

FISCHER-TROPSCH INDIRECT COAL LIQUEFACTION DESIGN/ECONOMICS - MILD HYDROCRACKING VS. FLUID CATALYTIC CRACKING

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In order to evaluate the economics of Fischer-Tropsch (F-T) indirect coal liquefaction, conceptual plant designs and detailed cost estimates were developed for plants producing environmentally acceptable, high-quality, liquid transportation fuels meeting the Clean Air Act requirements. The designs incorporate the latest developments in coal gasification technology and advanced (F-T) slurry reactor design. In addition, an ASPEN Plus process simulation model was developed to predict plant material and energy balances, utility requirements, operating and capital costs at varying design conditions. This paper compares mild hydrocracking and fluid catalytic cracking as alternative methods for upgrading the F-T wax.

FISCHER-TROPSCH PLANT DESIGN

Plant Configurations

Figure 1 is a block flow diagram showing the overall process configuration for the original design using mild hydrocracking. The plant contains three main processing areas. Area 100 generates a clean syngas from Illinois No. 6 coal from the Burning Star mine. Area 200 is the Fischer-Tropsch (F-T) synthesis area, and Area 300 is the product upgrading and refining area. Areas 100 and 200 are identical for both the mild hydrocracking and fluid catalytic cracking (FCC) cases. Utility plants and storage requirements in the offsites were estimated, but they are not detailed here.

1. **Area 100 - Syngas Production** -- Synthesis gas is generated in Shell gasifiers from ground, dried coal. Processing of the raw synthesis gas from the gasifiers is conventional, with Wet Scrubbing followed by single-stage COS/HCN Hydrolysis and Cooling, Acid Gas Removal by inhibited amine solution and Sulfur Polishing. *Sour Water Stripping and Sulfur Recovery units are included in this area.*
2. **Area 200 - The Fischer-Tropsch Synthesis Loop** -- This area includes the Fischer-Tropsch Synthesis, CO₂ Removal, Recycle Gas Compression and Dehydration, Hydrocarbon Recovery by deep refrigeration, Hydrogen Recovery and Autothermal Reforming. The Hydrocarbon Recovery unit includes deethanization, depentanization, fractionation and an oxygenates wash column. At low H₂/CO ratios, CO₂ is the primary byproduct of the F-T reaction (using an iron based catalyst) so a large CO₂ removal unit is required. The Autothermal Reformer converts the unrecovered light hydrocarbons to additional syngas which is recycled back to the F-T synthesis reactors.
3. **Area 300 - Product Upgrading**
Hydrocracking Design -- Figure 2 is a block flow diagram of Area 300 of the mild hydrocracking design. This area contains eight processing steps: 1) wax hydrocracking, 2) distillate hydrotreating, 3) naphtha hydrotreating, 4) naphtha reforming, 5) C₄ isomerization, 6) C₅/C₆ isomerization, 7) C₃/C₄/C₅ alkylation, and 8) saturated gas processing and product blending. The hydrocracked and hydrotreated naphthas are catalytically reformed to produce an aromatic gasoline blending component. The lighter materials are isomerized and alkylated to produce a high quality gasoline blending stock. Purchased butanes are required to alkylate all the available C₃/C₄/C₅ olefins.

Fluid Catalytic Cracking Cases -- Figure 3 is a block flow diagram of Area 300 for the Fluid Catalytic Cracking (FCC) cases. Two FCC upgrading cases are considered; one uses a beta zeolite cracking catalyst, and the other uses an equilibrium USY cracking catalyst. In these cases, the wax hydrocracker is replaced by a FCC unit, a MTBE (methyl-tertiary-butyl ether) plant, and a NExTAME (mixed C₅/C₆/C₇ ethers) plant. The other seven processing plants are unchanged.

The F-T slurry reactor is a bubble column reactor in which the slurry phase is a mixture of liquid hydrocarbons (molten wax) and catalyst. Synthesis gas provides the agitation necessary for good mixing and mass transfer of the reactants and products between the two phases. The slurry bed reactor design was chosen over a fixed bed reactor design based on an earlier DOE sponsored Bechtel study^{1,2}. The reactor design is based on Mobil's two-stage, slurry reactor pilot plant studies³. These results were the basis for the yield correlations contained in the F-T slurry bed reactor computer model used in this study⁴. Details concerning the overall design basis, process selection, and costs have been reported⁵.

Product and Byproduct Yields

A Fischer-Tropsch liquefaction facility can produce a wide variety of products of various qualities depending on the method used to upgrade the F-T wax.

In the mild hydrocracking case, the facility produces C₃ LPG, an upgraded C₅-350 °F naphtha and a 350-850 °F distillate. Liquid sulfur also is produced by the syngas production area. The hydrocarbon products have no measurable sulfur or nitrogen contents. Oxygen is removed to less than 30 ppmv. There are virtually no aromatics in the distillate. Both the naphtha and distillate products have low

residual olefin concentrations. The diesel fraction has a very high cetane number. The jet fuel and heavy distillate fractions have low smoke points. The naphtha product is a mixture of C3/C4/C5 alkylate, C5/C6 isomerate and catalytic reformate. It is basically a raw gasoline with a clear (R+M)/2 octane of about 88.

In the FCC upgrading cases, the facility produces a propylene product in addition to those produced in the hydrocracking case. Methanol is purchased and reacted with the tertiary C4, C5, C6 and C7 olefins to produce MTBE and a mixed C5/C6/C7 ethers stream from the NExTAME etherification plant. The ether streams are mixed with the C5-350 °F naphtha to form an oxygenated gasoline blending component which contains significant amounts of olefins and has higher octane numbers than in the mild hydrocracking case. Except for a lower pour point, the distillate fraction has about the same properties as that produced in the hydrocracking case.

PROCESS SIMULATION MODEL

The ASPEN Plus process flowsheet simulation model predicts the effects of key process variables on the overall material and utility balances, operating requirements and capital costs. It was developed as a planning/research guidance tool for use by the DOE and its subcontractors to explore, evaluate and define additional promising areas for future research in the production of liquid transportation fuels. The model is not a detailed plant design tool although it contains some design features. The F-T synthesis loop design is modeled in some detail, and Bechtel's slurry bed F-T reactor sizing and yield models have been incorporated into the ASPEN model. For the other plants, only overall yield, utility requirements and capital costs are estimated. Individual plant costs are prorated on capacity using cost-capacity exponents in conjunction with minimum and maximum single train capacity limits.

All plants in the three main processing sections are simulated either by stand-alone user Fortran blocks or a combination of ASPEN Plus process blocks and user Fortran blocks. Material balances, as well as utility consumptions, operating personnel requirements and ISBL costs for each plant are generated. The offsites, engineering and contingency costs are estimated as a percentage of the processing plant costs to generate the total installed cost of the facility. Detailed discussions of the ASPEN model development and simulation results have been presented in three separate papers⁶⁻⁸; the last of which discusses the beneficial effect of treating the F-T reactor vapor products in a close-coupled ZSM-5 reactor as an alternative product upgrading scheme.

A linear programming (LP) model of a typical PADD II refinery was developed using Bechtel Corporation's proprietary Process Industry Modeling System (PIMS) to assess the values of the F-T products from the mild hydrocracking case⁹. With the ASPEN and LP model results, a discounted-cash-flow analysis was carried out under a given set of financial assumptions to calculate the cost of F-T production for a 15% return on investment. Results are presented in terms of a Crude Oil Equivalent (COE) price which is defined as the hypothetical break-even crude oil price at which the liquefaction products are competitive with those produced from crude oil. Table 1 summarizes the overall simulation model results for the mild hydrocracking case and the two FCC upgrading cases; one of which uses a beta zeolite cracking catalyst, and the other uses an equilibrium USY cracking catalyst.

FLUIDIZED-BED CATALYTIC CRACKING OF F-T WAX

Fischer-Tropsch wax can be readily cracked in a FCC unit under normal petroleum feedstock operating conditions, as demonstrated by the Amoco Oil Company¹⁰. The product is rich in C4 to C7 reactive olefins which are valuable for oxygenates production. The hydrocracking design and the ASPEN Plus simulation model were modified to use FCC instead of mild hydrocracking for upgrading the F-T wax. In addition, both a MTBE plant and a NExTAME (mixed C5/C6/C7 ethers) plant were included in Area 300. Both other plants contain an associated selective hydrogenation unit to saturate diolefins in the feed.

Based on the Amoco data, two FCC cases were considered; a beta zeolite catalyst case and an equilibrium USY catalyst case. Although not in widespread commercial use, beta zeolite catalyst was selected for comparison with an equilibrium USY catalyst since it produces more olefins which can be converted to ethers for use as reformulated gasoline blending components. The propylene is purified and sold. The butenes are sent to the MTBE (methyl-tertiary-butyl ether) plant in which the isobutene is converted to MTBE, and the normal butenes are passed through to the alkylation unit. The C5, C6 and C7 olefins are sent to a NExTAME unit which converts most of the C5 olefins, less of the C6 olefins, and still less of the C7 olefins to ethers. This design produces significantly more gasoline blending components at the expense of distillate production than the hydrocracking design.

Amoco found that the F-T wax cracks so easily in a FCC unit that it does not produce enough coke to maintain the unit in heat balance. One solution to this problem is to supply additional fuel, sometimes called torch oil, to the regenerator to heat the regenerated catalyst to a high enough temperature to sustain the cracking operation. In a conventional petroleum refinery whenever torch oil is required, a low-value heavy material is used. However, in this stand-alone situation, no high-boiling low-valued streams are available from sources other than the FCC unit. Therefore, the heaviest portion of the potential distillate product is used as torch oil and burned in the regenerator to maintain the FCC unit heat balance.

Table 1 compares the model results for the wax hydrocracking case with those for the two FCC wax upgrading cases. In the hydrocracking case, approximately 3100 bbls/day of butanes are purchased and

isomerized for alkylation unit feed since the F-T reaction does not produce a sufficient amount to alkylate all the C3/C4/C5 olefins. The two FCC cases produce more olefins for alkylation unit feed, and as a result, still more butanes have to be purchased. Both FCC cases produce significantly more gasoline than the hydrocracking case. This additional gasoline is produced at the expense of distillate production which is reduced by over 60% resulting in gasoline to distillate ratios of over 4/1 compared to a 0.97/1 ratio for the wax hydrocracking case. In addition, the gasoline products are of better quality. They now contain oxygenates and have higher octanes, lower Reid vapor pressures, and contain less aromatics.

ECONOMIC COMPARISON

The predicted installed cost of each case is just under 3 billion dollars in mid-1993. The FCC upgrading cases have somewhat higher capital costs because of a larger alkylation plant, and the cost of the FCC plant and two etherification plants are more than the hydrocracker. These are preliminary cost estimates and have an accuracy range of +/- 30%. Most of the cost is in the syngas preparation and F-T synthesis areas. For the hydrocracking case, the entire product upgrading and refining area accounts for less than 8% of the ISBL cost.

A discounted-cash-flow economic comparison of the three cases was made using the spreadsheet program with previously reported economic assumptions⁸. Inflation projections are those of the Energy Information Administration¹¹. Results are reported in terms of a Crude Oil Equivalent (COE) price which is the hypothetical break-even crude oil price at which the F-T liquefaction products are competitive with those produced from crude oil in an average PADD II refinery.

The hydrocracking case has an expected COE price of 35.4 \$/bbl. The expected COE prices for the two FCC upgrading cases are the same at 34.5 \$/bbl. These COE prices were calculated using the same margins for the gasoline and diesel blending stocks that were calculated for the hydrocracking case at the typical PADD II refinery. The gasoline blending stocks produced in these two FCC upgrading cases are of better quality than those from the hydrocracking case and should be more valuable. However, the COE calculations for the two FCC cases did not account for this expected increased value. Thus, the calculated COE prices for both FCC cases are conservative in the sense that they are somewhat higher than they should be because the products probably are undervalued. In order to accurately evaluate these two FCC upgrading cases, additional refinery LP modeling studies are required to assess the value of these blending stocks properly, and they will be done under another DOE contract.

In addition, there is another significant difference between the beta zeolite and equilibrium USY catalyst cases which can influence the choice between them. Both FCC upgrading cases consume methanol and produce a propylene product; whereas neither component is present in the hydrocracking case. The beta zeolite catalyst case consumes about 54% more methanol and produces about 57% more propylene than the equilibrium USY catalyst case. For 1995, propylene prices have ranged between 350 and 495 \$/s-ton, and methanol prices have ranged at least between 0.47 and 1.35 \$/gal (141 to 406 \$/s-ton)¹². The above expected COE prices were calculated using the average propylene price of 422.5 \$/s-ton and the average methanol price of 0.91 \$/gal (273 \$/s-ton). The following table shows the effect of these variations in the methanol and propylene prices on the COE price for the two FCC upgrading cases.

	Most Optimistic	Average	Most Pessimistic
Propylene price, \$/ton	495	422	350
Methanol price, \$/ton	141	273	406
<u>COE Prices, \$/bbl</u>			
Beta zeolite catalyst FCC upgrading case	33.2	34.5	35.8
Equilibrium USY catalyst FCC upgrading case	33.7	34.5	35.3

Thus, the COE price for the beta zeolite catalyst FCC upgrading case can vary between 33.2 and 35.8 \$/bbl, a range of 2.6 \$/bbl. For the equilibrium USY catalyst case, the COE price can vary between 33.7 and 35.3 \$/bbl, a smaller range of only 1.6 \$/bbl. This leads to the conclusion that with all other factors being the same, the equilibrium USY catalyst FCC upgrading case is less risky based on recent prices since it minimizes the effect of price variations on the expected COE price.

In conclusion, FCC upgrading of the F-T wax appears to be preferable to upgrading it by mild hydrocracking. Recent wide variations in methanol and propylene prices have been shown to cause significant fluctuations in the COE price of the F-T liquefaction products. Additional petroleum refinery modeling studies are needed to determine more accurately the values of the FCC upgraded products and to define a more reliable COE price for both of the FCC indirect F-T liquefaction cases. It is expected that this will improve the economics of upgrading the F-T wax by fluid catalytic cracking.

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TABLE 1
Comparison of Mild Hydrocracking and Fluid
Catalytic Cracking Upgrading of Fischer-Tropsch Wax

Wax Upgrading Mode FCC Catalyst Type	Method of Upgrading the F-T Wax		
	Hydrocracking	FCC 1	FCC 2
	Hydrocracking	FCC	FCC
	--	Beta	Equilibrium
		Zeolite	USY
<u>Plant Input:</u>			
ROM Coal, TSD (MF)	18575	18575	18575
Methanol, TSD	0	321	209
Mixed Butanes, BSD	3110	5204	4327
Electric Power, Mwatts	54	58	56
<u>Plant Output:</u>			
Gasoline, BSD	23943	39723	39950
Distillate, BSD	24686	9764	9347
Propylene, BSD	0	5060	3215
Liquid Propane, BSD	1922	1573	1584
Sulfur, TSD	560	560	560
Slag, TSD (MF)	2244	2244	2244
Total Net C5+ Production, BSD	48629	49487	49297
Total Net C4+ Production, BSD	45519	44283	44970
<u>Blended Gasoline Properties:</u>			
Research Octane Number	90.9	96.8	95.8
Motor Octane Number	86.1	88.9	87.8
(R+M)/2 Octane Number	88.5	92.8	91.8
Reid Vapor Pressure, psi	5.0	4.7	4.7
Benzene, wt%	0.3	0.1	0.1
Aromatics, wt%	28.1	11.0	13.9
Olefins, wt%	0.0	12.7	15.5
Oxygen, wt%	0.0	3.3	2.1
<u>Blended Distillate Properties:</u>			
Pour Point, °F	-28	-40	-40
Cetane Index	74	74	74
Installed Plant Cost, MM\$ in mid-1993	2964	2987	2978

Figure 1
 Indirect Coal Liquefaction Baseline Study
 Overall Process Configuration

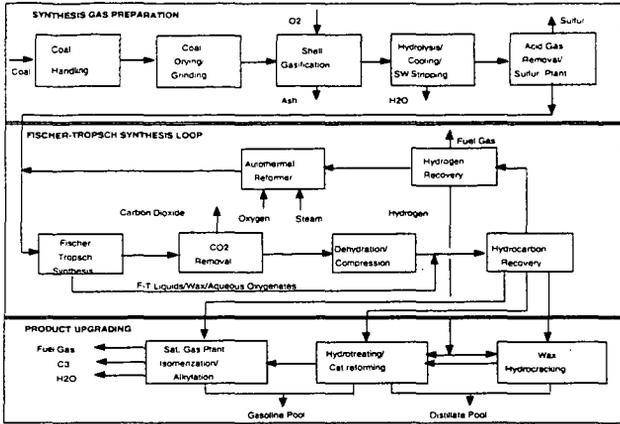


Figure 2
 Area 300 Block Flow Diagram - Baseline Design With Wax Hydrocracking

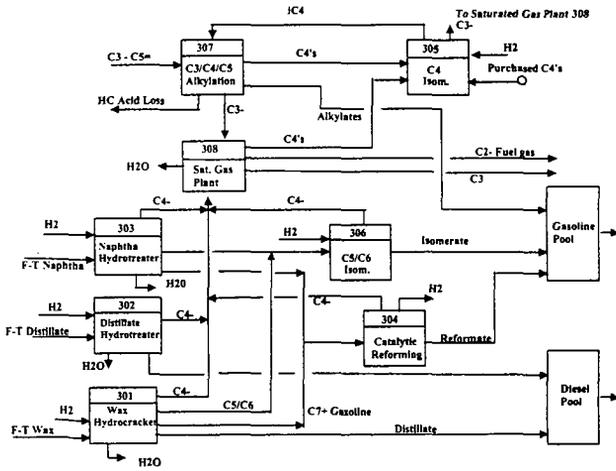


Figure 3
 Area 300 Block Flow Diagram - Fluid Catalytic Cracking

