

PRODUCT VALUATION
OF
FISCHER-TROPSCH DERIVED FUELS

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INTRODUCTION

The Clean Air Act Amendments (CAAA) of 1990 have placed stringent requirements on the quality of transportation fuels. Most petroleum refiners are scrambling to meet provisions of the Amendments to be implemented between 1995 and 2000. These requirements will also have significant implications for the production of alternative fuels. These have been examined for Fischer-Tropsch (F-T) derived fuels.

This analysis was conducted in conjunction with the U.S. Department of Energy (DOE) sponsored project, *Baseline Design/Economics for Advanced Fischer-Tropsch Technology*, conducted by Bechtel and Amoco^{1,2}. The goal of this study was to develop a baseline design for indirect liquefaction of Illinois No. 6 coal using gasification, syngas conversion in slurry reactors with iron catalysts, and conventional refinery upgrading of the F-T derived hydrocarbon liquids. One alternative case using ZSM-5 upgrading technology³ was also considered. This study included complete capital and operating cost estimates for the processes.

To perform economic analyses for the different design cases, the products from the liquefaction plant had to be valued relative to conventional transportation fuels. This task was accomplished by developing a Linear Programming (LP) model for a typical midwest refinery, and then feeding the F-T liquids to the refinery. In this way, the breakeven value determined for these materials is indicative of the price they could command if available in the marketplace.

Inputs to the LP model include: refinery size, configuration, feedstocks, products, specifications, prices, and operating and capital recovery costs. The model was set up to be representative of conditions anticipated for the turn of the century. This required inclusion of fuel specifications from the CAAA of 1990 which have or will come into force by the year 2000.

CAAA FUEL SPECIFICATIONS

Meeting the requirements of the 1990 CAAA have been the subject of negotiations between the government, the refining and transportation industries, and various environmental groups. At the time this study was conducted, agreement had only been reached in regards to fuel requirements up through 1995. Reduced summer gasoline volatility (RVP), a winter oxygenated gasoline program for CO non-attainment areas, and a low sulfur diesel program already have been implemented. A federal Phase I reformulation program is scheduled for implementation in 1995. It requires the production of reformulated gasoline for severe ozone non-attainment areas of the country.

The ultimate goal of the CAAA fuels program is the reduction of gasoline volatility, toxicity, and (more recently) NOx to below 1990 levels. These reduction goals are to be phased-in between 1995 and the year 2000 under the federal Phase II reformulation program. In December 1993, the U.S. Environmental Protection Agency published a first draft of the Complex Model which must be used by refiners before 2000 to establish reduction targets.

In addition to the federally mandated programs, California, through the California Air Resources Board (CARB), has promulgated its own Phase I and Phase II programs. In general, the requirements of the CARB programs are more strict than the federal programs. Fuels marketed in California will need to satisfy both the federal and CARB requirements. The CARB Phase I program coincides with the federal program, whereas the CARB Phase II program is to be implemented in 1996. The significance of the California programs is that the rest of the nation has in the past followed California's lead in setting environmental policy. Thus, many of CARB's more severe requirements could become effective nationwide sometime early in the next century.

At the time this study was conducted, little was known regarding the federal Phase II program. Therefore, two different scenarios were modeled with the LP spanning a range of possibilities. The first scenario (Scenario I) assumes fuel specifications in accordance with the federal Phase I program, and the second scenario assumes specifications similar to the CARB Phase II program. Table 1 lists key fuel specifications for gasoline and diesel fuel under the two scenarios.

LP MODELING

The crude capacity of the typical midwest refinery was set at 150,000 bbl/day for this study. A composite crude with an API gravity of 32.9° and total sulfur content of 1.30 wt% was used as the basis for the comparisons with F-T liquids. These properties were projected by extrapolating historical crude quality trends. The crude oil was given a nominal price of \$18 per bbl. Product values were based on current margins between crude and finished products and forecasts for incremental margins due to fuel reformulation. Product demands also were forecast for the year 2000. Table 2 lists the product rates used in the study.

Capital expansions will be required by U.S. refineries to make the fuels required by the CAAA. These were estimated in order to establish the base refinery configuration for the year 2000 and also to determine if any capital savings could be achieved from blending F-T derived fuels with their petroleum counterparts. Table 2 shows a comparison of the typical midwest refinery circa 1990 and 2000.

Table 2 shows that major expansion of refinery hydrotreating capacity will be needed to meet both reduced gasoline and reduced diesel sulfur limits. Associated with the increase in hydrotreating are increases in hydrogen production and sulfur recovery. Producing oxygenated gasoline will require the addition of MTBE (methyl tert-butyl ether) and TAME (tert-amyl methyl ether) units. These ethers are produced from purchased methanol and isobutylene and isoamylene available within the refinery from the catalytic cracking and delayed coking operations. Supplemental n-butane will also be purchased and converted to isobutylene to supply additional MTBE. Benzene levels in gasoline will be controlled by dehexanizing the catalytic reformer feed to remove benzene and its precursors.

F-T PRODUCT DESCRIPTION

The indirect liquefaction designs discussed above produce two distinct product slates. These are listed in the footnote beneath Table 3. For the most part, these streams have been fully upgraded at the liquefaction plant and are suitable for blending to finished fuels. Important properties of these blending components are shown in Table 3. These properties were estimated based on available data from previous DOE-sponsored projects.

In the baseline design, conventional upgrading of F-T liquids produces about one barrel of gasoline for every barrel of diesel. The components of the gasoline are alkylate, isomerate and reformate. These materials are essentially equivalent to their petroleum counterparts produced in a typical refinery. Alkylate, produced from reacting C3, C4, and C5 olefins with isobutane, is the highest octane component in the gasoline. Isomerate is produced from isomerizing normal pentane and hexane. It has a moderate octane rating but is relatively volatile. The reformate, on the other hand, has a high octane rating but contains undesirable aromatic components. The benzene content of the reformate is low due to the dehexanizing of the reformer feed. All of the gasoline blending components have zero sulfur and olefins, which is of considerable benefit when manufacturing CAAA mandated fuels.

Diesel produced from conventional upgrading of F-T products consists of hydrotreated straight-run distillate blended with distillate from wax hydrocracking. The F-T diesel has rather unique properties relative to petroleum-derived diesels. It is sulfur free, almost completely paraffinic, and has an extremely high cetane rating.

The alternative upgrading case using ZSM-5 produces a gasoline-to-diesel ratio of about 1.8, which is more typical of the U.S. transportation fuels market. The components of the gasoline are alkylate, ZSM-5 gasoline, and hydrocracker gasoline. The alkylate is of somewhat lower quality than alkylate produced from the conventional upgrading case due to dilution with C5 paraffins within the liquefaction plant. The ZSM-5 gasoline resembles cat cracker derived gasoline with a high octane rating, high olefins content, and moderate aromatics level. A lower yield loss is associated with the ZSM-5 upgrading compared to conventional catalytic reforming of the highly paraffinic F-T naphtha. The hydrocracker gasoline is of low quality and would be further upgraded in most petroleum refineries. It is the lowest octane material in either design case.

The diesel from the alternative upgrading case is identical to the hydrocracked component from the conventional case and has similar superior properties for diesel blending.

F-T PRODUCT VALUATION

The F-T derived materials were added to the blending pool of the midwest refinery model. After the introduction of these new blending stocks, the refinery configuration was re-optimized. Inclusion of these blending stocks resulted in reduced feedstock, operational, and capital costs. Thus, the F-T derived material was found to be more valuable than the refinery gasoline or diesel products. For example, the zero sulfur content of the F-T derived materials enable the refinery to reduce petroleum hydrotreating requirements, resulting in reduced capital and operating costs.

The results of the product valuation are shown in Table 4 for both Scenario I and Scenario II. This table shows that the F-T derived gasolines always command a premium over F-T derived diesel. Conventional wisdom has been that F-T derived gasoline is of low quality and F-T diesel production is preferable to gasoline production. This study suggest that this conventional wisdom is wrong for the U.S. fuels market. There are two explanations for this result. First, the U.S. market is skewed toward the production of gasoline which commands a higher price than diesel. Second, after upgrading F-T gasoline blending stocks are high quality components for blending to meet the CAAA gasoline specifications.

The ramifications of the price differential between gasoline and diesel can be further illustrated by comparing the alternative upgrading case to the conventional case for Scenario I. While the F-T gasoline from the alternative case is of lower value due to its low octane rating, the composite values for the gasoline and diesel are much closer due to the higher gasoline-to-diesel ratio for the alternative upgrading case. For Scenario II, the composite value for the alternative upgrading case is actually higher. This is a result of both the higher gasoline-to-diesel ratio and the negative effect of the high aromatics content of the F-T gasoline from the conventional upgrading case.

Alkylate and reformate are premium gasoline blending components and contribute significantly to the F-T gasoline value. Because of aromatics restriction in the CAAA, the reformate value, however, decreases in Scenario II. The ZSM-5 gasoline also was found to be a superior blending component. In Scenario I, the low value of the gasoline from the alternative upgrading was primarily a result of the low octane of the hydrocracker gasoline. However, in Scenario II this gasoline commands a substantial premium over the refinery gasoline product because of its zero sulfur and low aromatics contents, which are more critical in this scenario.

The high cetane and zero sulfur content of the F-T diesel blending stock was not found to have a significant effect on its value, which was only slightly higher than the price used for low-sulfur, on-highway diesel. The CAAA force the refiner to invest heavily in hydrotreating capacity both for gasoline and diesel sulfur reduction. Much of the desulfurization derives from gas oil (cat cracker feed) hydrotreating aimed primarily at lowering the sulfur content of the gasoline and hydrocracking aimed at increasing the gasoline yield. Any severe distillate hydrotreating required has the added benefit of improving the distillate cetane index. For these reasons, the refinery did not receive much benefit from the superior F-T diesel properties.

The implications of the F-T product values given in Table 4 on the economics of indirect liquefaction are reported elsewhere².

CONCLUSIONS AND RECOMMENDATIONS

The results of this study indicate that F-T derived materials look attractive for blending with conventional petroleum derived stocks to produce CAAA mandated transportation fuels. F-T derived gasoline blending stocks benefit the refinery due to their high octane, low sulfur content, and low olefins content. The F-T diesel, while superior to its petroleum counterpart, does not show much benefit to the typical refinery. However, it does command the same price as low sulfur diesel fuel. Further work is required to quantify the value of the high-cetane F-T diesel. Refinery specific situations might result in enhanced value for this material.

For Scenario I, the liquids from the conventional upgrading of the F-T product were more valuable than those from the alternative upgrading. This was reversed in Scenario II. Optimization of the F-T upgrading could improve the value of the gasoline from the alternative upgrading case. Octane improvement could possibly be achieved either by more severe ZSM-5 operation or by additional upgrading of the hydrocracker gasoline. Octane improvement for the conventional upgrading case is limited by the aromatics content of the reformate stream.

In addition, the alternative upgrading case results demonstrate the benefits of higher gasoline production from F-T upgrading. Other avenues for increasing the gasoline-to-diesel ratio from F-T upgrading include cat cracking F-T wax and low-wax F-T reactor operation. Both of these routes also could be used for the production of ethers for gasoline blending. Isobutylene and isoamylene can be converted directly to MTBE and TAME, whereas normal olefins must be converted to their iso-counterparts first. Skeletal isomerization could prove attractive for converting the large quantity of normal olefins obtained from iron-based F-T synthesis into etherification feedstocks.

Further work is necessary to optimize the production of transportation fuels from F-T synthesis. In addition to expanded LP studies including more upgrading options, experimental data are required to fill gaps in the existing LP data base and to confirm predictions from the LP model. Tests are necessary to establish the blending properties of the F-T derived materials. Additional testing of the ZSM-5 process for upgrading F-T liquids also should be performed.

The DOE-sponsored Refining and End Use Study of Coal Liquids will attempt to address some of the issues outlined above. Participants in this recently initiated project include Bechtel, Southwest Research Institute, Amoco, and M.W. Kellogg. Results from the present study indicate that Fischer-Tropsch synthesis could be an important technology for satisfying our nation's transportation fuel needs in the next century. The potential benefits of F-T derived fuels for meeting the environmental requirements of the CAAA have been quantified. More new insights are anticipated from the End Use Study.

REFERENCES

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TABLE 1: CAAA 1990 Fuel Specifications

Gasoline Pool [*] :	Conventional	Scenario I Reformulated (Fed. Phase I)	Scenario II Reformulated (CARB Phase II)
% Reformulated		15 %	70 %
Summer RVP, psi	8.7 max	7.1 max	7.1 max
90% Point, °F	330 max	330 max	300 max
Sulfur, ppm	339 max	339 max	30 max
Olefins, LV%	9.2 max	9.2 max	4 max
Aromatics, LV%	32 max	26.2 max	22 max
Benzene, LV%	1.5 max	0.95 max	0.8 max
Oxygen, Wt%	-	2.1 min	2.1 min
Diesel Pool:			
% Low Sulfur		83 %	83 %
Sulfur, Wt%	0.25 max	0.05 max	0.05 max
Cetane Index	40 min	40 min	48 min

*The gasoline pool was assumed to be 42% premium grade (92 octane) and 58% regular grade (87 octane) in 2000.

**TABLE 2: Typical Midwest Refinery Capacity and Production
(BPSD unless otherwise noted)**

Unit Capacity:	1990	2000
Atmospheric Distillation	150,000	unchanged
Vacuum Distillation	59,300	unchanged
C5/C6 Isomerization	11,200	11,200-12,700
Naphtha Hydrotreating	45,900	unchanged
Catalytic Reforming	39,400	unchanged
Total Distillate Hydrotreating	21,300	31,200-34,200
Catalytic Cracking	53,300	unchanged
Hydrocracking	7,500	16,000-21,200
Delayed Coking	16,800	unchanged
Gas Oil Hydrotreating	-	27,600-28,300
C4 Isomerization	-	2,700-8,800
IC4 Dehydrogenation	-	0-4,100
MTBE/TAME Production	-	1,400-6,700
Alkylation	11,900	unchanged
Hydrogen Production, MMSCFD	7	31-39
Sulfur Production, LT/D	120	195-201
Production:		
LPG	4,270	4,270
Total Gasoline	72,730	78,760
Jet Fuel	12,500	14,680
Conventional Diesel	29,130	5,410
Low Sulfur Diesel	-	33,610
Residual Fuel/Asphalt	9,560	8,560

TABLE 3: F-T Derived Gasoline and Diesel Quality

Gasoline Pool:	Conventional* Upgrading	Alternate** Upgrading
Road Octane No.	88.4	81.1
RVP, psi.	5.1	6.0
90% Point, °F	294	305
Sulfur, ppm	0	0
Olefins, LV%	0	6.3
Aromatics, LV%	23.2	13.0
Benzene, LV%	0.2	0.5
Oxygen, Wt%	0.0	0.0
Diesel Pool:		
Sulfur, Wt%	0	0
Cetane Index	74.1	73.1

*Gasoline Pool: 37% alkylate, 23% isomerate, 40% reformate;
Diesel Pool: 67% hydrocrackate, 33% distillate;
Gasoline-to-Diesel Ratio: 0.97.

**Gasoline Pool: 35% alkylate, 36% ZSM-5 gasoline, 29% hydrocrackate;
Diesel Pool: 100% hydrocrackate;
Gasoline-to-Diesel Ratio: 1.8.

**Table 4: Fischer-Tropsch Product Values
(dollars per barrel)**

Crude Oil & Refinery Products:	Scenario I	Scenario II
Crude Oil	18.00	18.00
Composite Gasoline	26.00	26.70
Conventional Diesel Fuel	22.70	22.70
Low Sulfur Diesel Fuel	24.80	24.80
F-T Conventional Upgrading:		
F-T Gasoline Blendstocks	27.02	28.07
F-T Diesel Blendstock	24.90	25.19
Composite for Conv. Upgrading	25.95	26.61
F-T Alternative Upgrading:		
F-T Gasoline Blendstocks	25.62	28.17
F-T Diesel Blendstock	24.91	25.19
Composite for Alt. Upgrading	25.36	27.10