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# ASSESSING THE ECONOMICS OF ADVANCED INDIRECT LIQUEFACTION PROCESS CONCEPTS

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Abstract

The objectives of this study are to estimate the cost of production of high quality transportation fuels from advanced coal-based indirect liquefaction processes and to determine the economic impact on the cost of these fuels that results from coproducing electric power using the once-through Fischer-Tropsch (OTFT) concept. Integrated computerized simulation models of commercial-scale indirect liquefaction facilities have been developed to accomplish these objectives. The baseline plant consists of Shell entrained coal gasification, slurry phase Fischer-Tropsch (FT) synthesis, and product upgrading, including wax hydrocracking, to produce gasoline, diesel and LPG. In addition to the baseline components that produce transportation fuels, the OTFT plant model includes gas turbines, heat recovery steam generators, and steam turbines that make up the combined-cycle section of the plant. In the OTFT mode, the synthesis gas is passed once through the slurry FT reactors, and the unconverted gas and lower hydrocarbon gases are combusted in the gas turbines to produce electric power. Using these simulation models, the impacts on the required selling price (RSP) of liquid fuels were quantified for various OTFT plant configurations. The reduction in RSP of the liquids depends on the quantity of electric power coproduced. For plants coproducing significant quantities of electric power (i.e., about 40 percent of their output), the reduction in the RSP of liquid fuels compared to the baseline plant is estimated to be about 18 percent.

Background

This analysis was undertaken 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.

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 Schulz-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.

Development of the Indirect Liquefaction Model

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. The MITRE gasification model simulates Shell gasifier performance from thermodynamic principles. This generalized gasification model combines inputs of coal, moisture or steam, oxygen, and transport gas to determine the quantities of $O_2$, $H_2$, and carbon by elemental balance. Nitrogen and sulfur present in the coal are assumed to react to $NH_3$ and $H_2S$, respectively. The exit temperature is varied iteratively until a temperature is found that simultaneously satisfies mass and energy conservation, under the assumption that CO, $CO_2$, $H_2$, $H_2O$, and $CH_4$ are either in equilibrium or a specified approach to thermodynamic equilibrium. Carbon utilization and external thermal losses may be varied by input. This theoretical model produces results that very closely match test data for the entrained Shell gasifier.

The model can utilize carbon dioxide, nitrogen or synthesis gas as the high-pressure coal transport gas. Nitrogen was used in the Shell pilot plant gasification tests.[3] However, since nitrogen is inert, it can only be removed from the system by bleeding that would result in high bleed losses and/or a synthesis gas stream containing high levels of $N_2$, which will increase pumping losses and take up reactor space in the F-T units. This study uses $CO_2$ as the transport gas because the $CO_2$ will be removed in the existing Selexol unit. The overall effect of the $CO_2$ on gasifier performance is small; the main effect is to alter the $H_2$:CO ratio of the new gas output. Shell suggests that product synthesis gas could also be used as high-pressure (HP) transport gas.

Raw gas exits the gasifier at about 1482°C (2700°F) and is cooled with recycle gas to 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 $H_2S$ and some $CO_2$. 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 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 $H_2$ are sent to a Benfield $CO_2$ removal system, a hydrocarbon recovery unit, and a 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 4 shows the slurry F-T reactors where finely divided catalyst is suspended in a wax medium through which the synthesis gas is bubbled. This is the heart of the indirect liquefaction process where the actual hydrocarbon synthesis takes place. The model simulates reactors based upon input dimensions. The results presented in the report use reactor dimensions suggested by Mobil in their 1985 report.[4] These reactors are 4.42 m (14.5 ft) in diameter and 10.67 m (35 ft) in height with an upper disengaging section 4.87 m (16 ft) in diameter and 4.27 m (14 ft) tall. Suspended within the reactor are the steam tubes for the removal of the heat of reaction. Fischer-Tropsch synthesis is very exothermic with approximately 20 percent of the combustion energy of the feed gas appearing as heat of reaction.

The wax produced in the F-T reaction that will not vaporize and be carried overhead under reaction conditions is continuously removed from the reactor slurry and pumped to a hydroclone where most of the suspended F-T catalyst is returned to the reactor. The wax is then filtered to remove the residual catalyst particles.

Slurry reactors are complex because, in addition to the usual chemical kinetic and mass diffusion constraints, the reactor hydrodynamics also impart a constraint. The model simulates the performance of the slurry reactors with respect to kinetics and hydrodynamics by using data taken from operations of the 2-inch diameter reactor of Mobil.[4,5] Most of the runs in this unit were operated at superficial gas velocities in the range 4 to 10 centimeters per second. Until more definitive data concerning the hydrodynamics of these reactors are available, the model assumes the hydrodynamic limitations discussed by Kolbel and Ralek[6] during operations of the Rheinpreussen-Koppers slurry F-T pilot plant.

The model calculates the number of reactors required to process a certain volume of synthesis gas at a certain temperature and pressure for a given catalyst loading (weight percent of catalyst in the slurry) and for certain reactor wax and catalyst densities. The kinetic information in the program calculates the synthesis gas conversion per pass for a given input value of the catalyst rate constant.

The final consideration in the reactor system is the removal of the heat of reaction during synthesis. The model assumes a constant operating temperature in the reactor, and thus the rate of heat generated is equal to the rate of removal. This is determined using the basic heat transfer equation and by assuming a value for the overall heat transfer coefficient.

Figure 5 shows the details of the raw F-T product upgrading and refining section of the conceptual plant. Raw liquid production is fractionated to produce a light stream $C_5^-$ for polymerization, a $C_5$-$C_6$ stream for isomerization, and a naphtha ($C_7$ - $C_{11}$) and diesel ($C_{12}$ - $C_{18}$) stream for hydrotreating and reforming. The wax ($C_{19}^+$) is selectively hydrocracked to produce additional middle distillate and naphtha.

Heating and cooling requirements are calculated for each stream in the integrated plant from gasifier input through F-T product separation. Waste heat from stream cooling that is not required for gas-to-gas heating is used for boiler feed water (BFW) heating and steam generation to produce high, medium, and low pressure steam. The major heat sources are the gasifier exit stream and the F-T synthesis reactors.

The model also includes all the necessary off-site units for a totally integrated, grassroots facility. The major off-sites are oxygen production, coal handling, cooling water system, waste water treatment, power generation and distribution, and F-T catalyst preparation. In the baseline model, power is produced using medium pressure steam turbines. Power requirements for all operations are estimated, and excess is sold as a by-product.

In the economic section of the model, construction costs, capital and operating costs are estimated. To calculate the required selling prices (RSP) of products from the plant, certain financial parameters need to be specified. These are the debt to equity ratio, project life, tax life, income tax rate, general inflation, escalations of feedstocks and products over and above general inflation, return on equity, debt interest, and period of construction. These parameters are then used in the model as input to the discounted cash flow (DCF) analysis. These can be changed as required to reflect any set of financial conditions. These financial parameters allow the capital recovery factor (CRF) to be calculated. The CRF determines the capital component of the plant annual revenue requirement. The other component is the operating costs. The sum gives the total annual revenue requirement from which the required selling prices of products are calculated.

For the baseline plant that essentially produces only transportation fuels and liquified petroleum gas (LPG), 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 $H_2$ 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 Kolbel,[6] Farley and Ray,[7] and Bukur.[8] Raw product refining data were obtained from Mobil,[9] and wax hydrocracking data were obtained from UOP.[10]

Since an objective of this present study is to investigate the economic potential of OTFT with coproduction of electric power, it was necessary to extend the baseline model to include combined-cycle electric power generation units. Figure 6 is a block flow diagram of the OTFT plant simulated in the model. 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 were 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. The OTFT plant then can sell both electric power and high quality transportation fuels.

The OTFT configuration differs from the baseline plant in several respects. Primarily, since the F-T reactors are operated once-through, all equipment related to recycling of unconverted synthesis gas is eliminated. This includes carbon dioxide removal and autothermal reforming. In addition, the OTFT configuration has an additional major source of high temperature waste heat from the gas turbine exit. This is used to produce steam for electric power generation in a combined-cycle configuration. Since the combined-cycle system has to be included, steam drivers for oxygen production that were used in the baseline case have been replaced by electric motors.

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 simulate a plant that eliminated the F-T synthesis and upgrading section altogether. The resultant coal gasification/combined-cycle plant simulation model was then used to develop realistic costs of electric power that could be used in the OTFT coproduction cost models.

## Results of the Analysis

### Baseline Case

This section reports on the results obtained using the MITRE model to investigate the performance and economics of the baseline case, of the combined-cycle only case, and of several OTFT cases with cogeneration of electric power.

Figure 7 summarizes the material flows that result from application of the model to the baseline case. After upgrading the raw F-T products, approximately 83,500 BPD of refined liquid fuels are produced. Overall efficiency to liquid products is about 57 percent on a higher heating value basis.

Table 1 summarizes the baseline plant construction costs and capital required. A construction cost of $2,830.5 million is required. Data on the cost of Shell gasifiers were taken from a recent EPRI report prepared by Florida Power and Light Company with input from Shell Oil Company.(12) For this baseline plant the total capital required is $4,405 million. Table 2 shows the computation of gross and net annual operating costs for the baseline plant. After by-product credits, the net annual operating costs are about $450 million. Table 3 shows the baseline economic assumptions used in the DCF analysis. General inflation is assumed to be 3 percent and no escalation over and above inflation for feedstocks or products is assumed. Table 4 shows the calculated required selling prices (RSP) for refined products. These are calculated from the annual revenue requirements shown in the lower part of the table. On a Btu basis, where the thermal value of all products in Btus are used, the RSP would be $8.34 per million Btus. For $C_3$-$C_4$ valued at $4.84/MM Btu and other fuels equal on a volume basis, the RSP is $46.22 per barrel. This is equivalent to crude oil at $36.28/barrel.

It has been assumed in the base case that the raw F-T products will be refined on site at a dedicated refinery. This situation exists at SASOL II and III where dedicated refineries upgrade the raw products to gasoline and diesel. The baseline plant therefore includes a refinery in the capital cost estimate as described. If the raw F-T products could be refined at an existing refinery, then no on site refinery would be required and the plant capital cost could be reduced. Liquid products could be transported to the refinery by pipelines, but the 50% solid wax obtained in the baseline case would probably have to be hydrocracked on site or be transported to refineries by other means. Also, about 10 percent of the raw product is $C_3$ and $C_4$ material that must be polymerized to produce liquids. A no-refinery case would probably make more sense for a product distribution that did not produce wax. There are many opportunities for blending the raw F-T products with both petroleum-derived products and liquids from direct coal liquefaction, and future studies should address these possibilities.

## Results of the Analysis

### Once-Through Fischer-Tropsch

In order to investigate the economics of the OTFT concept, the model was used to estimate the RSP of electric power produced from the gasification/combined-cycle plant configuration. This configuration used Shell gasifiers, gas cleanup to remove 90 percent of the sulfur and a gas turbine/steam turbine combined-cycle plant. The RSP of electricity calculated from this configuration was used in the subsequent OTFT cases that coproduced electricity and F-T liquids for sale.

Three OTFT/combined-cycle cases were investigated in this study. In case 1, the synthesis gas is passed once through the F-T reactors, and the effluent gases are separated so that the $C_1$-$C_4$ hydrocarbon gases and unconverted synthesis gas are passed to the gas turbine combustors. The $C_5^+$ raw F-T product is sent to the refinery to produce gasoline and diesel. The same F-T selectivity as was used in the baseline case is used in case 1, and the wax (~50 wt% of total product) is hydrocracked as in the base case. Figure 8 summarizes the material flows in case 1. In this case, 947 MW of electric power are coproduced together with 60,800 BPD of transportion fuels.

In case 2, the effluent from the F-T reactor is separated so that $C_1$-$C_7$ hydrocarbons and alcohols are combusted in the gas turbines, and the $C_8^+$ hydrocarbons are sold unrefined as raw diesel blend stock. In case 2 the F-T selectivity is changed so that essentially no wax is produced. This case produces 1951 MW of electric power and 33,600 BPD of liquid transportation fuel. Figure 9 summarizes the material flows for this case.

In case 3, the effluent from the F-T reactors is separated so that the $C_1$-$C_6$ hydrocarbons are combusted in the gas turbines, and the $C_7^+$ hydrocarbon liquids and alcohols are sold as unrefined products. Figure 10 summarizes the flows for this case where 1674 MW of electric power and 42,900 BPD of liquids are produced.

Table 5 compares the economics of the baseline case to the three OTFT cases described above. The by-product credit for electric power is that developed for a 1000 MW coal gasification/combined-cycle plant and is 0.0534 $/KWh.

Figure 11 shows the sensitivity of liquid cost in dollars per barrel of equivalent crude price 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 revenue. The reference power values shown on Figure 11 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 $0.534, $.0452, and $0402 per KWh 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.

This analysis concludes that the OTFT concept that coproduces electric power and high quality transportation fuels can significantly reduce the cost of F-T liquids. For example, in case 1 that coproduces almost 1000 MW of power, the RSP of liquids is reduced by 11 percent from the base case, all liquids plant.

**Acknowledgement**

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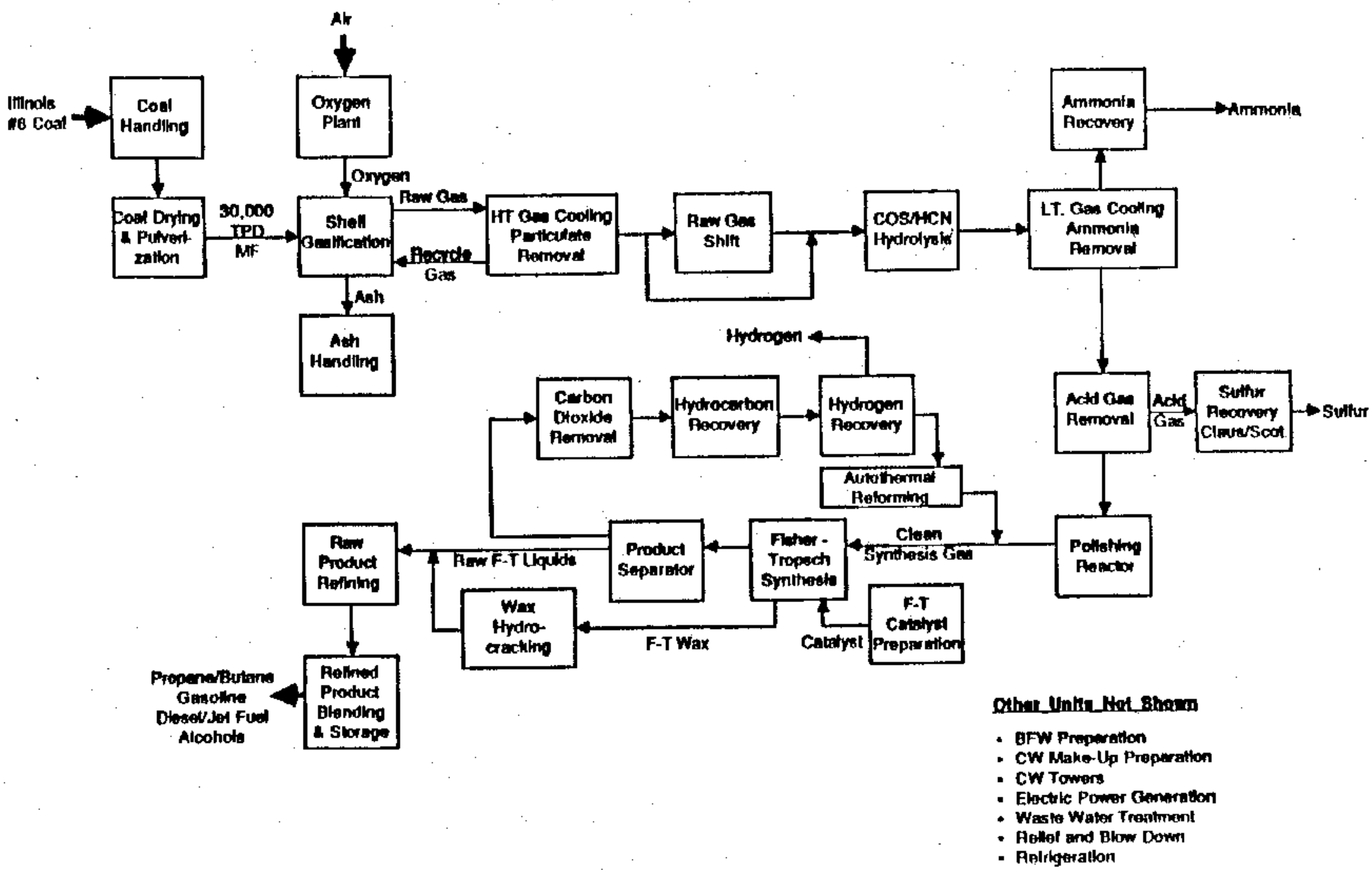



**Figure 1**
**Components of MITRE Indirect Coal Liquefaction Model**
**(Base Case)**

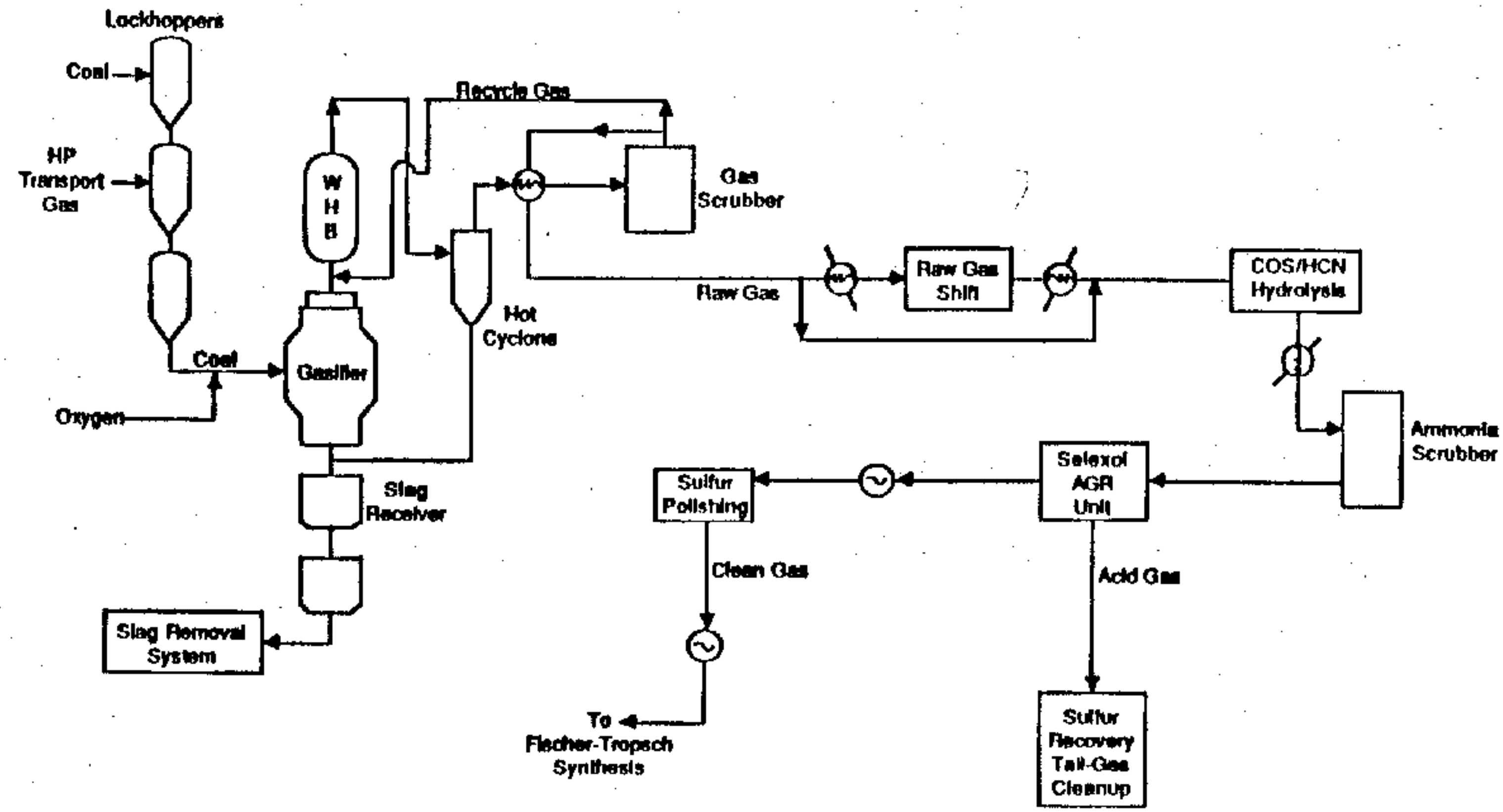



**Figure 2**
**Detail of Clean Synthesis Gas Production**
**(Shell Gasifiers)**

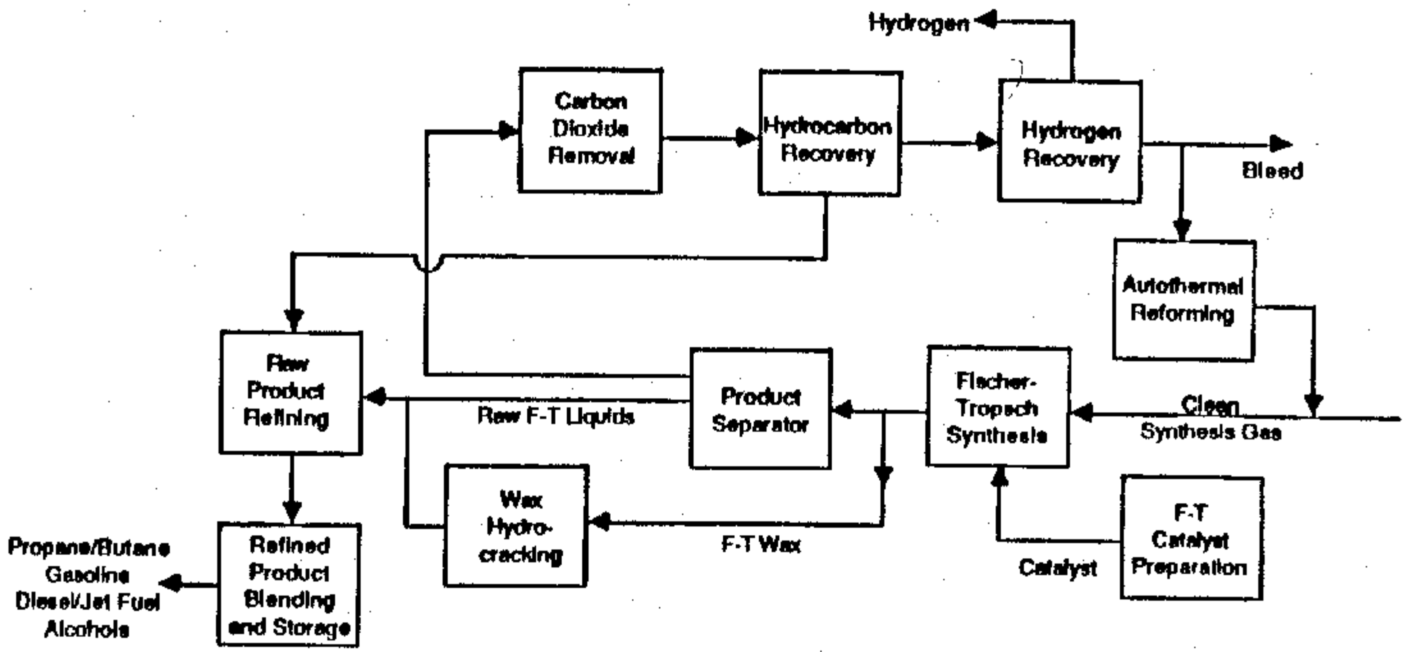



**Figure 3**
**Fischer-Tropsch Recycle Loop Details**

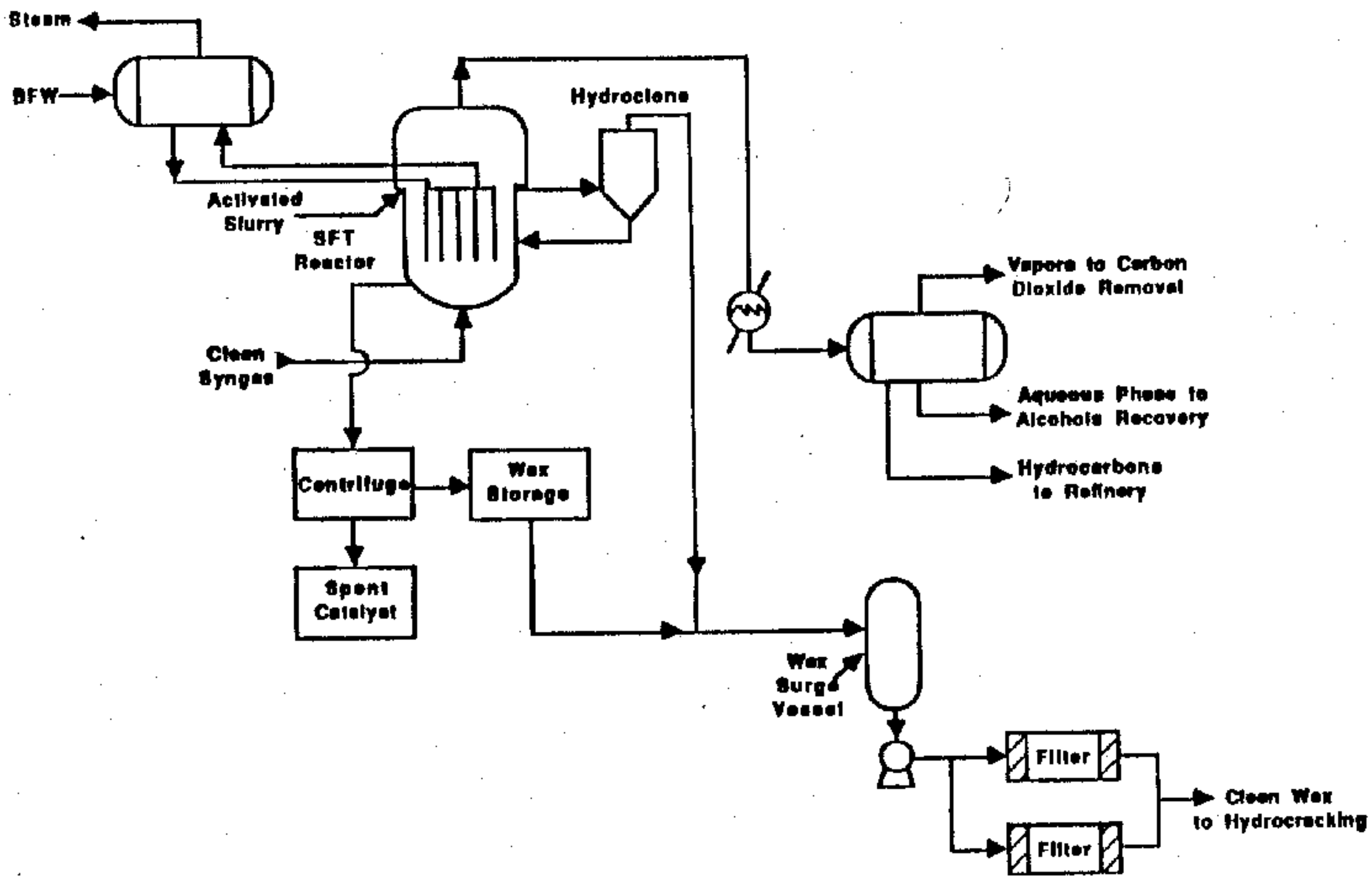
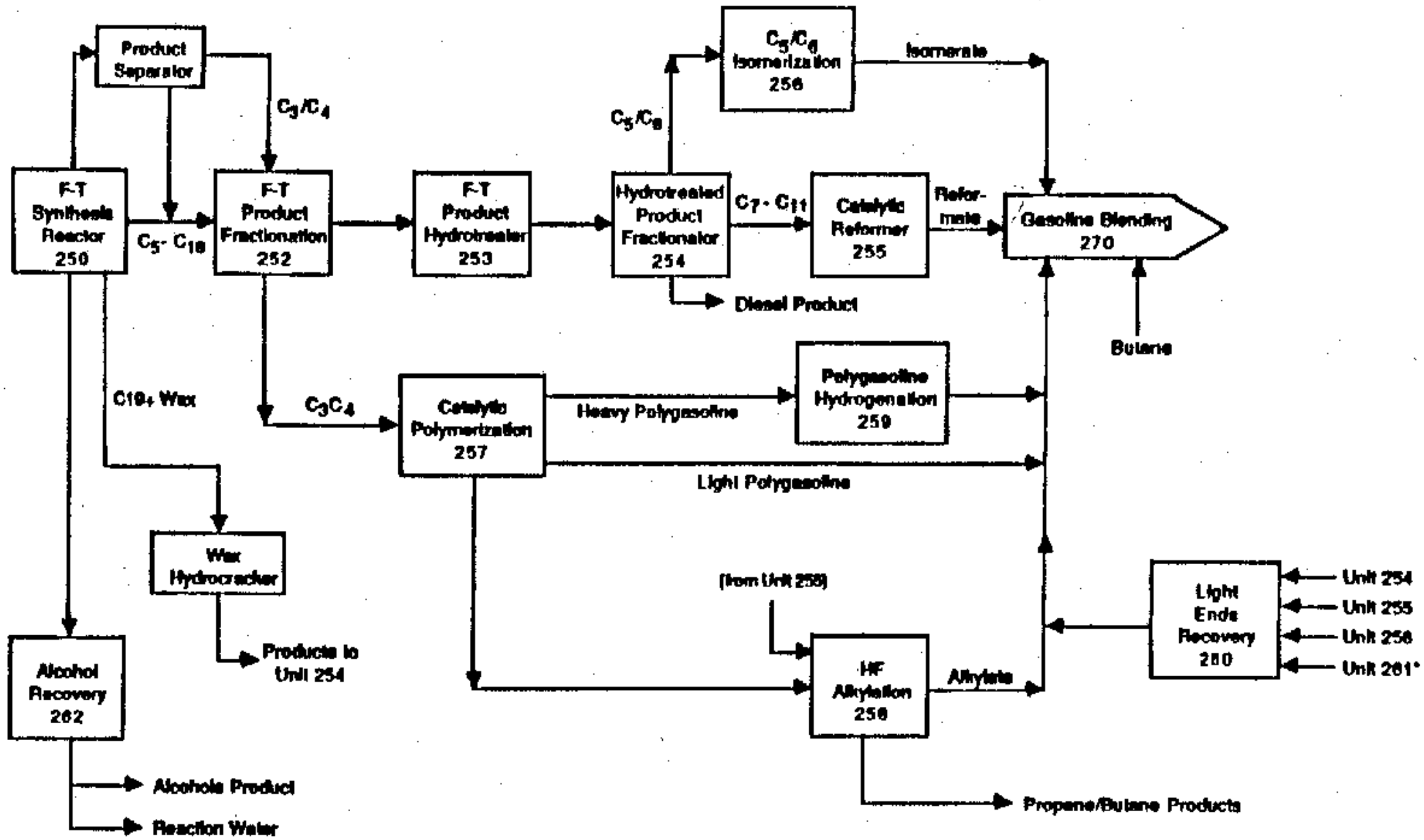



**Figure 4**
**Detail of Slurry Fischer-Tropsch Reactor System**




* Unit 261 Hydrogen Purification not shown.

**Figure 5**
**Raw Fischer-Tropsch Product Refining**

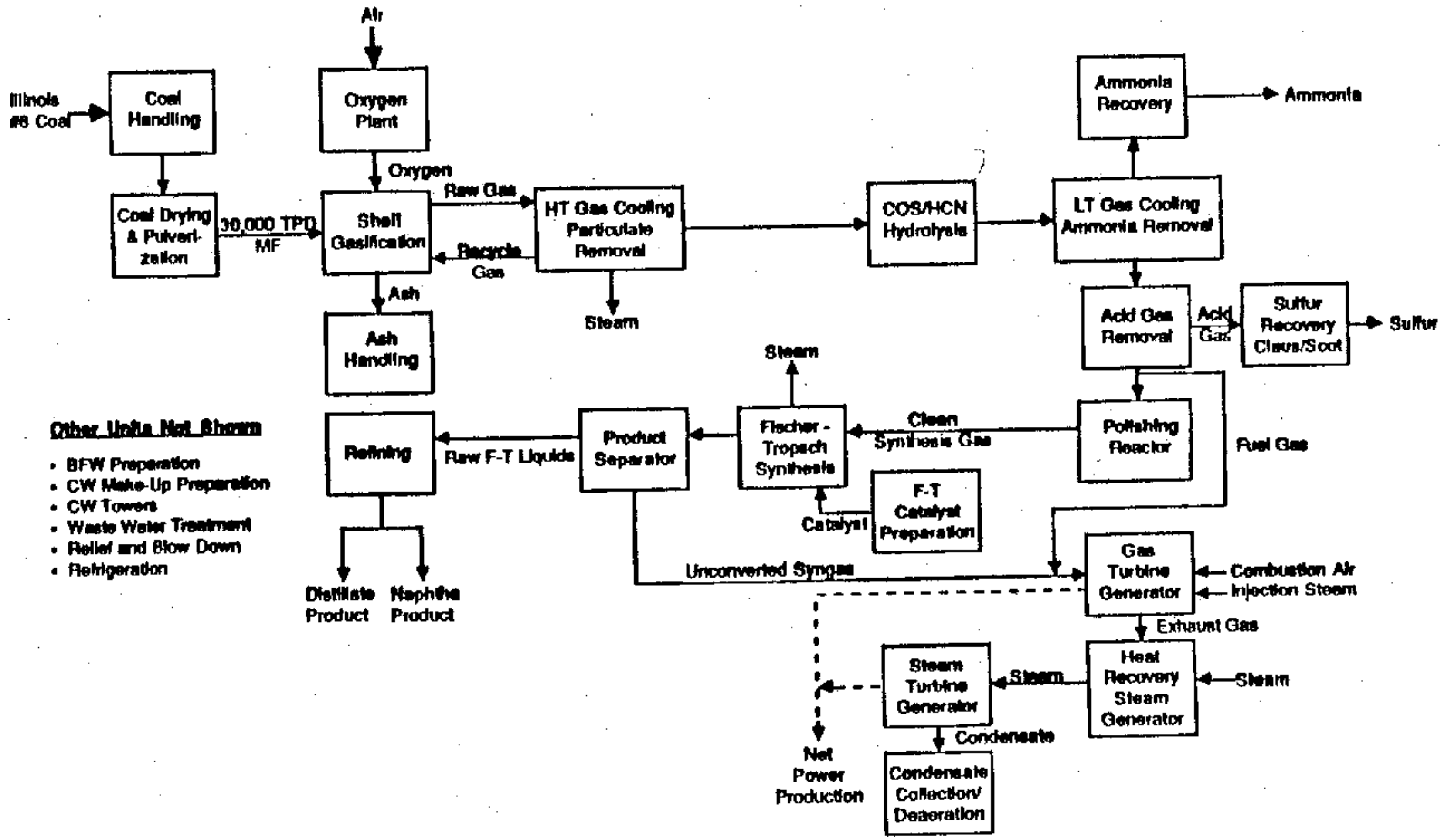



**Figure 6**
**Overall Block Flow Diagram Once-Through Fischer-Tropsch Electricity Generation**

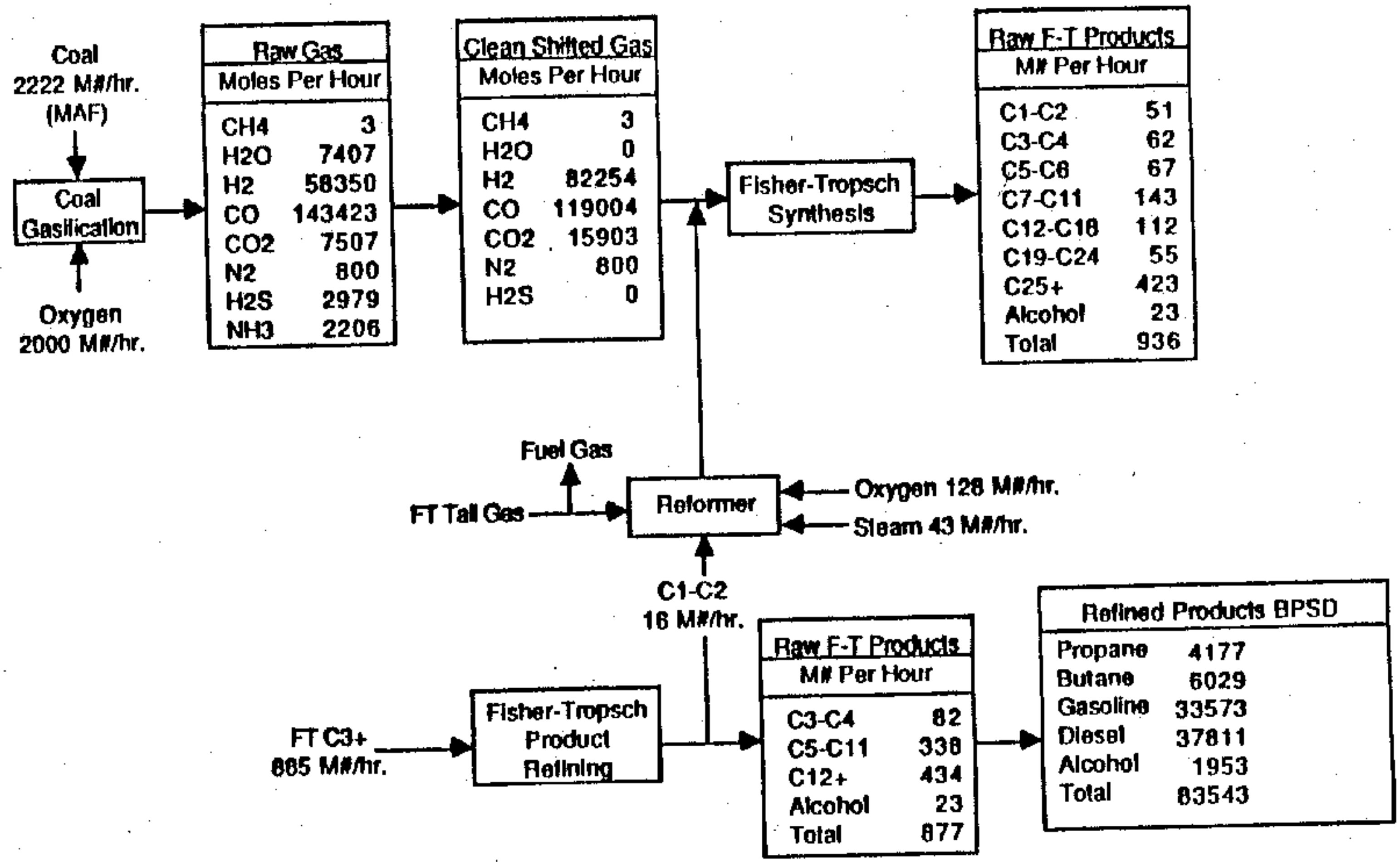



**Figure 7**
**Summary of Materials Flows**
**(Base Case)**

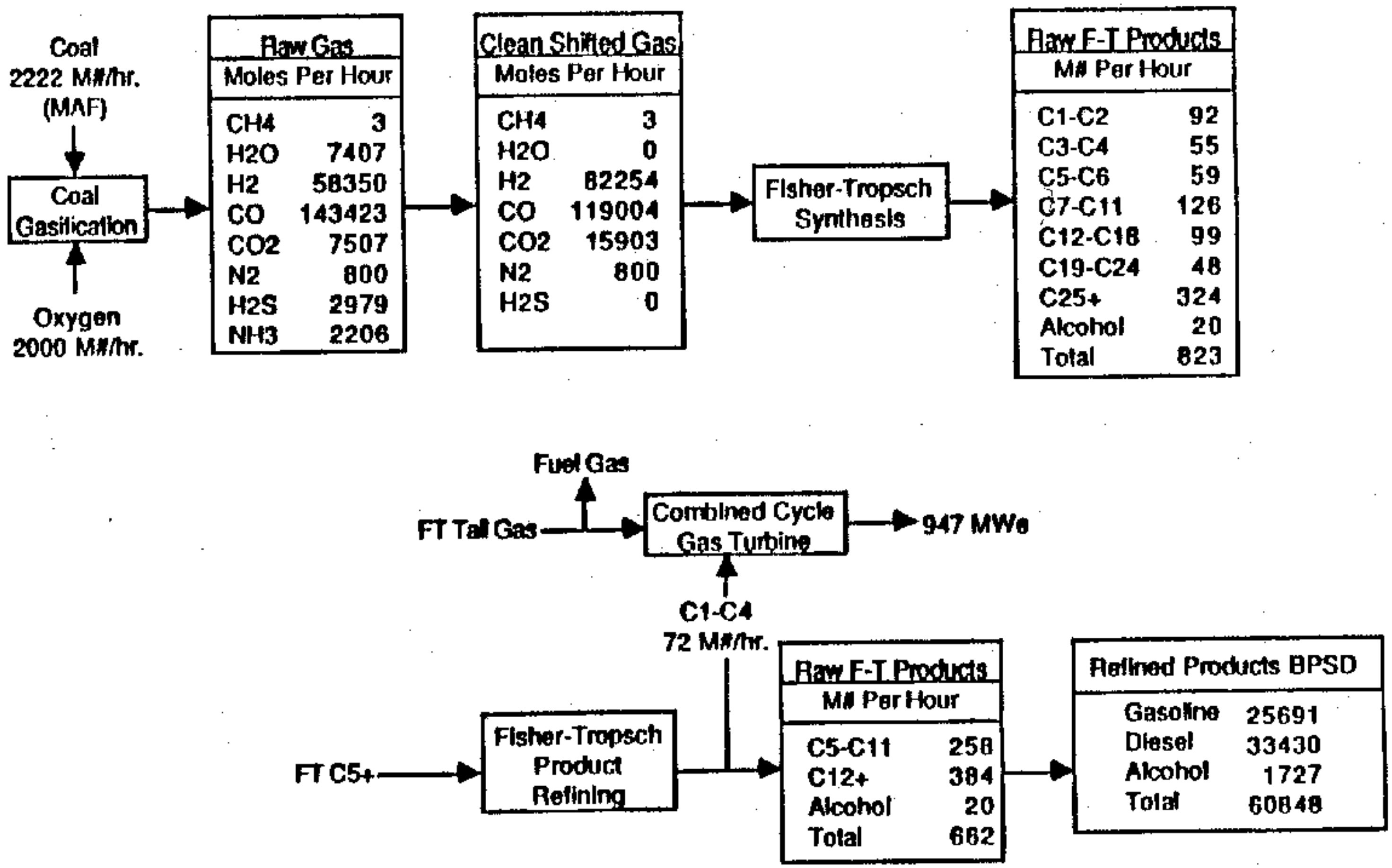



**Figure 8**
**Summary of Materials Flows**
**High Alpha: Refining of $C_5^+$ Product (Case 1)**

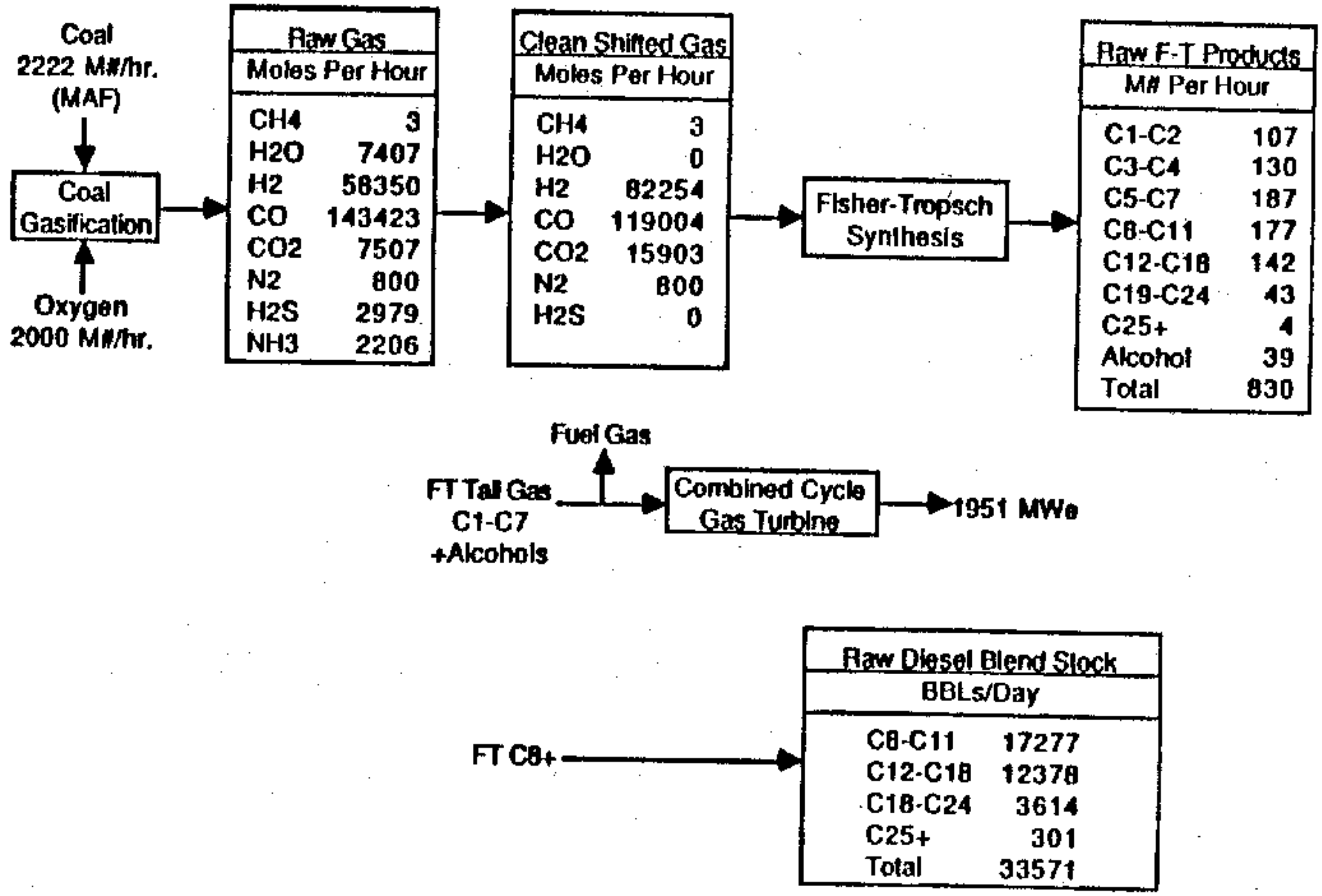



**Figure 9**
**Summary of Materials Flows**
**Low Alpha: Unrefined $C_8^+$ Product (Case 2)**

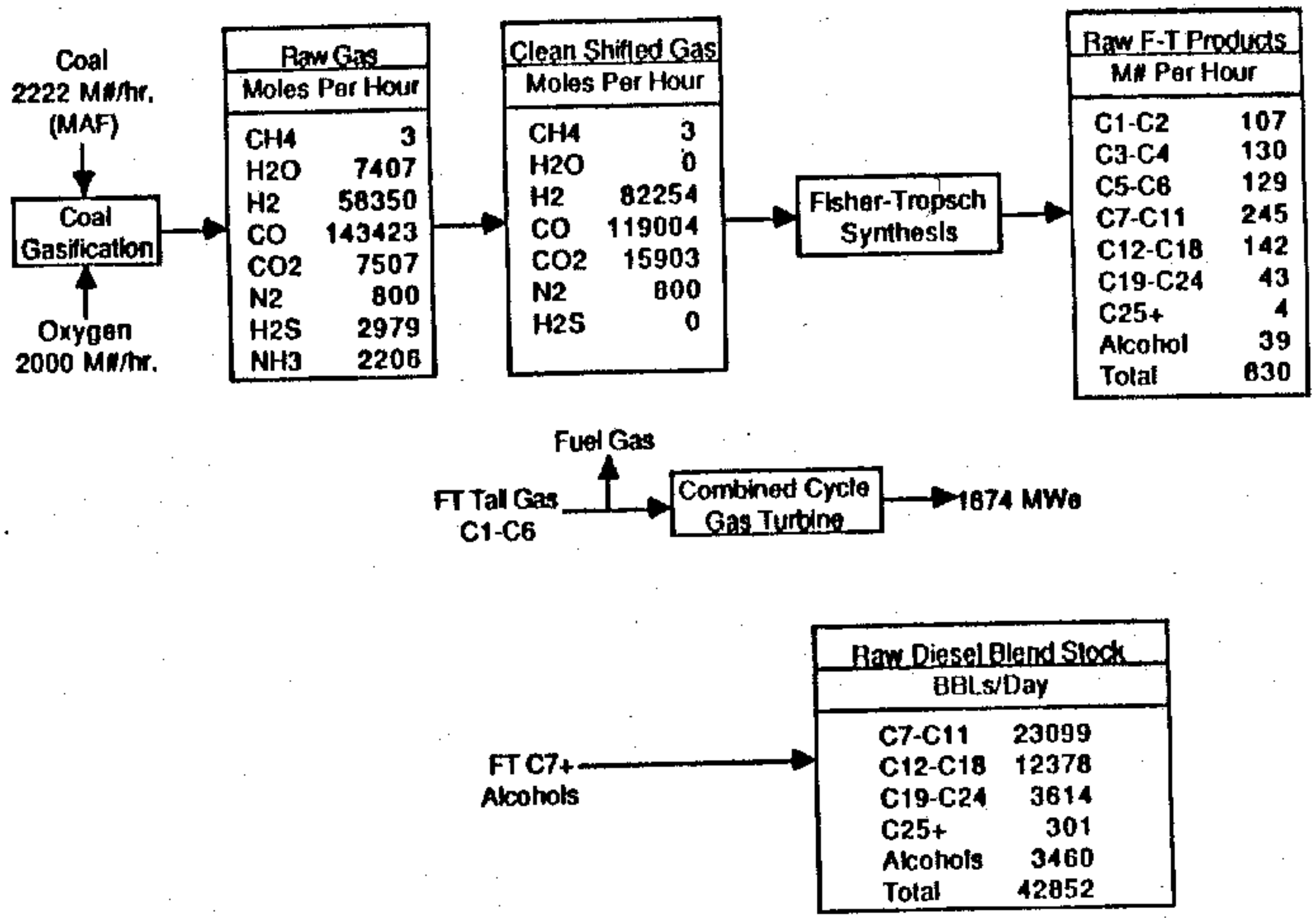



**Figure 10**
**Summary of Materials Flows**
**Low Alpha: Unrefined $C_7^+$ /Alcohol Product (Case 3)**

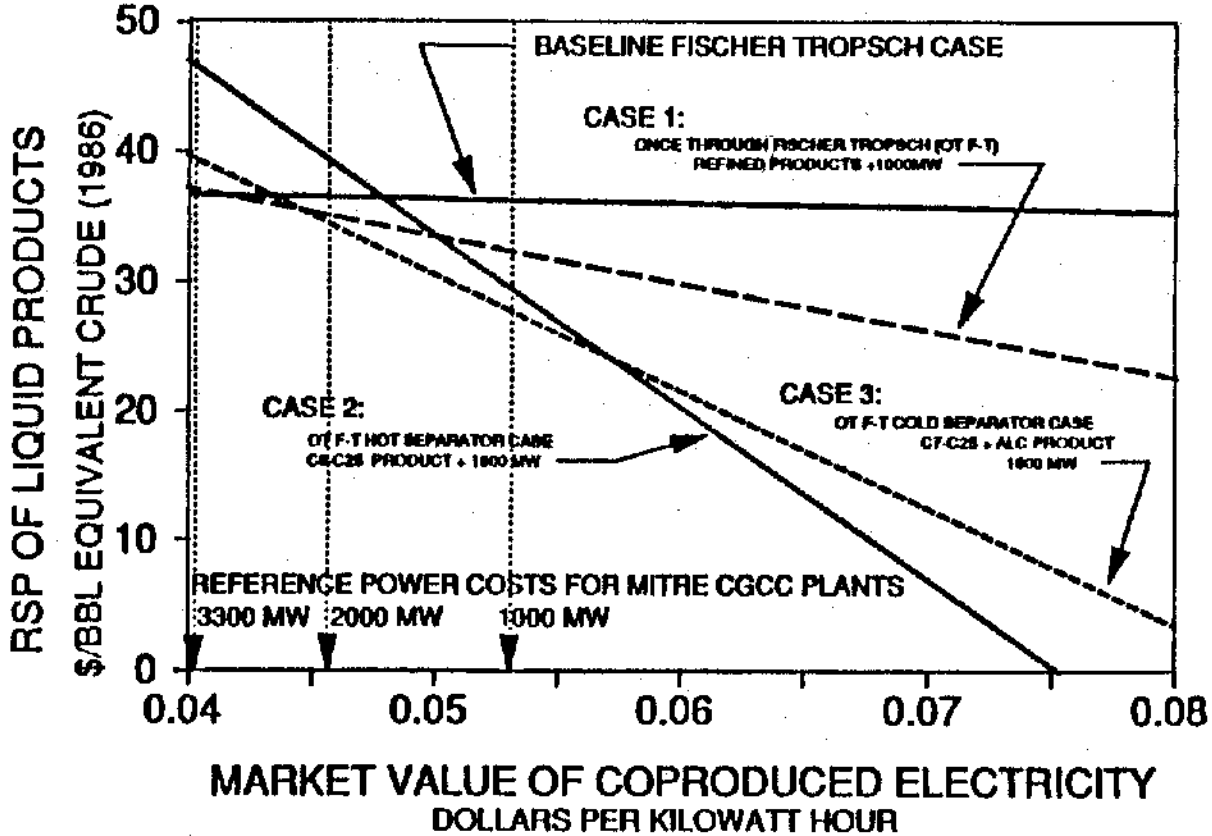



**Figure 11**
**RSP of Liquid Products vs Market Value of Coproduced Electric Power**

Table 1
Baseline Plant Construction Cost and Capital Estimate
($MM 1986)

| | |
|---|---|
| Clean Synthesis Gas Production | 804.50 |
| By-Product Recovery | 65.12 |
| Fischer-Tropsch Synthesis | 520.24 |
| F-T Product Refining | 368.24 |
| Oxygen Production | 437.78 |
| Coal Handling | 188.51 |
| Other Off-Sites | 266.58 |
| F-T Catalyst Preparation | 40.25 |
| Infrastructure & Miscellaneous | 93.80 |
| Autothermal Reforming | 45.46 |
| **Total Construction Cost** | 2,830.50 |

**Capital Requirements (Baseline Plant $MM)**

| | |
|---|---|
| Construction Cost | 2,831 |
| Engineering Design and Project Contingency | 708 |
| **Total Plant Investment** | 3,539 |
| Allowance for Funds Used During Construction | 598 |
| **Total Depreciable Capital** | 4,136 |
| Start-up Costs | 104 |
| Working Capital | 131 |
| Initial Charge of Catalyst & Chemicals | 34 |
| **Total Non-Depreciable Capital** | 269 |
| **TOTAL CAPITAL REQUIRED** | 4,405 |

**Table 2**
**Calculation of Gross and Net Operating Costs**
**($M1986 Per Annum) Baseline Plant**

| | |
|---|---|
| Coal - $22.70/ton As-Received | $258,780 |
| Catalyst, Chemicals and Water | 34,253 |
| Process Operating Labor | 17,691 |
| Overhead & G&A - 60% Process Labor | 10,614 |
| Maintenance - 3.5% TPI | 123,834 |
| Local Taxes & Insurance - 2% TPI | 70,763 |
| Solids Disposal - $6.00/ton | 5,867 |
| **TOTAL GROSS ANNUAL OPERATING COSTS (GAOC)** | **$521,802** |
| Sulfur - $100/ton | $37,601 |
| Ammonia - $150/ton | 22,280 |
| Electric Power | 11,833 |
| **TOTAL BY-PRODUCT CREDITS** | **$ 71,714** |
| **TOTAL NET ANNUAL OPERATING COST** | **$450,089** |

Table 3
Baseline Economic Assumptions

| | |
|---|---|
| Equity | 25 percent |
| Project Life | 25 years |
| Tax Life | 16 years |
| Income Tax Rate | 34 percent |
| Price Escalation* | 0 |
| O & M Escalations | 0 |
| Fuel Escalation | 0 |
| General Inflation | 3 percent |
| Return on Equity | 15 percent |
| Interest on Debt | 8 percent |
| Construction Period | 5 years |

*Escalation defined as inflation over and above general inflation.

**Table 4**
**Required Selling Price of Fuels**
**(Baseline Case)**

| | | |
|---|---|---|
| Required Selling Price, Btu Basis | \$8.34/MM Btu | |
| | \$/Bbl | \$/Gal |
| $C_3$-$C_4$ Valued @ \$4.84 MM Btu, Other Fuels Equal on Volume Basis RSP = | \$46.22 | \$1.10 |
| Equivalent Crude | \$36.28 | |
| ANNUAL REVENUE REQUIREMENTS (\$M) | | |
| Capital @ 0.167 CRF* | \$ 735,568 | |
| Coal @ \$22.7/Ton | \$ 258,780 | |
| Other O & M | \$ 191,304 | |
| TOTAL | \$1,185,657 | |

*CRF = Capital Recovery Factor.

Table 5
Comparison of Once-Through F-T Cases
and Baseline Case

| | Baseline | OTFT Case 1 | OTFT Case 2 | OTFT Case 3 |
|---|---|---|---|---|
| Net Electric Power Produced (MW) | 37 | 947 | 1951 | 1674 |
| Capital Cost ($MM) | 4405 | 4624 | 4581 | 4433 |
| Gross Annual Operating Cost ($MM/Yr) | 522 | 532 | 530 | 522 |
| Byprod. Credits: Sulfur/Ammonia | 60 | 60 | 60 | 60 |
| Electric Power* | 12 | 401 | 825 | 708 |
| Net Operating Costs | 450 | 71 | -355 | -246 |
| Total Liquids Produced BPSD | 83,500 | 60,800 | 33,600 | 42,900 |
| RSP of Liquid Products ($/Bbl) | 46.20 | 42.00 | 37.00 | 34.90 |
| Equivalent Crude ($/Bbl) | 36.30 | 32.30 | 29.40 | 27.50 |

*Electric Power at .0534 $/KWh