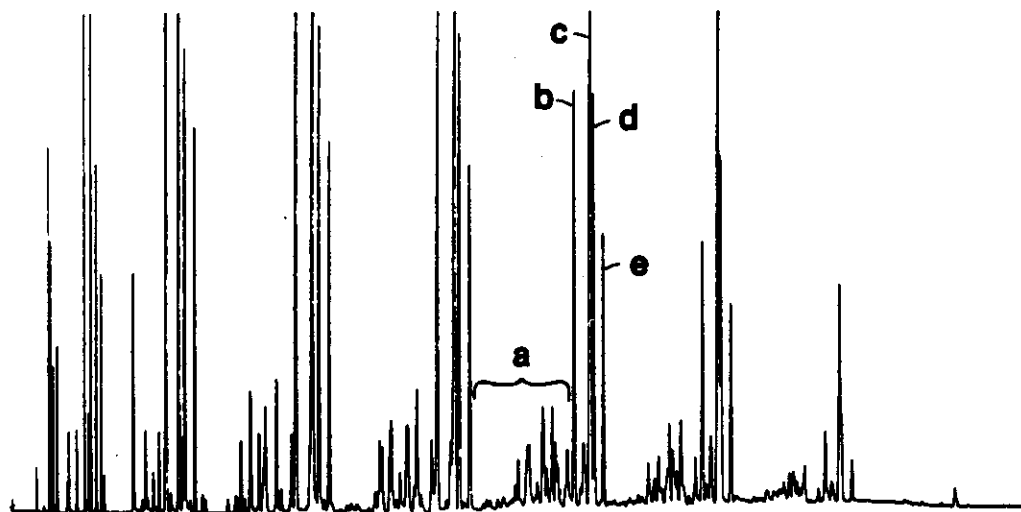
a) C_9 isoolefins + isoparaffins   d) C_9 t-β-olefin
b) C_9 α-olefin   e) C_9 c-β-olefin
c) C_9 n-paraffin

(B) PARAFFINS ONLY
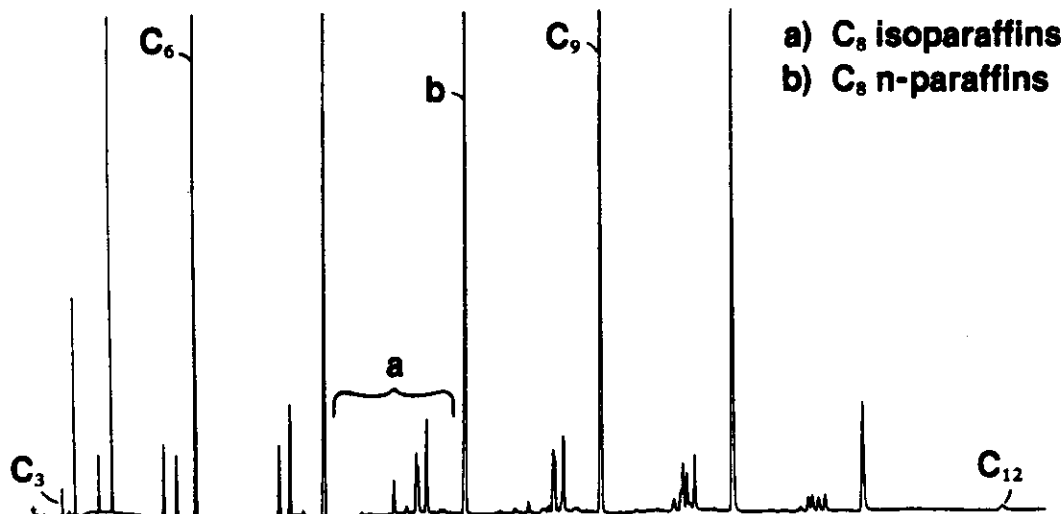
a) C_8 isoparaffins
b) C_8 n-paraffins

FIGURE 64

GAS CHROMATOGRAM OF A HEAVY REACTOR-WAX

WITHOUT BASELINE SUBTRACTION

WITH BASELINE SUBTRACTION

Min ⟶
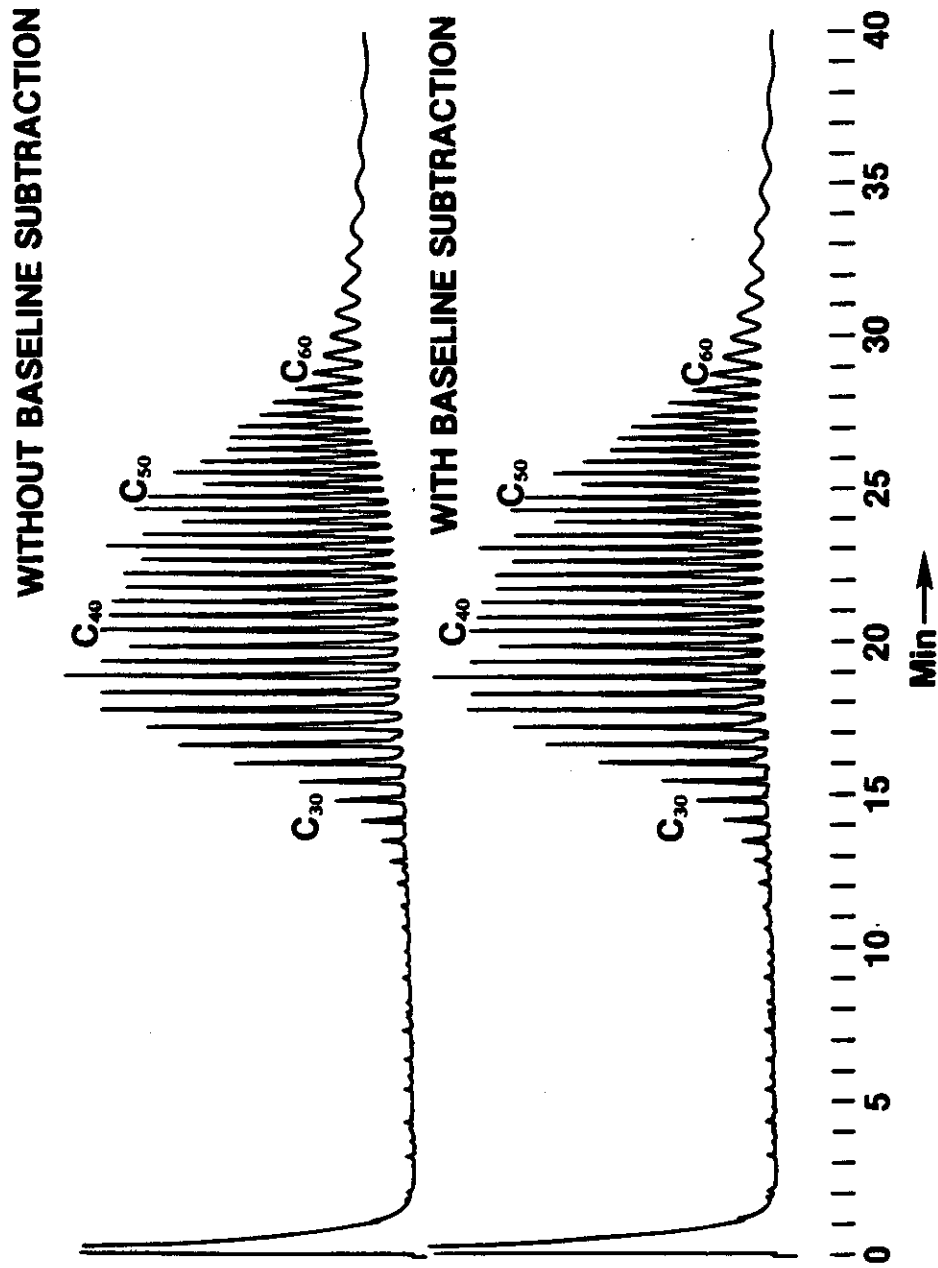
then obtained by FS-GC with cool on-column injection. Alcohols and ketones (major oxygenates) can be distinguished chromatographically.

Other analyses for the F-T reactor-wax are Kinematic Viscosity, Surface Tension, Vacuum and Analytical Distillation, and Specific Gravity.

D.   Second-Stage ZSM-5 Products

The products from the second-stage ZSM-5 reactor are separated into three streams, i.e., gaseous, aqueous, and liquid hydrocarbons. Analysis of the gaseous product is similar to that of the first-stage gaseous product using an on-line GC system. A typical chromatogram is included as (B) of Figure 58. The aqueous stream from the ZSM-5 reactor contains insignificant amounts of oxygenates and only its pH values are occasionally measured.

Analyses of the liquid hydrocarbon product from the ZSM-5 reactor is more complex. A three-column GC system and an olefin scrubber are used. This setup is similar to a system employed for the Methanol-to-Gasoline process (Bloch, et al., 1977). The system is highly automated and can identify individual components up to approximately C_{10}.

The small amount of components boiling above 204°C are determined by capillary column GC and identified by GC-MS. Finally, a LC method has been developed for the determination of trace oxygenates which may be present.

Other analyses employed for the second-stage liquid hydrocarbon product include Research and Motor Octane Numbers, and Acid Number.

X. Characterization of Gasoline Product

A. Raw Gasoline Characterization Tests

In addition to gasoline yield, the performance of the second-stage ZSM-5 reactor must also be judged by the quality of the gasoline product. In the two-stage BSU, the total gasoline is obtained by combining many streams. The major stream is the C_5+ in the raw gasoline (60-65 wt %) collected in ambient and chilled condensers. Other streams include the C_5+ hydrocarbons in the vapor product, the alkylate produced by alkylating butenes and propylene with i-butane, and the butanes added to achieve proper gasoline vapor pressure. The yields and properties of the finished gasoline can be estimated from material balance data.

A detailed blending calculation was carried out to establish the design base data for the conceptual commercial plant design. It was shown that 63 wt % of the finished 10 RVP (Reid Vapor Pressure) gasoline consisted of C_5+ hydrocarbons from the ambient and chilled condensers. Fifteen percent of the remaining constituents was C_5+ hydrocarbons from the gaseous product stream, 18% was from alkylate, and 4% was n-butane. The properties of the finished gasoline are summarized as follows:

Research Octane, Clear		89
Motor Octane, Clear		83
RVP, psia		10
PONA, vol %		67/13/4/16

Distillation, °C	ASTM	TBP
10 vol %	43	29
30 vol %	59	61
50 vol %	93	72
70 vol %	116	92
90 vol %	141	159

The estimated octane number (R+O) of the total gasoline was very close to that of the raw gasoline, and the final gasoline exhibited similar characteristics of conventional petroleum-derived gasoline. Consequently, it was sufficient to judge the performance of the second-stage ZSM-5 reactor by characterizing the qualities of the raw gasoline samples collected from the two-stage pilot plant.

The properties of raw gasoline collected during Runs CT-256-1, -2, and -3 are summarized in Tables B-8, C-5 and D-8, respectively.

The high aromatic content and high octane number of the raw gasoline collected during Run CT-256-1 reflects strongly the consequence of high severity operation in the second-stage reactor. The unleaded research octane numbers ranged from 95 to 97, while the leaded research octane numbers (R+3) ranged from 100 to 105. The severity indexes of the second stage reactor operation, measured as molar i-butane/(propylene + butenes) ratio, ranged from 1 to 8. An index higher than 1.0 generally reflects a high severity operation which results in low propylene and butene yield and thus low alkylate yield. A low alkylate yield usually coincides with a low total gasoline yield. In Run CT-256-1, the C_5+ hydrocarbon including alkylate was about 73 wt % of the total hydrocarbons produced. The gasoline yield increases with lowering the operating severity, as demonstrated in Runs CT-256-2 and -3.

From the ASTM distillation data, it can be seen that during Runs CT-256-1, -2 and -3, the end point of all samples was higher than the ASTM gasoline end-point specification of 225°C. The analyses of these samples showed that they contained about 3-5 wt % of hydrocarbons with boiling points greater than 225°C. These heavier hydrocarbons were, however, 2-3 wt % of the final total finished gasoline and can be removed easily by simple distillation.

As described in Subsection VI.D.3, the first three samples of Run CT-256-1 exhibited foaming at the end of ASTM D-86 distillation and distillations were stopped prematurely. This unusual phenomenon may be related to the fact that these three samples were obtained under the most severe condition in the second-stage operation, and that their aromatic content was very high. The foaming was not experienced with gasoline samples of Runs CT-256-2 and -3.

Another important property of the raw gasoline was its acid content. Except for a few samples, the acid numbers of the majority of the raw gasoline samples were less than 0.19 mgKOH/g. As described before in Subsection VI.B.3, these acids can be removed by simple water washing. In one instance, a raw gasoline sample (20 g) with an acid number of 0.19 mgKOH/g was washed twice with fifty grams of distilled water. The acid number was reduced to zero after the washing.

Figure 25 (Subsection VI.D.3) shows the research octane numbers, aromatic content, and olefin content of the raw gasoline collected during Run CT-256-3 as a function of second-stage operating severity index. The octane numbers during Runs CT-256-2 and -3 range about 90-94 with severity index of 0.5-2.

B. Raw Gasoline Product Stability Tests

Raw gasoline product samples, taken from Runs CT-256-2 and -3, were tested for existent and total gums (ASTM D381) and oxidation stability (ASTM D525).

Metal deactivator at 0.5 lb per 1000 bbl and antioxidant at 2.5 lb per 1000 bbl were used in one portion and the antioxidant level was increased to 15 lb per 1000 bbl in a second portion. As shown in Table 41, existent (heptane-washed) gum contents of 1 to 4 mg/100 cm^3 were found in all samples, thus meeting the 5 mg/100 cm^3 maximum specification of ASTM D439 for automotive gasolines. However, total residues on evaporation were very high (ranging up to 170 mg/100 cm^3) in several of the tests, indicating the presence of high-boiling, heptane soluble materials. The higher antioxidant usage rates were only partially effective for reducing the total residue levels. The high-boiling materials were confirmed by subsequent ASTM D86 distillations, in which end points up to 249°C were measured. The drastic differences in the total gums for some of the samples may be due to operating condition differences in the second stage reactor.

The ASTM D525 procedure provides an indication of gasoline tendencies to react with oxygen to form gum during storage. ASTM D439 specifications require 240 minutes or more for the stability period in this test; time periods of 305 to 825 minutes were obtained for these samples, indicating acceptable performance.

Long-term storage stability tests were conducted on a water-washed composite sample (ASTM D974 total acid number of 0.05 mgKOH/g) of Run CT-256-3 to determine the stability of the gasoline product under accelerated oxidation conditions. Metal deactivator at 1 lb per 1,000 bbl and two different antioxidants at 10 lb per 1,000 bbl were added to two separate portions of the unit product prior to the test.

This long-term test involves storage of the test fuel at 43°C with measurement of gum formation during a sixteen week period. Samples are taken at the start and at incremental periods for total and existent gum contents (ASTM D381). Based on our experience, the amount of gum formed during the storage test provides a good correlation with the gum formation during ambient field storage conditions for approximately one year.

Existent (heptane-washed) gum (ASTM D381) contents of 1 to 3 mg/100 cm^3 were found in all samples at the start of the storage tests, thus meeting the 5 mg/100 cm^3 maximum specification of ASTM D439 for automotive gasolines. The existent gums increased less than 1 mg/100 cm^3 after sixteen-weeks of elevated temperature storage, well within the guideline limits (increase of $\leq$ 2 mg/100 cm^3) for commercial motor gasolines. Thus,

Table 41

Raw Gasoline Short-Term Stability Tests

| Mat. Balances | DOS | Additive Pkg. No.* | ASTM D381 GUMS, mg/100 cm³ | | ASTM D525 Oxidation Stab., Mins. |
			Existent	Total (Unwashed)	
CT-256-2-7	6.9	1	2	117	620
CT-256-2-7	6.9	2	1	120	725
CT-256-3-6	8.6	1	1	170	425
CT-256-3-6	8.6	2	1	142	425
CT-256-3-22	21.1	1	3	11	305
CT-256-3-22	21.1	2	1	10	355
CT-256-3-57	66.5	1	4	119	620
CT-256-3-57	66.5	2	4	81	710
CT-256-3-63	78.5	1	1	37	660
CT-256-3-63	78.5	2	2	12	825

*Additive Package No. 1 -- 0.5 lb/1000 bbl metal deactivator +
2.5 lb/1000 bbl antioxidant.

*Additive Package No. 2 -- 0.5 lb/1000 bbl metal deactivator +
15 lb/1000 bbl antioxidant.

satisfactory stability performance would be expected for the products during conventional field storage at ambient temperatures. However, samples taken at the start and at incremental periods contained high-boiling, heptane soluble materials which resulted in very high and unsatisfactory total residues on evaporation (approximately 150 mg/100 cm^3 throughout the test period) in the ASTM D381 test. Federal Specification VV-G-1690B for automotive gasolines, for example, limits the total residue on evaporation to 10 mg/100 cm^3 maximum. These high boiling materials would be removed by simple distillation in commercial plants.

In addition to the long-term storage tests, short-term accelerated oxidation stability (ASTM D525) tests were also conducted on these samples. Induction times of 510 to 560 minutes was obtained, verifying that the product has satisfactory resistance to oxidation.

Standard N.A.C.E. (National Association of Corrosion Engineers) corrosion tests were conducted on a water washed composite raw gasoline sample (ASTM D974 total acid number of 0.05 mgKOH/g) of Run CT-256-3 to determine the corrosion tendencies. The N.A.C.E. test method involves contacting a cylindrical steel specimen with a constantly stirred mixture of 91% distilled water (maintained at 38°C) for a period of 3 1/2 hours. Performance is expressed by a scale dependent on a visual observation of the rust on the steel specimen surface.

Metal deactivator at 1 lb. per 1000 bbl. and two different antioxidants at 10 lb. per 1000 bbl. were added to two separate portions of the sample. The N.A.C.E. corrosion tests were conducted on duplicate samples from these two portions and on an additized petroleum-sourced unleaded gasoline. Tests were also run on these fuels with a commercial corrosion inhibitor at a conventional level of 2.1 lb. per 1000 bbl. The steel specimen surfaces were severely rusted in tests of fuel samples without corrosion inhibitor. Testing of the fuels containing the corrosion inhibitor, on the other hand, indicated satisfactory protection, showing zero to less than 0.1% (2 or 3 spots of no more than 1 mm diameter) of the surface rusted. Based on these results, it is concluded that the use of a commercial corrosion inhibitor will satisfactorily control the fuel's corrosion tendencies.

In addition to these tests, two raw gasoline samples from Run CT-256-1 were examined which had ASTM D-974 acid numbers of 0.15 (forty-eight DOS) and 0.28 (twenty-eight to thirty DOS) mgKOH/g. Because of limited sample size available at the time, standard corrosion tests could not be run; however, modified in-house tests were conducted to obtain relative comparisons of corrosion tendencies for the two acid number levels and a conventional petroleum sourced unleaded gasoline. The modified

test used a tall bottle with a galvanized iron strip standing in a bottom water layer, with the gasoline sample above, and with air exposure at the top. Results, judged after four weeks storage at 43°C, indicated trace-to-light corrosion for the 0.15 and 0.28 acid number samples and reference unleaded gasoline. Similar gasoline samples of 150 cm^3 were then washed first with 15 cm^3 of 15 wt % caustic soda solution and then with 15 cm^3 of distilled water, and finally subjected to the same test. However, no significant improvements in the test results were observed.

XI. Conceptual Process Design and Scoping Cost Estimate

A. Introduction

A conceptual process design and scoping cost estimate for a commercial plant producing 27,000 BPSD of 10 RVP gasoline plant has been developed for the two-stage slurry F-T/ZSM-5 process. The objectives of the study are two-fold. One is to study the layout of all the processing units and equipment; the other is to provide guidances for future research and development. The design of the plant is as a battery limit part of a complete coal conversion complex. The feed to this plant is a clean synthesis gas derived from a BGC (British Gas Corporation)/Lurgi slagging gasifier which is not included in this design and cost estimate. The composition and quantity of the feed-gas are those used in a study in a report by Gray, et al. (1980).

The data base used for the conceptual design was obtained from Run CT-256-3 and represents a gasoline mode operation. The data for the first-stage slurry F-T reactor were taken from material balance no. 22, which is typical of 1.48 MPa (200 psig) operation at 260°C. The data for the second-stage ZSM-5 reactor were taken from material balance no. 34, which is typical of operation at a target operational severity-index $(i\text{-}C_4/(C_3^= + C_4^=)$ molar ratio) of about 0.9. The data base was established by adjusting the raw data for atomic balances.

The plant consists of a reactor section and a product recovery section. The reactor section, the integrated two-stage slurry F-T and fixed-bed ZSM-5 reactors, consists of forty slurry F-T reactors and five ZSM-5 reactors. The product recovery section consists essentially of conventional distillation facilities. A CO_2 removal unit and an alkylation unit are also included. The cost of battery limit facilities is estimated at $700 million using mid-1983 instantaneous cost basis at a Wyoming location. This is strictly a scoping cost estimate and shall not be used for absolute comparisons of investments from other studies or for purposes other than the objectives mentioned above.

For convenience, the conventional engineering units are used throughout this chapter.

B. Scope of Study

The study covers development of a conceptional design and cost estimate of the battery limits facilities for the Mobil two-stage process. The synthesis gas feed is assumed available at the required conditions from advanced gasifiers of the BGC/Lurgi type. Basis of the study and the scope of the

facilities are summarized below:

- The capacity and feed-gas composition have been selected to be compatible with the coal gasification complex in the MITRE Corporation study (Gray, et al., 1980) for DOE.

- The synthesis gas feed from the gasification complex is assumed to be clean and desulfurized.

- The processing scheme, operating conditions, and yields used in this design are data derived from the two-stage bench scale pilot plant experiments. Other aspects of the design, such as the configuration of SFT reactor internals, were obtained from information available in the published literature.

- Product recovery and separation is by conventional distillation. The carbon dioxide produced in the F-T reaction is removed using a hot potassium carbonate absorption system. The recovered propylene, butene, n-butane, and i-butane fractions together with small quanitity of imported i-butanes are processed in an alkylation unit to maximize gasoline production. Light hydrocarbon gases are available as an offgas stream for further upgrading to SNG.

- The waxy hydrocarbon stream from the SFT reactors is recovered and filtered for removal of traces of catalyst. The filtered wax is stored for use in preparation of fresh slurry and the balance is assumed exported for further upgrading.

- Facilities are included for the periodic removal of the deactivated F-T catalyst and for preparation and activation of fresh catalyst in a separate system. Also included are ZSM-5 catalyst regeneration and nitrogen circulation facilities. Catalyst manufacturing facilities are not included in the scope of the work.

- The cost estimate of the battery limits facilities is based on instantaneous 1983 costs and a Wyoming location.

C. Conceptual Process Design

1. Feed-Gas Basis

The synthesis gas composition is based on gasification of a Wyoming subbituminous coal from advanced gasifiers of BGC/Lurgi type. The gas is treated for sulfur-compound and

carbon dioxide removal and delivered at the required temperature and pressure for this plant. Composition of the clean synthesis gas to the plant used for design purposes is as follows:

	Rates Lb-Mol/Hr	Composition Mol %
Hydrogen	31,841	29.83
Methane	7,490	7.02
Carbon Monoxide	64,319	60.26
Carbon Dioxide	2,360	2.21
Nitrogen	365	0.34
Ethene	26	0.02
Ethane	341	0.32
Total	106,742	100
Total Lb/Hr	2,111,070	

To raise the H_2/CO ratio in the feed gas used in the design study from 0.5 to the 0.67 basis practiced in the laboratory experiments for the SFT/ZSM-5 process, sufficient steam is added with the gas to promote the water-gas shift reaction within the SFT reactor. The assumption that this reaction takes place adequately at the SFT reactor conditions without affecting the F-T catalyst activity is supported by Koelbel and Ralek (1980) and in-house Mobil research work.

2. Reactor Yields

The first-stage SFT and the second-stage ZSM-5 reactor yields used in the design are shown in Tables 42 and 43, respectively. The yield data and reactor conditions used are derived from process studies in the two-stage bench-scale pilot unit. The overall yield distribution and composition of the hydrocarbon products are as follows:

	Overall Yields Wt % of(H_2+CO)[1]	Hydrocarbon Composition Wt %
H_2O	0.81	---
CO_2	65.81	---
C_1 + C_2	2.37	11.6
$C_2^=$	0.37	1.2
C_3	0.43	4.3
$C_3^=$	1.92	5.5
C_4	0.47	13.2
$C_4^=$	1.51	4.8
C_5	2.01	18.4
C_6^+	13.85	41.0
Total	89.55	100.0

(1) Based on 90% CO conversion.

Table 42

First-Stage Slurry F-T

Reactor Yields

Components	Mol.-Wt.	Lb-Mol
Water	18.02	0.7885
Hydrogen	2.02	8.0730
CO	28.01	5.9880
CO2	44.01	26.2889
Methane	16.04	1.8839
Ethene	28.05	0.2298
Ethane	30.07	0.4020
Propene	42.08	0.7660
Propane	44.10	0.1782
N-Butane	58.12	0.1435
C4 Olefins	56.11	0.4739
N-Pentane	72.15	0.1213
C5 Olefins	70.14	0.3777
N-Hexane	86.18	0.0979
C6 Olefins	84.16	0.2533
N-Heptane	100.11	0.0562
C7-Olefins	98.19	0.1244
N-Octane	114.23	0.0574
C8-Olefins	112.21	0.1204
N-Nonane	128.26	0.0530
C9-Olefins	126.24	0.0944
C10-C15 (P+O)	167.82	0.3805
C16-C20 (P+O)	245.95	0.0901
C21-C25 (P+O)	311.75	0.0157
C26+ (P+O, Excl. Wax)	384.55	0.0012
Methanol	32.04	0.0801
Formic Acid	46.03	0.0037
Ethanol	46.07	0.1429
Acetic Acid	60.05	0.0092
Acetone	58.08	0.0241
N-Propanol	60.10	0.0710
I-Propanol	60.10	0.0163
Propanoic Acids	74.08	0.0034
C4-C9 (Oxygenates)	94.24	0.1206
C10-C15 (Oxygenates)	181.43	0.0274
C16-C20 (Oxygenates)	261.93	0.0028
C21-C25 (Oxygenates)	330.75	0.0002
Slurry Reactor Wax	389.05	0.0829

Lb-Mol per 100 Lb-Mol Feed   47.6438

Table 43

Second Stage ZSM-5

Reactor Yields

Components	Mol.-Wt.	Lb-Mol
Water	18.02	1.3138
Hydrogen	2.02	8.0794
CO	28.01	5.9928
CO2	44.01	26.3099
Methane	16.04	1.8928
Ethane	30.07	0.4046
Ethene	28.05	0.1516
Propane	44.10	0.4561
Propene	42.08	0.3724
N-Butane	58.12	0.2934
I-Butane	58.12	0.5278
N-Butene	56.11	0.3116
N-Pentane	72.15	0.2762
I-Pentane	72.15	0.4208
N-Pentene	70.14	0.0102
I-Pentene	70.14	0.2273
Cyclopentane	70.14	0.0129
N-Hexane	86.18	0.1136
I-Hexane	86.18	0.1843
N-Hexene	84.16	0.0046
O-Hexene	84.16	0.0362
Methylcyclopentane	84.16	0.0460
Cyclohexane	84.16	0.0009
Benzene	78.11	0.0415
N-Heptane	100.21	0.0542
I-Heptane	100.21	0.0894
N-Heptene	98.19	0.0045
I-Heptene	98.69	0.0357
Demethyl-Cyclopentane	98.19	0.0350
Methylcyclohexane	98.19	0.0082
Toluene	92.14	0.1307
N-Octane	114.23	0.0183
I-Octane	114.23	0.0310
N-Octene	112.22	0.0073
I-Octene	112.21	0.0573
C8-N5	112.22	0.0232
C8-N6	112.24	0.0054
P-Xylene	106.17	0.1090
O-Xylene	106.17	0.0347
Ethylbenzene	106.17	0.0471
N-Nonane	128.26	0.0054
I-Nonane	128.26	0.0180
N-Nonane	126.24	0.0034
I-Nonene	126.24	0.0268
C9-N5	126.24	0.0057

Table 43 (Cont'd)

Second Stage ZSM-5

Reactor Yields

Components	Mol.-Wt.	Lb-Mol
C9-N6	126.27	0.0013
N-Propylbenzene	120.20	0.0039
Methyl-Ethyl-Benzene	120.20	0.0658
Trimethyl-Benzene	120.20	0.0483
I-Decane	142.28	0.0054
N-Decene	140.27	0.0010
I-Decene	140.27	0.0080
C10-N5	140.30	0.0017
C10-N6	140.30	0.0004
I-Butylbenzene	134.22	0.0214
Tetramethylbenzene	134.22	0.0062
Diethylbenzene	134.22	0.0025
C11-Alkylbenzene	148.25	0.0298
C12-Paraffin	170.38	0.0087
C12-Alkylbenzene	162.30	0.0183
C13-Paraffin	184.41	0.0040
C13-Alkylbenzene	176.33	0.0084

Lb-Mol per 100 Lb-Mol Feed   48.4664

3. Reactor Conditions

The process design conditions for the first- and second-stage reactors are shown below.

	First-Stage SFT	Second-Stage ZSM-5
Inlet Pressure, Psia	250	235
Inlet Temperature, °F	440	700
Outlet Temperature, °F	500	767
H_2/CO Ratio, Molar	0.67[1]	N/A
Space Velocity	2.75[2]	1.65[3]
Catalyst	$Fe/Cu/K_2CO_3$	ZSM-5 Class
Heat of Reaction Btu/Mol (H_2+CO) In SFT Feed	23,000	520

4. Material Balances

The overall design material balance for the battery limits plant in this study is shown below:

	Lb/Hr	Sp. Gr. (Mol. Wt.)	BPSD (SCFD X10^6)
Feeds			
Synthesis Gas	2,111,070	(19.8)	(973.5)
Steam	121,351	(18.0)	(0.6)
I-butanes	10,671	(58.1)	1,299
	2,243,092		
Products			
Offgas	392,634	(15.7)	(227.4)
Propane LPG	22,528	0.501	3,087
Mixed Butanes	7,524	(0.584)	883
10 RVP Gasoline	274,380	0.701	26,869
Distillate	3,926	0.753	357
Wax	30,260	(389.1)	2.400
Waste Water	16,314	1.0	1,126
Carbon Dioxide	1,495,526	(44.0)	(291)
	2,243,092		

(1) Assumed attained after the shift.
(2) In NL/gFe-hr.
(3) In WHSV based on hydrocarbons in feed.