

TITLE: ECONOMICS OF ADVANCED INDIRECT LIQUEFACTION PROCESSES

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OBJECTIVE:

The objectives of this work are to estimate the cost of production of high quality liquid transportation fuels from advanced coal-based indirect liquefaction processes and to determine the economic impact of coproducing electric power using the once-through Fischer-Tropsch (OTFT) concept.

TECHNICAL APPROACH:

Previous MITRE studies have shown the potential of advanced entrained gasifiers and slurry-phase Fischer-Tropsch (F-T) synthesis processes to significantly improve the efficiency and reduce the costs of indirect liquefaction plants compared to the SASOL technology commercialized in South Africa.^(1,2) The overall economics are very sensitive to the production of light hydrocarbon gases (methane and ethane), and therefore gasifiers and F-T synthesis conditions that produce less of these components are economically preferred. Production of large quantities of wax followed by selective hydrocracking to middle distillate product is a practical method of reducing methane and ethane, and overcoming the Schultz-Flory selectivity limitations. The present MITRE study is an extension of the previous studies and represents the most detailed computer model so far developed at MITRE for the evaluation of indirect liquefaction.

Figure 1 shows the components of the MITRE indirect coal liquefaction model of the baseline case for a conceptual commercial plant producing liquid fuels. The baseline plant consists of three totally integrated sections. The first section simulates the preparation of clean synthesis gas using Shell gasification of coal, the second section simulates the F-T synthesis, and the third section the upgrading of raw F-T products, including wax, to gasoline and diesel. The model is totally integrated

from input coal to finished products and contains all necessary off-sites for a grassroots facility. Figure 2 shows details of the Shell entrained coal gasification facility and gas cleanup section. Raw gas exits the gasifier at about 2700°F and is cooled with recycle gas to be below the ash deformation temperature. High pressure steam is produced in the gasifier waste heat boiler (WHB), and the cooled gas is scrubbed to remove fly ash. After raw shift and COS hydrolysis, the gas is treated with a Selexol system to remove H₂S and some CO₂. Sulfur is recovered using a Claus process, and the tail gas is treated with a SCOT unit. The clean gas containing about 1 ppm of sulfur is then polished with ZnO to obtain an ultraclean gas with 0.06 ppm total sulfur to protect the F-T catalyst.

Figure 3 shows details of the slurry phase F-T reactor including wax separation facilities. Figure 4 shows the details of the F-T recycle gas loop. The effluent gases from the F-T reactor that include light hydrocarbons and unconverted CO and H₂ are sent to a Benfield CO₂ removal system, hydrocarbon recovery unit and hydrogen recovery unit before being autothermally reformed back to synthesis gas and recycled to the F-T reactor. In this way all hydrocarbon gases are reformed, and the plant produces only liquid products.

Figure 5 shows the details of the raw F-T product upgrading and refining section of the conceptual plant. Raw liquid product is fractionated to produce a light stream C₅ for polymerization and a naphtha (C₈ - C₁₁) and diesel (C₁₂ - C₁₈) stream for hydrotreating and reforming. The wax (C₁₉⁺) is selectively hydrocracked to produce additional middle distillate and naphtha.

Table 1 lists the parameters used in the development of the baseline plant. In the syngas preparation section, 30,000 TPD of moisture-free Illinois #6 coal are gasified in Shell gasifiers. Data on the gasifier performance obtained from Shell were used to verify the results of the MITRE gasification model.⁽³⁾ The synthesis gas was cleaned to 0.06 ppm sulfur and adjusted to have a H₂ to CO molar ratio of 0.67 before entering the synthesis reactor. The F-T synthesis section used slurry-phase reactors sized to be the same as recommended by Mobil.⁽⁴⁾ Catalyst activity and selectivity data were obtained from results obtained by Kuo.⁽⁵⁾ Hydrodynamic data on the performance of slurry reactors were obtained from several sources notably from Kölbel,⁽⁶⁾ Farley and Ray,⁽⁷⁾ and Bukur.⁽⁸⁾ Raw product refining data were obtained from Mobil⁽⁹⁾ and SASOL, and wax hydrocracking data were obtained from UOP.⁽¹⁰⁾

Table 2 lists the characteristics of the MITRE indirect liquefaction simulation model, and Table 3 lists the sensitivities that can be performed and the parameters that can be investigated using the model.

Since an objective of this present study is to investigate the economic potential of Once-Through F-T (OTFT) with coproduction of electric power, it was necessary to extend the baseline model to include combined-cycle electric power generation units. The OTFT plant includes gas turbine packages (combustors, gas turbines and generators), heat recovery steam generators, and extraction-induction-condensing steam turbines with generators. Performance data on combined cycle systems was obtained from EPRI.⁽¹¹⁾ In the OTFT mode, the synthesis gas is passed once through the F-T reactors, and the unconverted gas and various lower carbon number hydrocarbons are combusted in the gas turbines to produce electric power.

In order to determine a value for the cost of electricity produced from a coal gasification/combined cycle plant, the model was further modified to eliminate the F-T synthesis and upgrading section. The resultant coal gasification/combined cycle model was then used to develop realistic costs of electric power that will be used in the OTFT coproduction cost models.

The economic section of the model provides estimates of the plant construction cost, total plant capital required, operating costs, and required selling prices (RSP) of the products. Details of the economic section are similar to those described in previous MITRE reports. (12)

SIGNIFICANT ACCOMPLISHMENTS:

The MITRE model has been used to investigate the performance and economics of the baseline case, combined cycle only and of several OTFT cases with cogeneration of electric power. Figure 6 summarizes the material flows that result from application of the model to the baseline case. After upgrading the raw F-T products approximately 83,000 BPD of refined liquid fuels are produced. Figure 7 illustrates the transformation of coal into products at several stages during the indirect processing. Overall efficiency to liquid products is seen to be about 56 percent.

The economics of the baseline plant are summarized in Tables 4, 5, 6, and 7. Total capital for the plant is estimated at about \$4,411 million (1986) and net annual operating cost at about \$420 million. Using economic parameters of 25 percent equity, 15 percent return on equity, 8 percent debt interest, and 3 percent general inflation, the required selling price of liquid products is about \$45 per barrel. This is equivalent to crude at about \$35/Bbl.

Table 8 lists the cases analyzed in this paper in addition to the all-liquid product F-T baseline case. The gasification/combined cycle case was analyzed to develop a cost of electric power. Three OTFT cases were examined. In OTFT case 1, the off-gases from the F-T synthesis (this included unconverted synthesis gas, and hydrocarbon gases from C_1 to C_4) were sent to the gas turbine combustor to produce electric power. The C_5^+ liquids were refined as in the baseline case. This case produced about 950 MW of electricity. In OTFT case 2, the selectivity of the F-T product was changed to produce only 6 wt percent liquid wax. A hot separator after F-T synthesis was used to produce a C_8^+ liquid product that was sold as diesel in an unrefined state. The C_8^- material was burned in the gas turbine combustor to produce electric power. In this case approximately 1900 MW of electricity was coproduced. In OTFT case 3, a cold separator was used to save the C_7 hydrocarbons and alcohols, and the lower hydrocarbons were sent to electric power production. In this case approximately 1600 MW of power were produced.

Figure 8 is a block flow diagram of the OTFT concept used in the model. Figures 9, 10, and 11 show the material flows for the three OTFT cases analyzed. Table 9 summarizes the economics of OTFT cases 1 and 2 and compares their economics to that of the baseline case. In all of these cases the price obtained for electric power is that developed from the 1000 MW coal gasification/combined cycle plant and is 0.0534 \$/KWhr.

Figure 12 shows the sensitivity of liquid cost in dollars per barrel equivalent crude to the market value of coproduced electric power. As electric power value increases, the plants producing more electricity will be able to sell liquid fuels at lower cost to meet the required annual revenue.

The reference power values shown on Figure 12 are the required selling prices for combined cycle power plants designed by MITRE using the same technical and economic assumptions as were used for the Fischer-Tropsch plants. These costs are \$.0534, \$.0452, and \$.0402 per KWhr for plants sized to produce 1000, 2000, and 3300 MW respectively. The 3300 MW plant would consume the same 30,000 ton/day of dry coal feed as the combined cycle/F-T plants previously presented.

The economic impact of using utility financing assumptions for the power production portion of the cogeneration plants will be considered in the ongoing study.

REFERENCES

1. Gray, D., M. Lyton, M. B. Neuworth, and G. C. Tomlinson. *The Impact of Developing Technology on Indirect Liquefaction*. MITRE Report MTR80W326, November 1980.
2. Gray, D., M. B. Neuworth, and G. C. Tomlinson. *Further Studies on Developing Technology for Indirect Liquefaction*. MITRE Report MTR82W32, March 1982.
3. *Evaluation of U.S. Coal Performance in the Shell Coal Gasification Process (SCGP)*. Volume 2: *Illinois No. 5 Seam Coal*. Report prepared for EPRI by Shell Oil Company. EPRI AP-2844, Vol. 2, February 1984.
4. Kuo, J. C. W. *Two-Stage Process for Conversion of Synthesis Gas to High Quality Transportation Fuels*. Report prepared for DOE by Mobil Research and Development Corporation. DOE/PC/60019-9, October 1985.
5. Kuo, J. C. W. *Slurry Fischer-Tropsch/Mobil Two-Stage Process of Converting Syngas to High Octane Gasoline*. Report prepared for DOE by Mobil R&D Corporation. DOE/PC/30022-10, June 1983.
6. Kölbel, H. and M. Ralek. "The Fischer-Tropsch Synthesis in the Liquid Phase." *Catalysis Reviews, Sci. Eng.*, 21(2), 225-274, 1980.
7. Farley, R. and D. J. Ray. "The Design and Operation of a Pilot-Scale Plant for Hydrocarbon Synthesis in the Slurry Phase." *Journal of Inst. of Pet.*, Vol. 50, Number 482, February 1964, p. 27.

8. Bukur, D. B., J. G. Daly, S. A. Patel, M. L. Raphael, and G. B. Tatterson. *Hydrodynamics of Fischer-Tropsch Synthesis in Slurry Bubble Column Reactors*. Report prepared for DOE by Texas A&M University, Department of Chemical Engineering. DOE/PC/10027-10, June 1987.
9. Schreiner, M. *Research Guidance Studies to Assess Gasoline from Coal by Methanol-to-Gasoline and SASOL-Type Fischer-Tropsch Technologies*. Report prepared for DOE by Mobil R&D Corporation. FE-2447-13, August 1978.
10. Shah, P. P., G. C. Sturtevant, J. H. Gregor, M. J. Humbach, F. G. Padra, and K. Z. Steigleder. *Fischer-Tropsch Work Characterization and Upgrading*. Report prepared for DOE by UOP and Allied-Signal EMRC. DOE/PC/80017-T1, June 6, 1988.
11. *Shell-Based Gasification - Combined Cycle Power Plant Evaluations*. Report prepared for EPRI by Fluor Engineers Inc. EPRI AP-3129, June 1983.
12. Gray, D. and G. C. Tomlinson. *Assessing the Economic Impact of Two-Stage Liquefaction Process Improvements*. MITRE Report WP87W00215. Published as Sandia Contractor Report SAND87-7147, August 1988.

PUBLICATIONS

David Gray and Glen Tomlinson, *Assessing the Economic Impact of Indirect Liquefaction Process Improvements: Volume I: Development of the Integrated Indirect Liquefaction Model and Baseline Case (Draft)*. MITRE Technical Report No. WP89W00144-I, June 1989.

"Economics of Direct and Indirect Liquefaction: Prospects for Cost Reduction through R&D." Briefing presented to the Committee on Production Technologies for Liquid Transportation Fuels, National Research Council, Energy Engineering Board, 9 June 1989.

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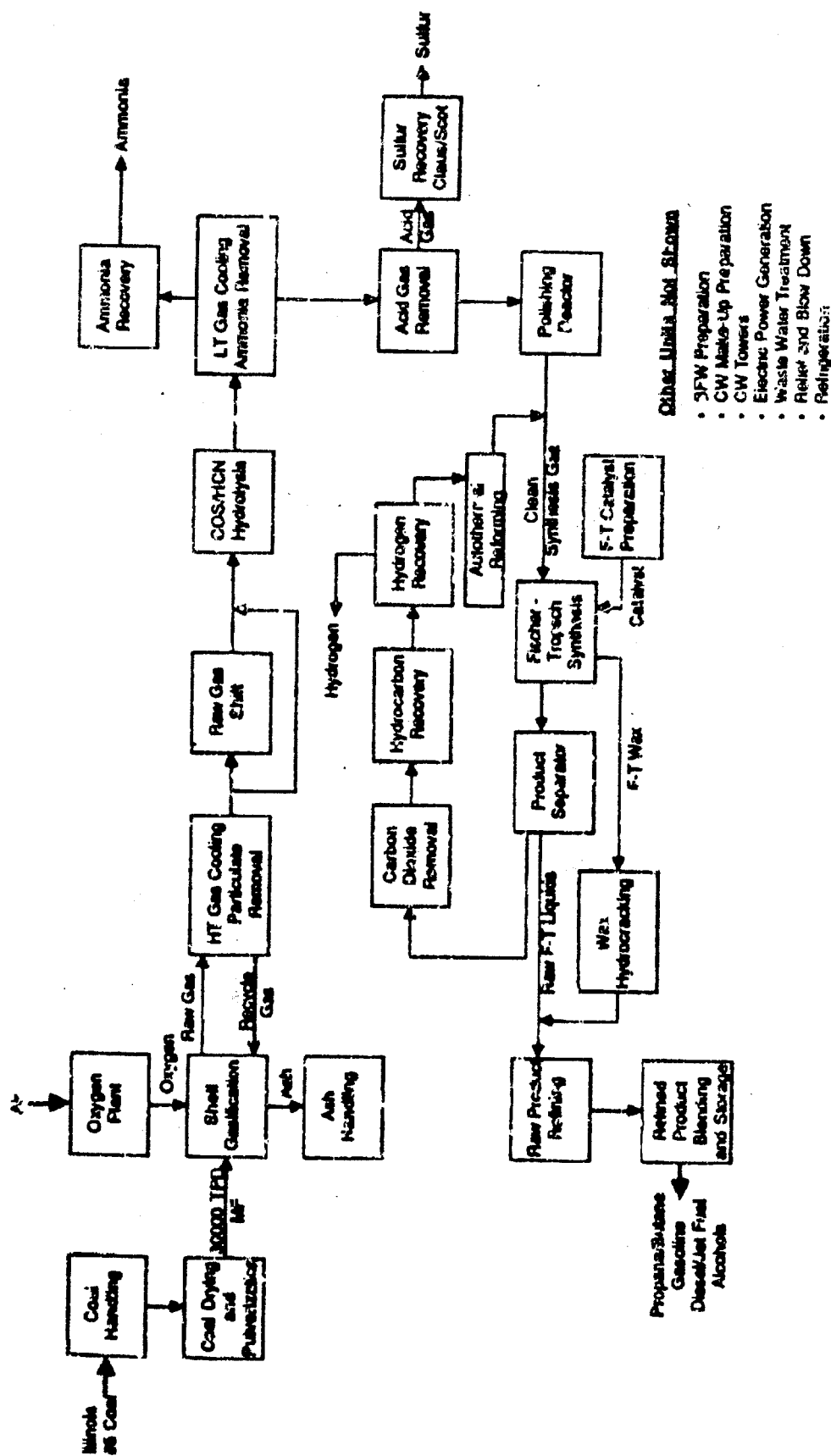


Figure 1
Components of MITRE Indirect Coal Liquefaction Model (Base Case)

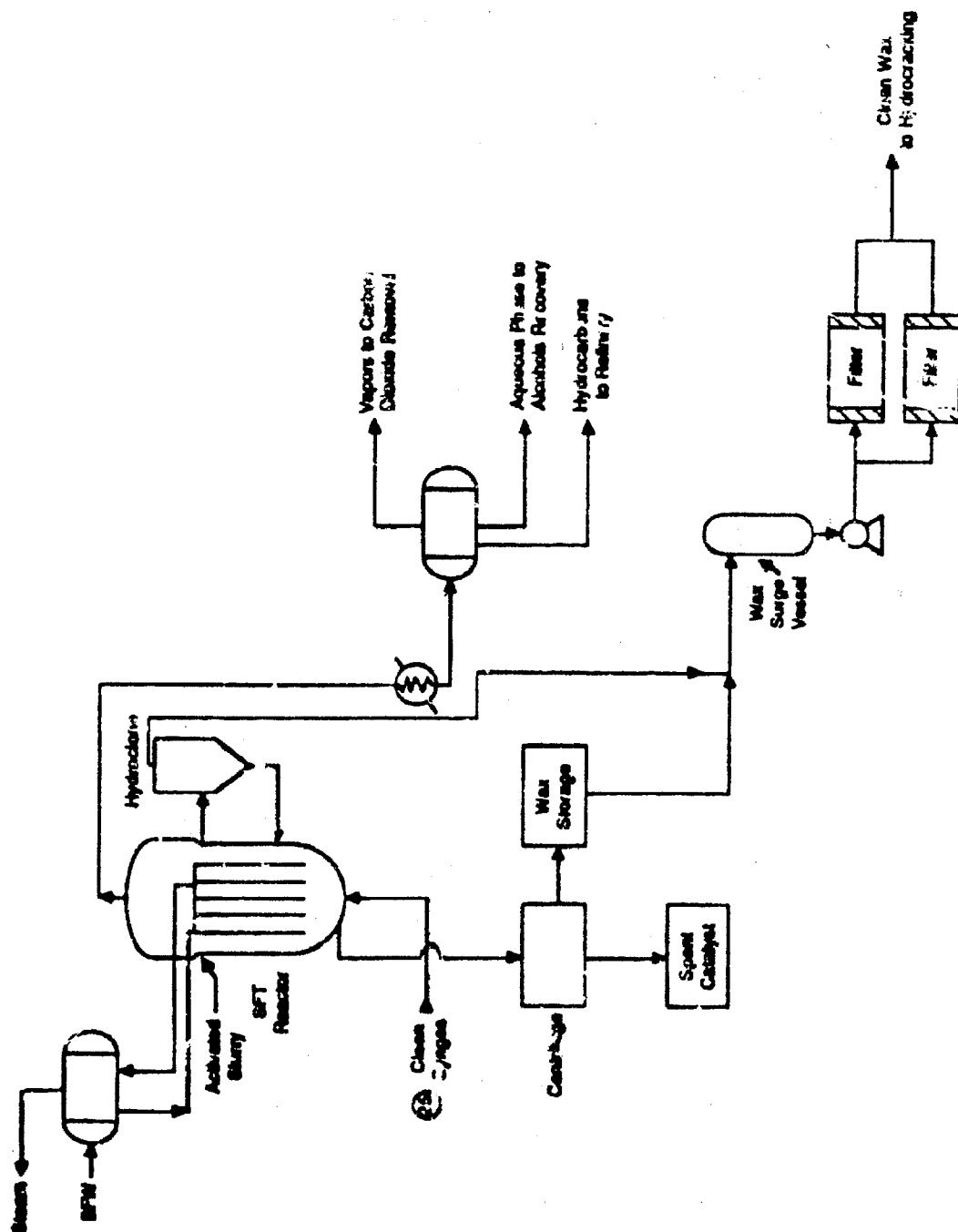
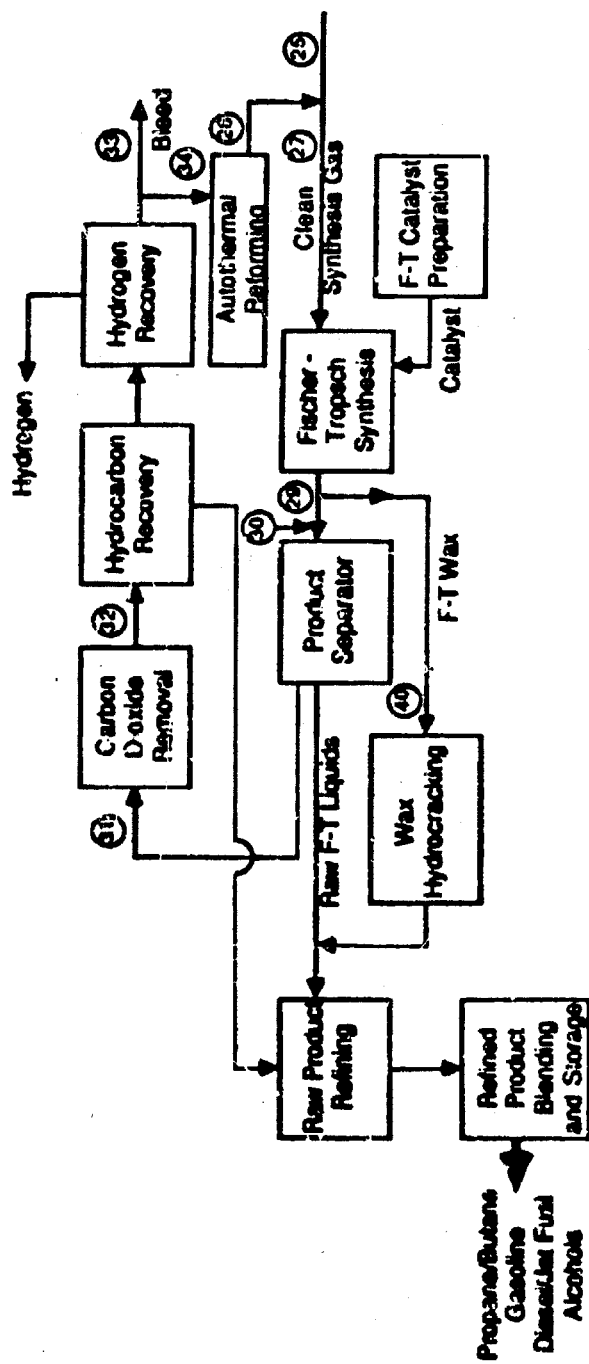


Figure 3
Detail of Slurry Fischer-Tropsch Reactor System



○ Stream numbers correspond to computer spreadsheet.

Figure 4
Fischer-Tropsch Recycle Loop Details

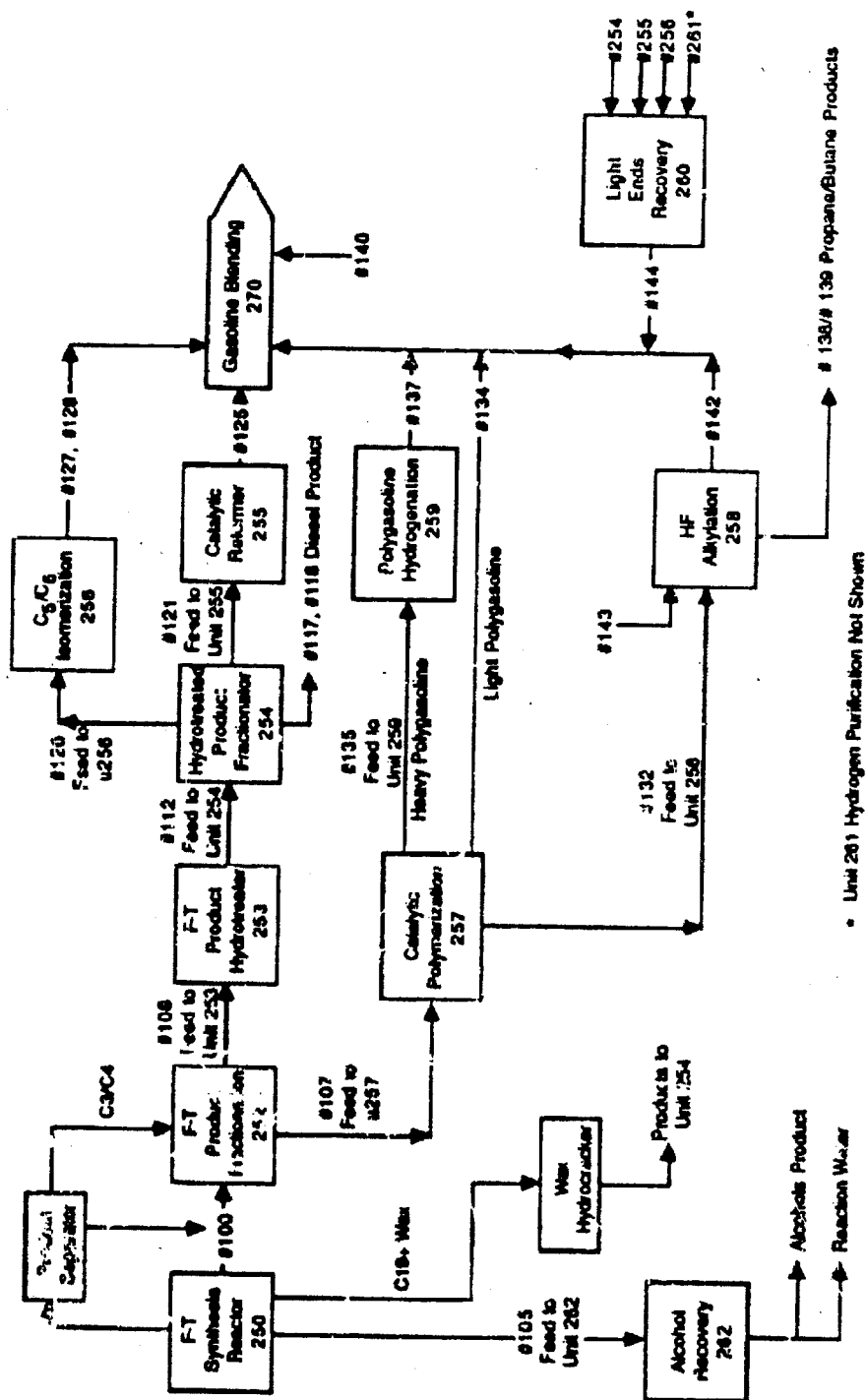


Figure 5
Raw Fischer-Tropsch Product Refining

Table 1
Baseline Plant Parameters Used

Syngas Preparation

- o Illinois #6 coal feed 30,000 TPD (MF).
- o Shell gasification 2500 TPD per gasifier.
- o Gasification coal feed 5 wt% moisture.
- o Overall carbon conversion in gasifiers 99%.
- o Radiant and convective waste heat boilers produce 1450 psi steam at 900°F.
- o Total sulfur in syngas feed to F-T units 0.06 ppm vol.
- o Carbon dioxide used as HP coal transport gas.
- o Feed gas H:CO molar ratio 0.67.

F-T Synthesis

- o Slurry Fischer-Tropsch reactor size 14.5 ft diameter by 35 ft high.
- o Catalyst ppt iron type at 16.7 wt percent loading.
- o Gas holdup correlation - Bach and Pilhofer.
- o CO + H₂ conversion per pass 90%.
- o Unconverted gases recycled.

Table 1
Baseline Plant Parameters Used - Concluded

- o First order reaction kinetics assumed to relate catalyst reaction rate constant to space velocity. Mobil bench-scale data used.
- o Overall heat transfer coefficient from Farley and Ray.

Refining

- o Wax hydrocracking data from UOP results on Mobil wax.
- o Other refining units are conventional practice at SASOL.

Plant Integration

- o Grassroots facility--all energy needs balanced.
- o All electric power generated on site.
- o No coal-fired steam generation used.

Table 2
Characteristics of Current Indirect Liquefaction
Simulation Model

- o Simulation is a totally integrated complete system model from input coal to finished products.
- o Model is grassroots; all power and energy requirements are generated within the system and all material, and energy needs are balanced.
- o Model is flexible enough to allow numerous sensitivities to be investigated, i.e., "what if" questions can be answered.
- o Model can be readily updated as new R and D information becomes available.
- o In the economic section financial assumptions can be easily changed.

Table 3
Sensitivities That Can Be Investigated
Using the Model

- o Coal Feedstock characteristics/coal feed rate/plant size.
- o H:CO ratio of synthesis gas, i.e., increase, decrease, or eliminate shift.
- o Change gas cleaning unit operations.
- o Change raw F-T selectivity.
- o Change F-T catalyst activity.
- o Change Slurry F-T reactor parameters: size, catalyst loading, relationship for gas holdup, superficial gas velocity, overall heat transfer coefficient, and pressure.
- o Raw F-T product refining configuration can be changed. Unit operations can be eliminated or new ones added.
- o Option to recycle unconverted syngas or once-through.
- o Option to autothermally reform C1/C2 gases.
- o Change wax hydrocracking selectivity.
- o Include gas turbine/steam turbine combined cycle system.
- o Eliminate F-T/Refining Section.

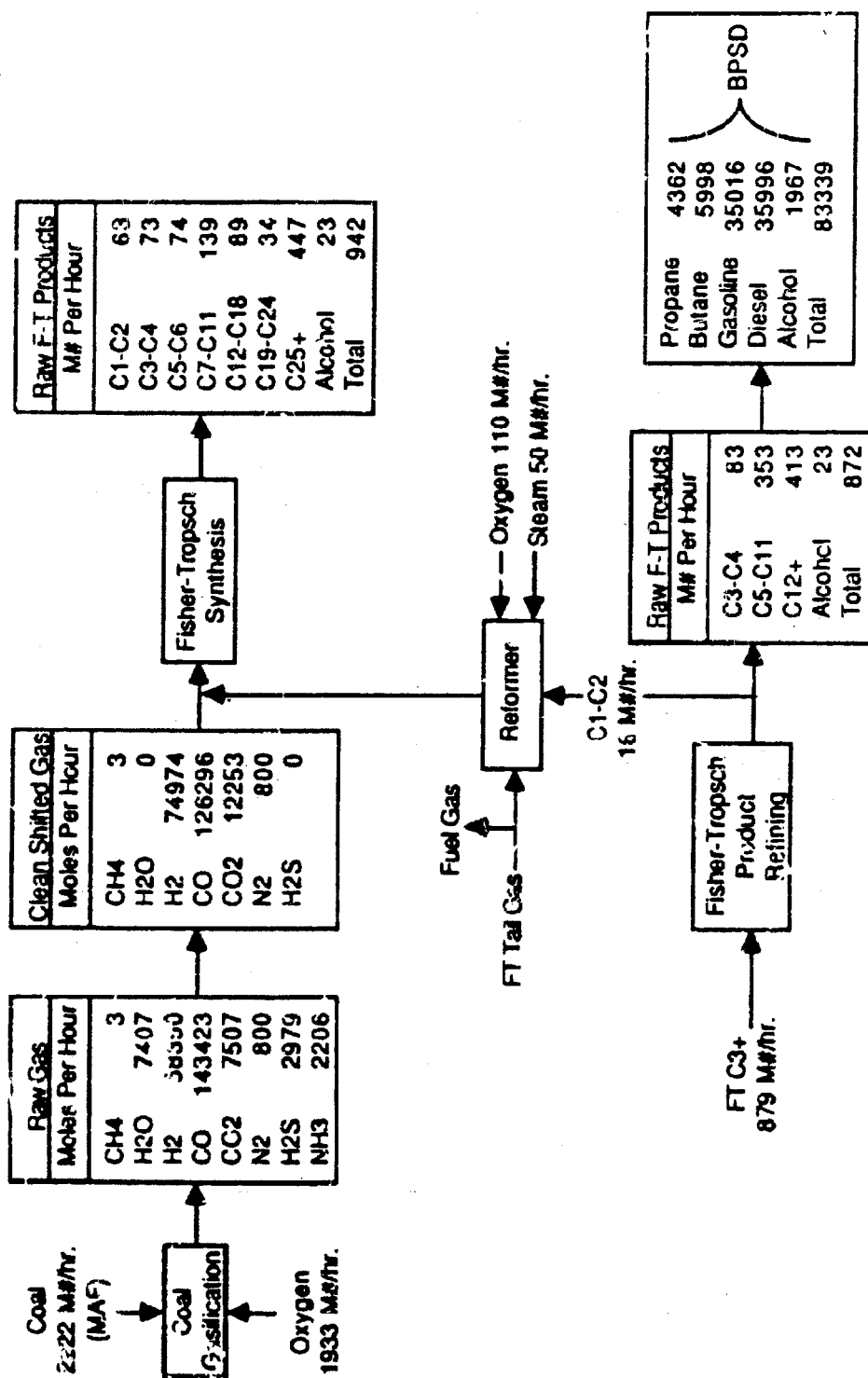


Figure 6
Summary of Materials Flows (Base Case)

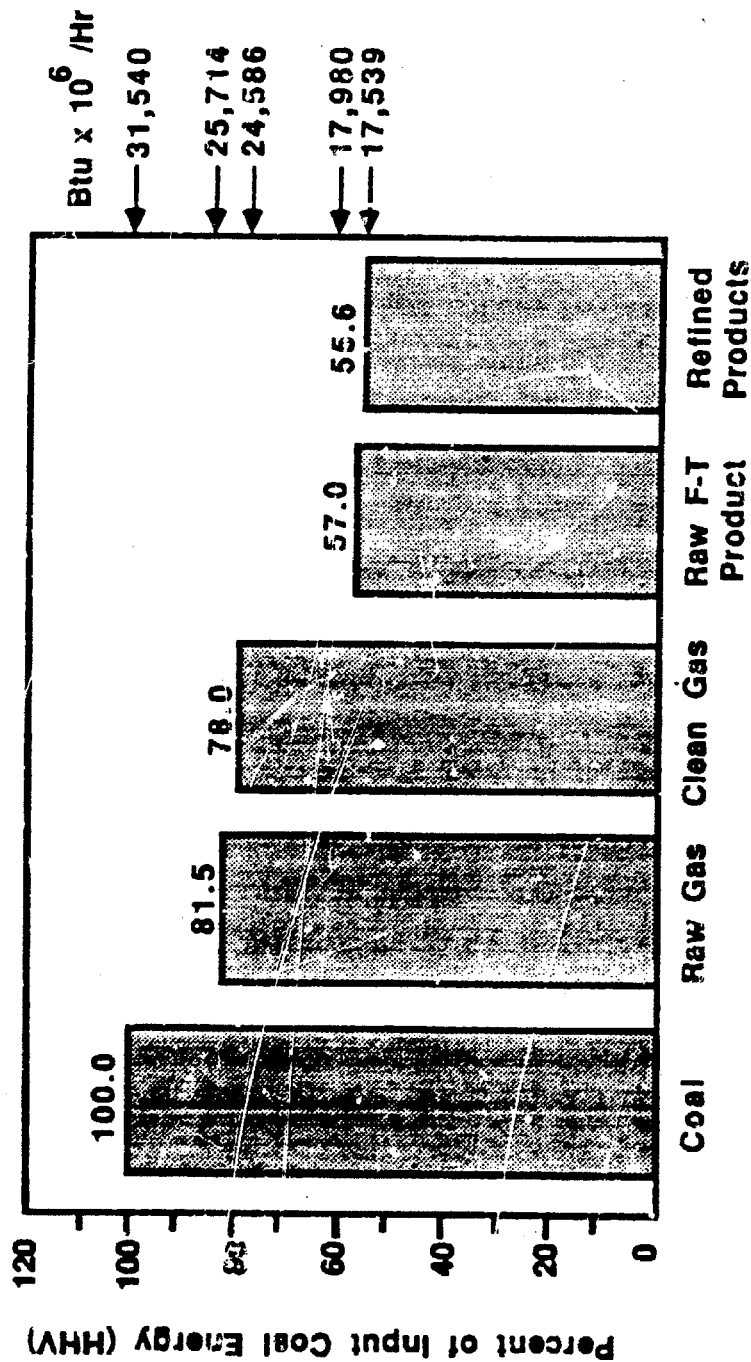


Figure 7
Percent of Coal Energy Remaining During
Transformation (Base Case)

Table 4
Baseline Plant Construction Cost Estimate
(\$MM 1986)

Clean Synthesis Gas Production	782.10
By-Product Recovery	65.27
Fischer-Tropsch Synthesis	523.07
F-T Product Refining	370.18
Oxygen Production	424.04
Coal Handling	188.51
Other Off-Sites	256.20
F-T Catalyst Preparation	40.46
Infrastructure & Miscellaneous	136.24
Autothermal Reforming	<u>48.29</u>
Total Construction Cost	<u>2,834.46</u>

Table 5
Capital Requirements (Baseline Plant \$MM)

Construction Cost	2,834
Engineering Design and Project Contingency	<u>709</u>
Total Plant Investment	3,543
Allowance for Funds Used During Construction	<u>599</u>
Total Depreciable Capital	4,142
Start-up Costs	104
Working Capital	131
Initial Charge of Catalyst & Chemicals	<u>34</u>
Total Non-Depreciable Capital	269
TOTAL CAPITAL REQUIRED	4,411

Table 6
Calculation of Gross and Net Operating Cost
(\$MM Per Annum) Baseline Plant

Coal Cost	258.78
Cat, Chem, Water	34.61
Other Operating	229.08
Total Gross Annual Operating Cost	522.47
By-Product Credit	105.10
Net Operating Cost	<u>417.37</u>

Table 7
Required Selling Price of Fuels for Baseline Case

	<u>\$/Bbl</u>	<u>\$/Gal</u>
C ₃ -C ₄ Valued @ \$4.70/MM Btu,*		
Other Fuels Equal on Volume Basis	45.17	1.07
Equivalent Crude	35.27	
ANNUAL REVENUE REQUIREMENTS		
Capital @ 0.167 CRF**	\$ 737 (64%)	
Coal @ \$22.7/Ton	259 (22%)	
Other O & M	<u>158 (14%)</u>	
TOTAL	\$1,154	

 *80% of Equivalent Crude Price, Btu Basis.

**CRF = Capital Recovery Factor.

Table 8
Cases Analyzed

1. Baseline F-T Case

- Shell gasification
- Gas cleaned to 0.06 ppm sulfur
- Slurry F-T synthesis
- Autothermal reforming of F-T offgases
- Refining of F-T products

2. Gasification/Combined Cycle Case

- Shell gasification
- Gas cleaned for 90% sulfur removal
- Gas turbine/steam turbine combined cycle plant

3. Once-Through F-T/Combined Cycle Cases

- No bleed, 50% wax, refining of C_5^+ (Case 1)
- No bleed, hot separator, 6% wax, C_8^+ product (Case 2)
- No bleed, cold separator, 6% wax, C_7^+ product and alcohols (Case 3)

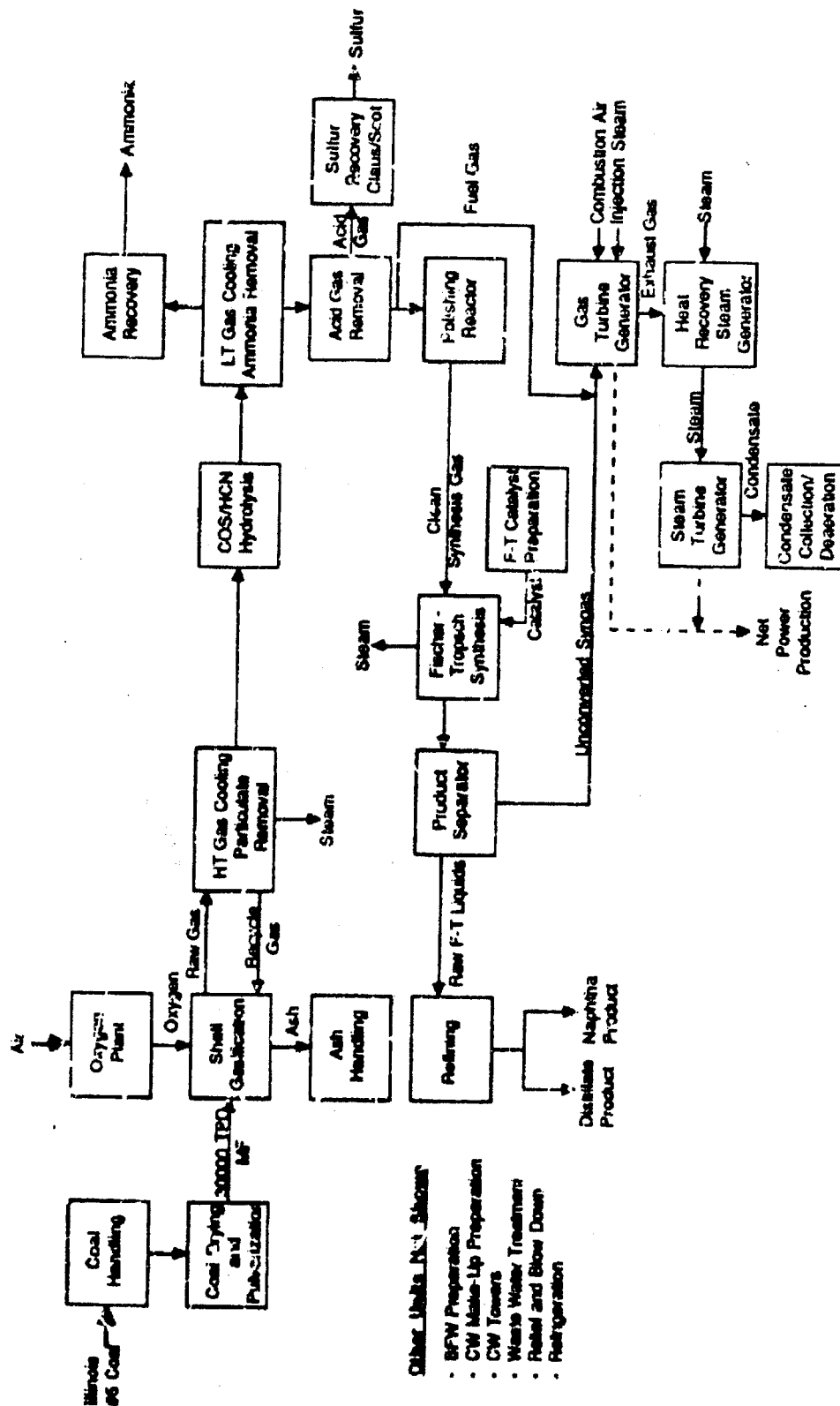


Figure 8
Overall Block Flow Diagram Once-Through Fischer-Tropsch
Electricity Generation

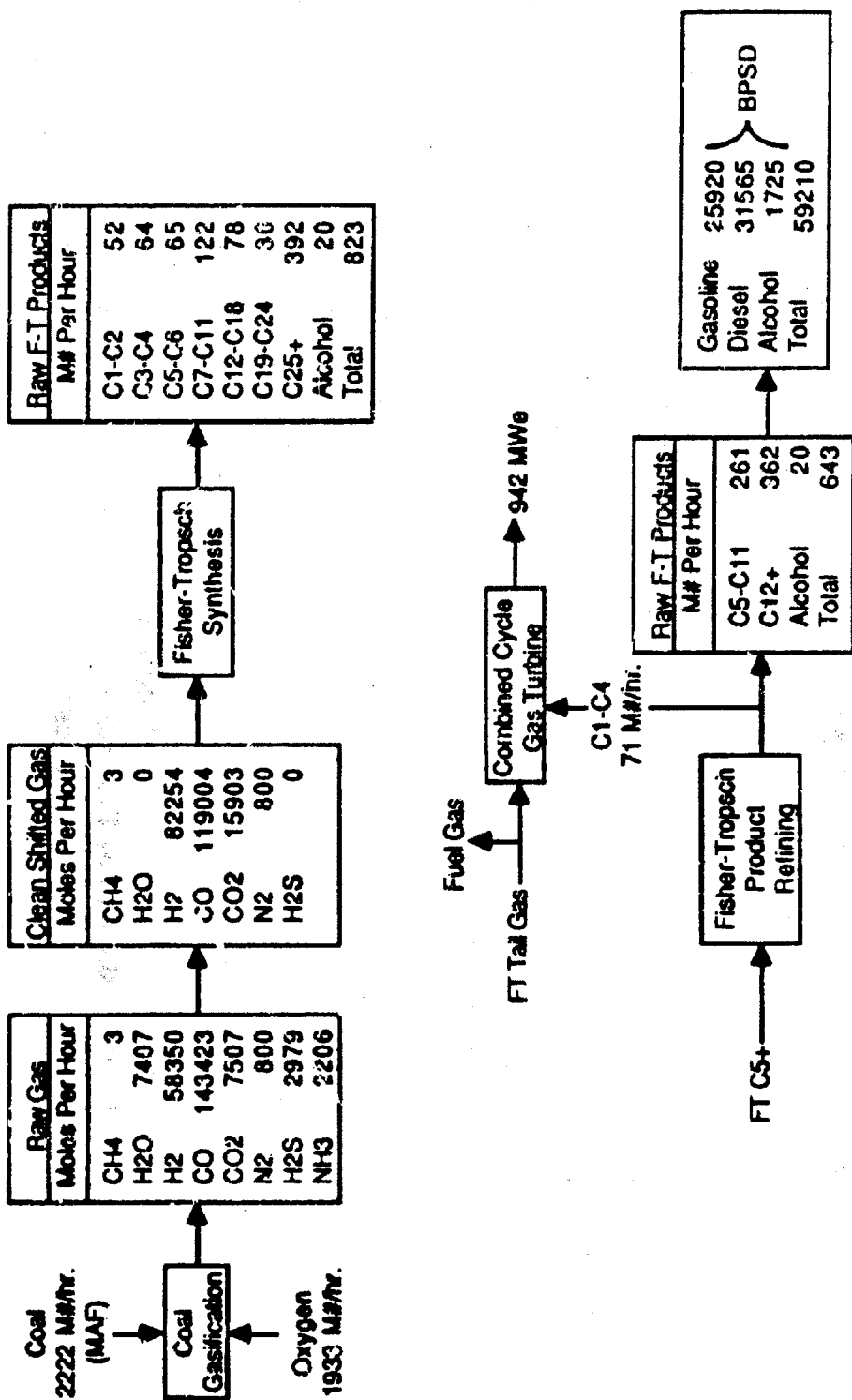


Figure 9
Summary of Materials Flows (Case 1)

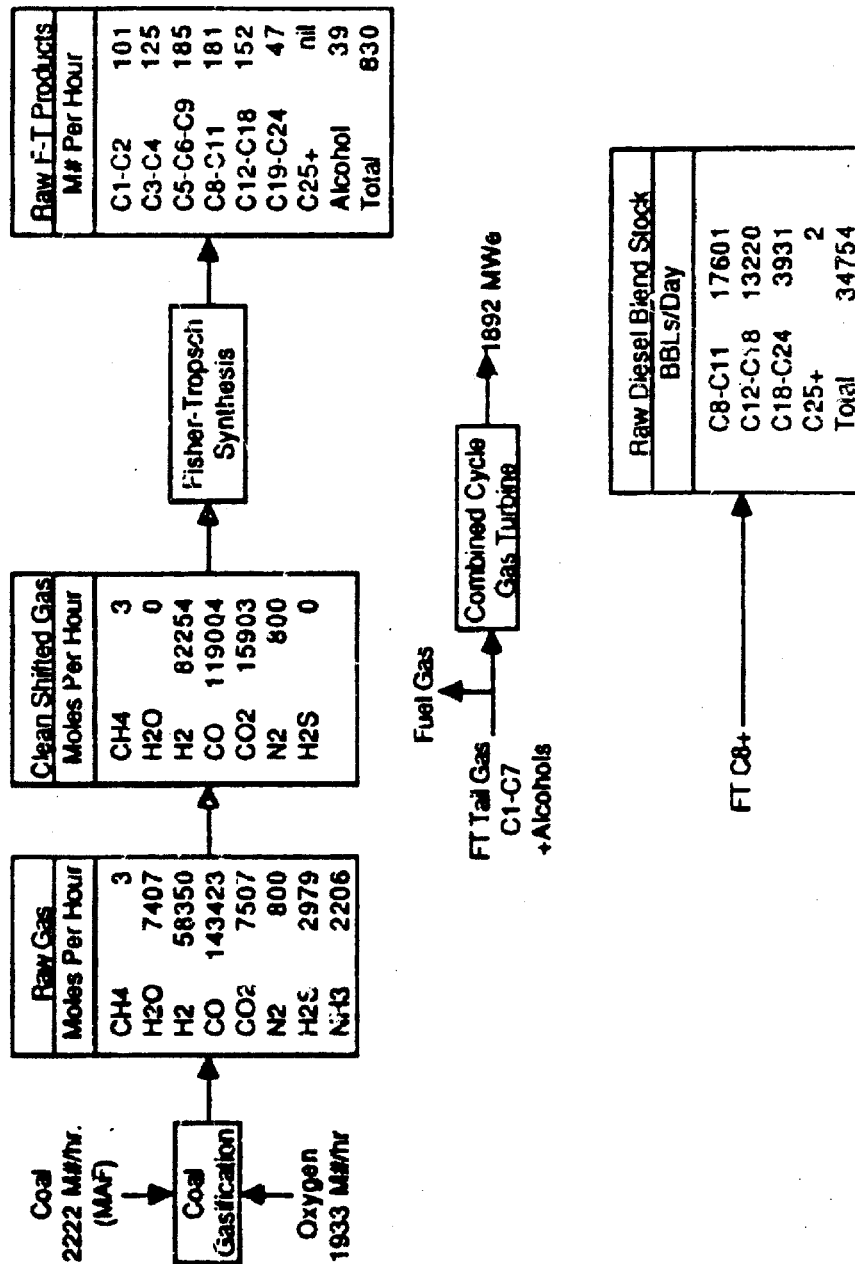


Figure 10
Summary of Materials Flows Hot Separator (Case 2)

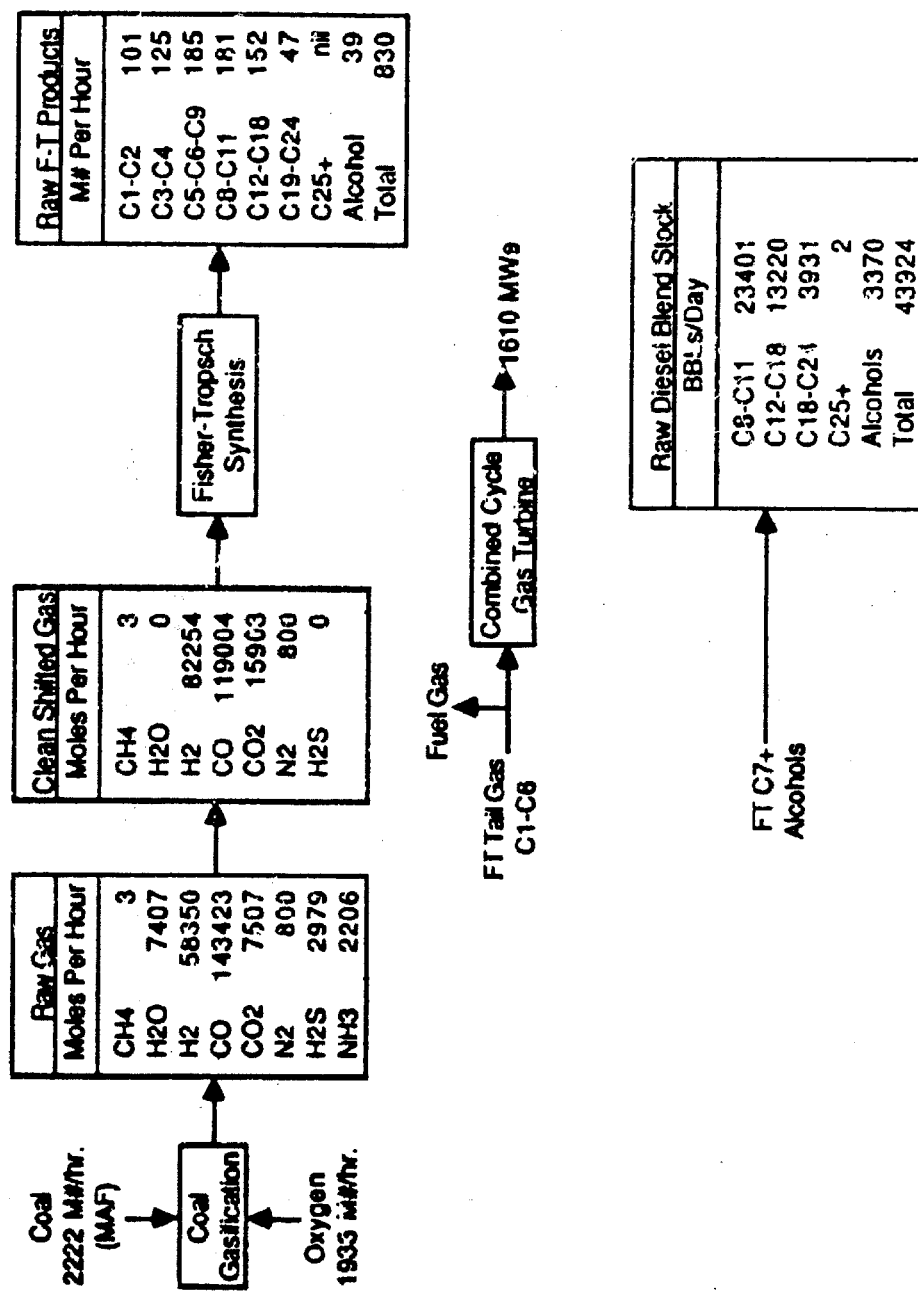


Figure 11
Summary of Materials Flows Cold Separator (Case 3)

Table 9
Comparison of Once-Through F-T Cases
and Baseline Case

	<u>Baseline</u>	<u>OTFT Case 1</u>	<u>OTFT Case 2</u>
Net Electric Power Produced (MW _e)	107	942	1892
Capital Cost (\$MM)	4411	4634	4546
Gross Annual Operating Cost (\$MM/Yr)	522.47	532.65	528.08
Byprod. Credits: Sulfur/Ammonia	60.03	60.03	60.03
Electric Power.*	45.06	398.58	800.37
Total Byproduct Credit	105.09	458.61	860.40
Annual Revenue Required (\$MM):			
Capital	737	774	759
Operating	317	74	-332
Total	1154	848	427
RSP of Liquid Products (\$/Bbl)	45.17	43.40	37.22
Equivalent Crude (\$/Bbl)	35.27	33.57	29.68

*Electric Power at .0534 \$/KWh

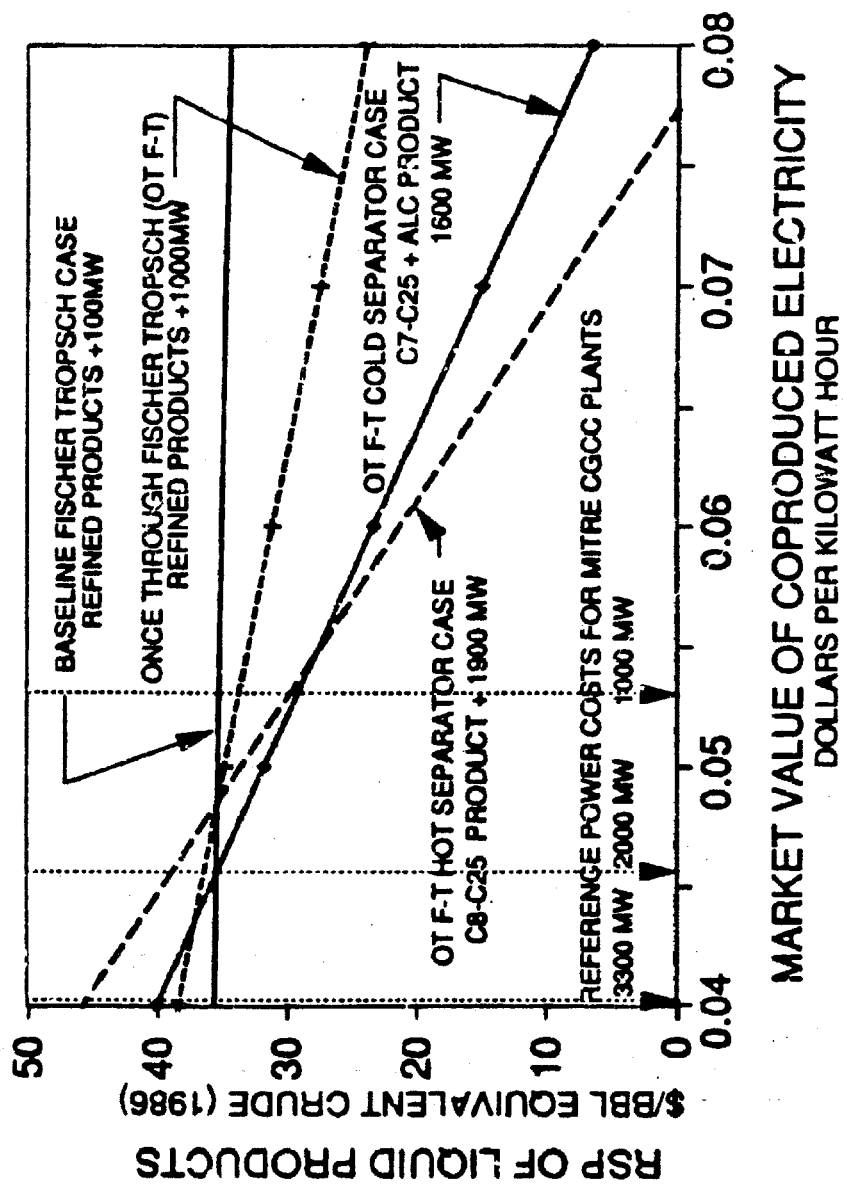


Figure 12
Sensitivity of RSP of Liquids to Electricity Value