EXECUTIVE SUMMARY

This report documents the development of an integrated indirect liquefaction systems model. The model was developed at the request of Sandia National Laboratories and the United States Department of Energy to provide guidance for indirect liquefaction research and development. The model simulates a conceptual commercial indirect liquefaction plant from input coal to refined liquid products. A major requirement of the model is that it be flexible enough to allow a large number of sensitivity studies to be performed. In this way the model can be used to investigate the impact, on the overall system economics, of projected advances in specific areas of the technology. These "what if" sensitivities can be readily performed to evaluate their potential impacts on system efficiency and economics. If the sensitivity is favorable, then making it a technical reality becomes a research objective.

The indirect plant conceptualized in the model is totally integrated from coal to products, and all power and energy requirements are generated within the plant. Excess electric power is sold as a by-product together with sulfur and ammonia. For the purpose of explanation, the plant can be considered as being divided into three main sections, although there is complete integration among these sections with respect to mass and energy flows. The first section simulates the preparation of clean synthesis gas. This is accomplished using Shell gasification of coal followed by shift of the raw product gas, gas cooling and cleaning, and sulfur and ammonia recovery. The second section simulates the Fischer-Tropsch (F-T) synthesis. Slurry-phase synthesis units are used to produce the raw products. This section also simulates the raw F-T product separation, recycle of unconverted synthesis gas, carbon dioxide removal, hydrogen recovery, and autothermal reforming of the C_1 and C_2 hydrocarbon gases. The third section simulates the raw F-T product refining to produce diesel, gasoline, and liquified petroleum gas (LPG). This section includes a complex refinery that polymerizes and alkylates light ends, hydrogenates the raw product, reforms and isomerizes naphtha, hydrocracks the F-T wax, and recovers the alcohols.

A complete utility balance is performed for all the unit operations in the plant. High- and medium-pressure steam are generated from waste heat from the gasification, autothermal reforming, and F-T sections. The steam produced in these plant areas is more than sufficient to power the turbines for oxygen and electricity production and for steam users throughout the plant.

In addition to the three main sections described above, the model includes the necessary off-site supporting units. The major units are the oxygen

plant for the gasification section, coal handling and drying, the cooling and boiler feed water systems, wastewater treatment, power generation and distribution, F-T catalyst preparation, refrigeration, storage, and infrastructure.

The economic section of the model provides estimates of the plant construction cost, total plant capital required, operating and maintenance costs, annual revenue required, and required selling prices (RSP) of the products. Total plant construction cost is estimated by using cost data of unit operations obtained from various open literature sources. These are scaled based on capacity, adjusted to the reference calendar year, and summed to give the total cost of construction. Total capital is calculated from the construction cost by adding engineering design and contingency costs and funds used during construction. Addition of the non-depreciable capital (start-up cost, working capital, and initial catalyst and chemical cost) gives the total capital required. Gross annual operating costs are calculated as the operating and maintenance expenses minus the by-product credits. The annual revenue required is the sum of the capital and operating cost components. The capital component is calculated from a discounted cash flow (DCF) analysis using specified financial parameters. The RSPs of the products are then calculated from the total plant product outputs and the annual revenue requirement.

Responding to the need for flexibility, MITRE has designed the model to allow several "sensitivities" to be investigated. The major ones are plant size, coal feedstock, raw F-T selectivity, catalyst activity, slurry reactor hydrodynamics, refinery operations, and economic parameters.

The operation of the model has been applied to a baseline plant case. In the baseline case, the conceptual indirect liquefaction plant processes 30,000 tons per day of moisture-free (MF) Illinois coal in 12 Shell gasifiers operating at 400 psig pressure. The raw gas (approximately 200,000 moles per hour) is shifted to a hydrogen to carbon monoxide molar ratio of 0.67 and cleaned to 0.06 ppmv total sulfur and fed to slurry-phase F-T reactors. These reactors contain 18.5 percent by weight of iron-based F-T catalysts suspended in reactor wax at a pressure of 17 bar and a temperature of 243°C. The F-T selectivity produces a product containing approximately 50 percent wax, and the catalyst activity matches that obtained by Mobil in their slurry-phase F-T bench-scale unit. The plant recycles unconverted synthesis gas and autothermally reforms the C_1 and C_2 hydrocarbons so that no methane and ethane are coproduced. The raw F-T products are sent to a refinery where the wax is hydrocracked to give diesel and naphtha range materials. The other raw F-T products are refined to produce high octane gasoline, high cetane diesel blending stock and LPG.

Table ES-1 summarizes the results obtained using the model on the baseline case. Approximately 83,500 barrels per stream day of products are produced from the 30,000 tons per day of moisture-free coal, and the overall efficiency to products is 56.9 percent on a higher heating value basis. Total capital for the plant is estimated at $4,405 million (1986), and net annual operating cost is $450 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, if LPG is $4.84 per million Btu, is $46.22 per barrel. This is equivalent to crude oil at $36.28 per barrel.

The conceptual baseline commercial plant modeled here consists of a large number of unit operations, each at a different stage of commercial and technical development. These stages normally range from the "commercially available right now" category to the "only demonstrated for limited time period in a bench-scale unit" category. Some of the unit operations have only been demonstrated at a small scale, and many of the assumed integrations have never been demonstrated. In addition to the uncertainty in many of the technical performances assumed in the model conceptual plant, the costs of many of the unit operations are not known with any precision. This is particularly the case for the F-T slurry reactors where detailed open literature cost information is not available. For the above reasons, it should be emphasized that the absolute costs of products derived by using this model are only as precise as assumed performance and current unit operation cost data allow. Although the absolute cost numbers produced by using the current model may not be precise, the value of the model is to quantify differences in costs that are derived by evaluating the impact of advances in technology. The model can then act as a road map to chart research direction; this is its primary purpose, and when used in this manner the results obtained are precise and meaningful.

During the development of this model, insufficient data necessitated making several assumptions regarding the technical performance of many of the unit operations. The recommendations for additional research primarily relate to investigating the validity of these assumptions. Table ES-2 lists the major recommendations for research and development. Since the greatest uncertainties are in the Fischer-Tropsch area, most of the recommendations are directed at obtaining a better understanding of the slurry reactor system and the development of appropriate F-T catalysts to use in these reactors.

This indirect model will be used in future work to investigate the potential economic impact of several of these sensitivities on the overall indirect liquefaction system. In addition, the model will be extended in capability so that the potential of once-through F-T with coproduction of

Table ES-1
Summary of Model Results for Baseline Case

Input			
Coal Feed (31,540 MM Btu/hr)	(30,000 TPD MF)	2,222,000	lb per hour MAF
Oxygen Feed	(24,000 TPD)	2,000,000	lb per hour
Clean Gas			
Carbon Monoxide	(1090 MM SCF/day)	126,512	moles per hour
Hydrogen	(644 MM SCF/day)	74,759	moles per hour
Products (Barrels Per Stream Day)			
Propane		4,177	
Butane		6,029	
Gasoline		33,573	
Diesel		37,811	
Alcohols		1,953	
TOTAL		83,543	
Overall Efficiency (HHV) 56.9 percent			
Economic Summary			
Construction Cost $MM (1986)		2,831	
Total Capital $MM (1986)		4,405	
Net Annual Operating Cost $MM/year*		450	
Required Selling Price of Products			
C_3-C_4 Valued at $4.84/MM Btu			
Other Fuels Equal Volume basis $/Bbl		46.22	
Equivalent Crude $/Bbl		36.28	

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*Coal cost $22.70/ton.

Table ES-2
Recommendations for Future Research and Development

1. **Design, build and operate a Slurry-Phase F-T bench-scale unit large enough to investigate the following:**

    - Effect on hydrodynamics of superficial gas velocity, catalyst loading, pressure, and physical properties of components.
    - Estimation of overall heat transfer coefficient.
    - Continuous addition and removal of catalyst.
    - Continuous withdrawal of wax and catalyst/reactor wax separations.
    - Activation of F-T catalysts.
    - Interphase mass transfer coefficients.

2. **F-T Catalyst Developments:**

    - Develop supported or fused (Synthol type) catalysts for use in slurry F-T reactors.
    - Develop reproducible F-T catalyst based on precipitated iron or other.
    - Develop sulfur-tolerant F-T catalyst.
    - Characterize catalyst for fundamental understanding of catalyst performance.

3. **F-T Kinetic Investigations:**

    - Investigate relationship between space velocity and synthesis gas conversion for standard F-T catalyst.
    - Determine pressure effect on selectivity and activity.
    - Determine effects of synthesis gas H_2:CO ratio on catalyst activity/selectivity.

Table ES-2
Recommendations for Future Research and Development (Continued)

4. Systems Studies:

   - Improve estimates of slurry-phase Fischer-Tropsch and fixed-bed reactor costs including ancillary equipment.
   - Investigate optimum configuration for conceptual plants producing high wax.
   - Investigate potential of once-through F-T with cogeneration of electricity.

electric power can be examined. Substitution of the slurry F-T units with fixed-bed ARGE reactors or liquid-phase methanol reactors could also be investigated using the model when sufficient cost and performance data are available.

SECTION 1

INTRODUCTION

Previous MITRE studies performed in the early 1980s at the request of the Department of Energy estimated the potential effect that the use of advanced gasifiers and Fischer-Tropsch synthesis processes would have on the economics of indirect coal liquefaction.[1,2] Savings of about 35 percent on the required selling price of liquid products compared to the conventional SASOL configuration were shown. Much of this savings (about 60 percent) resulted from the use of high-pressure entrained gasifiers like the Shell system, and the additional savings came from use of advanced slurry-phase Fischer-Tropsch (F-T) synthesis reactors. These early MITRE studies used a detailed report by Mobil Research and Development Corporation (MRDC)[3] as the data base for much of the technical and cost information. The objectives of the MITRE reports were first to determine if advanced gasifiers and slurry F-T synthesis would result in substantial cost benefits, and second to identify research and development directions that had the potential to further improve the overall indirect liquefaction system. On the basis of these studies MITRE recommended that research into the use of slurry-phase F-T reactors with appropriate catalysts be pursued.

In a later study,[4] MITRE was requested by Sandia National Laboratories and the Department of Energy to develop a Techno-Economic Fischer-Tropsch (TEFT) simulation model that would be flexible enough to allow several sensitivity studies to be investigated. These sensitivities included changing the F-T catalyst activity and selectivity, and estimating the impact of these changes on the required selling price of liquid products. In this TEFT model, only the slurry-phase F-T reactor system and the raw product refining were simulated. Since the front-end gasification and gas cleaning sections were not included, no overall systems integration of the plant could be performed.

Sandia and the Department of Energy recognized the need for an overall integrated indirect liquefaction systems model that could be used as an important research and development guidance tool. This integrated model would conceptualize the transformation of input coal to finished liquid products using indirect liquefaction technologies, and integrate and balance all plant energy requirements. The model would also estimate construction costs, total capital and operating costs, and calculate the required selling prices of products for a variety of economic assumptions. The model would be flexible enough to perform sensitivity analyses and to answer "what if" type questions. Sufficient detail would be necessary to assess the impact of changing the plant subsystems and substituting new ones when required. The integrated model would also be capable of incorporating the results of new research and development initiatives as they become available and of using new cost numbers for unit operations so that constant updating is possible. This type of model could predict the potential economic and technical impact of advances in indirect liquefaction technology, and thus provide an important research and development guidance tool for both Sandia and the Department of Energy.

In response to the need for such a model, MITRE has developed a detailed, yet flexible computer-based integrated system model that meets all of the above requirements. This report documents the development of this integrated indirect liquefaction model and presents some preliminary results for a baseline indirect liquefaction plant. These results include the expected mass and energy flows for the baseline plant, together with an estimate of the capital and operating costs, and hence the required selling prices of liquid products from the plant.

SECTION 2

DEVELOPMENT OF THE INTEGRATED INDIRECT LIQUEFACTION SYSTEM MODEL

2.1 INTRODUCTION

The MITRE integrated indirect liquefaction system model is a grassroots model that simulates the processing of coal from coal handling and preparation to production of finished transportation fuels and liquified petroleum gas. The model therefore includes the production of clean synthesis gas from coal, Fischer-Tropsch (F-T) synthesis and raw F-T product refining. For the purposes of explanation, the model can be divided into three main sections, although it must be understood that there is complete integration among these sections with respect to mass and energy flows. The first section conceptualizes the preparation of the plant input coal for gasification, the gasification of the coal using Shell entrained gasifiers, and the shifting and cleaning of the raw gas to provide a synthesis gas acceptable for F-T slurry-phase reaction. The second section simulates the slurry-phase F-T reactors, raw F-T product separation, recycle of unconverted synthesis gas, carbon dioxide removal, hydrogen recovery, and autothermal reforming of the methane, ethane, and ethylene. The third section simulates the raw F-T product refining to diesel, LPG and gasoline, including the hydrocracking of the F-T wax produced in the slurry-phase reactors.

The model is developed on a personal computer using standard spreadsheet software. The advantages of the model can be stated as follows:

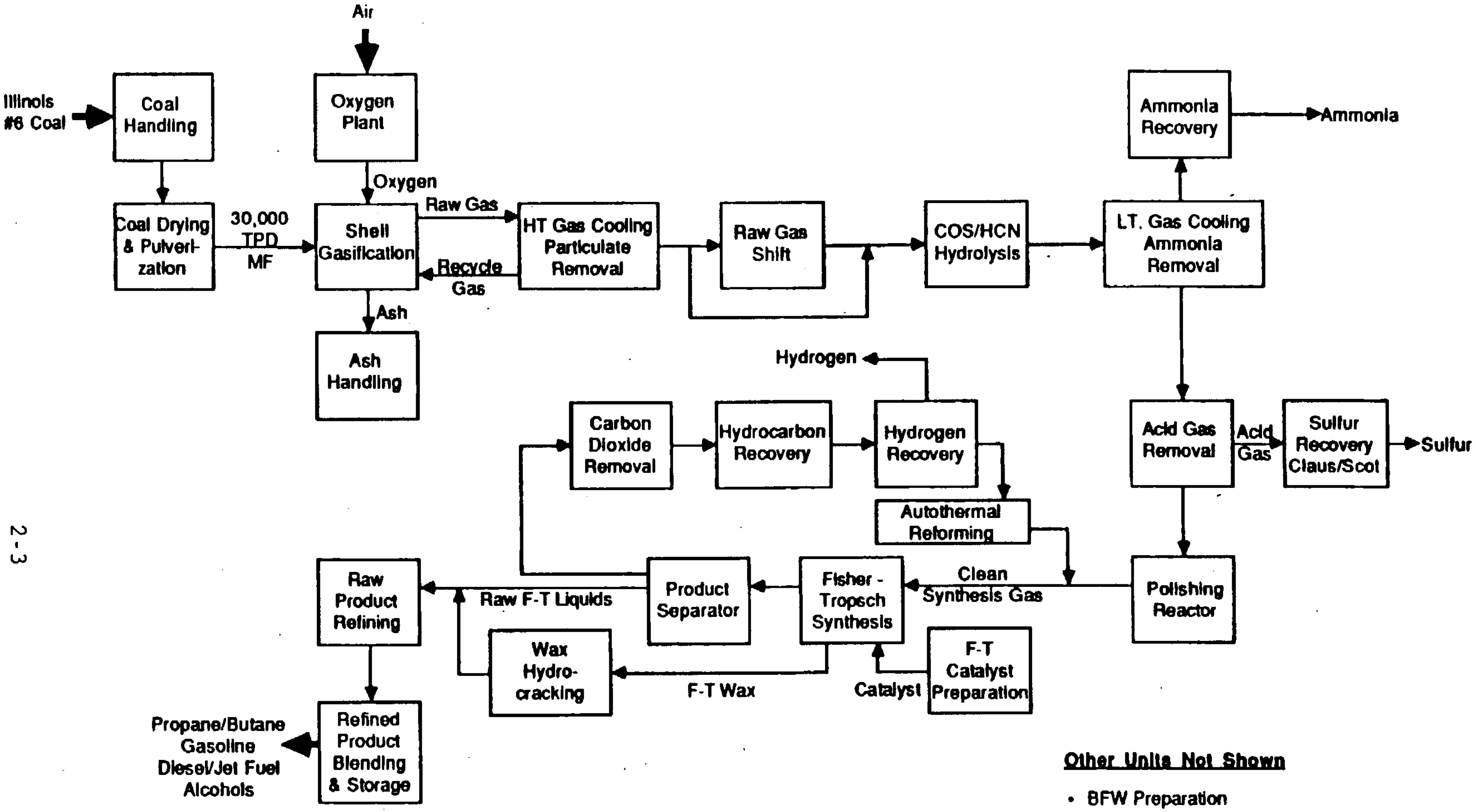
- The model is totally integrated from input coal to finished products.
- The model is grassroots, and all power and energy requirements are generated within the conceptual commercial plant. Excess power is sold as a by-product.
- The model is flexible enough to allow numerous sensitivity studies to be investigated and "what if" questions to be answered.
- The model can be readily updated as new research and better cost information become available.
- In the model, the financial assumptions can be easily changed.

Currently the major limitations of the model are the lack of reliability of the available cost data for some of the unit operations in an indirect coal liquefaction system, technical uncertainties as to the performance of slurry F-T reactors and catalysts, and the question of plant scaling factors. MITRE has used various sources for cost data in the development of the economic section of this model. Some of the data were generated several years ago and apply to units considerably smaller than the current model scale. The major data source, the Mobil Research and Development Corporation (MRDC) report of 1978,[3] conceptualized an indirect plant of approximately half the current model scale. There is thus some uncertainty as to whether the scaling factors used for some process equipment are applicable. As far as the costs of slurry-phase F-T reactors are concerned, there is currently no reliable data. More discussion of the economic data base is found in the economic section of this report.

The technical uncertainties apply mostly to the performance of the slurry F-T reactors and their catalysts. Definitive hydrodynamic data from large scale slurry-phase F-T reactors are unavailable. Most of the data are from cold non-reacting systems and very small (2-inch diameter) reacting bubble columns. The data from the Liquid Phase Methanol unit at La Porte, Texas are probably not applicable to slurry F-T processes because of the different properties of the materials and the smaller gas volume contraction during methanol synthesis. Until better hydrodynamic data are available, the model will use the hydrodynamic assumptions detailed below. The slurry F-T catalysts most often utilized in the DOE program have been the precipitated promoted iron type. Some of these have shown very adequate performance in the slurry system in terms of both their activity and selectivity. However, catalyst stability and the reproducibility of performance from batch to batch have yet to be demonstrated.

2.2 DESCRIPTION OF THE COMPONENTS OF THE INDIRECT LIQUEFACTION MODEL

This section of the report briefly describes the model development for the three major sections of the conceptual commercial plant. Figure 2-1 shows a block flow diagram of the general plant configuration that is simulated in the indirect liquefaction model. Coal that has been pulverized and dried is gasified with oxygen in Shell entrained flow gasifiers, and the raw gas is cooled, shifted, and cleaned of ammonia, particulates and sulfur to a level of 0.06 ppm by volume.[5] The cleaned synthesis gas is then reacted over catalysts in the F-T units to produce the raw hydrocarbon and oxygenate products. Unconverted synthesis gas, methane, ethylene, and ethane are separated and passed to carbon dioxide removal and autothermal reforming where the C_1 and C_2 hydrocarbons are reformed back to carbon monoxide and hydrogen and recycled to the F-T reactors. The raw F-T products (C_3 and higher hydrocarbons, plus alcohols) are then sent to a complex refinery for upgrading to LPG, gasoline, alcohols and diesel fuels. Other off-site units modeled but not shown in figure 2-1 are listed at the bottom of the figure.



Other Units Not Shown

- BFW Preparation
- CW Make-Up Preparation
- CW Towers
- Electric Power Generation
- Waste Water Treatment
- Relief and Blow Down
- Refrigeration

Figure 2-1
Components of MITRE Indirect Coal Liquefaction Model (Base Case)

2.2.1 Clean Synthesis Gas Production Section of the Model

Data on Shell gasification of Illinois coal are available from test results published by the Electric Power Research Institute (EPRI).[6] These tests were conducted in the 6 metric ton per day Shell gasification process development unit (PDU) in Amsterdam, The Netherlands. According to Shell, the cold gas efficiency (defined as the quotient of the thermal energy in the synthesis gas and the thermal energy of the input coal times 100) of a commercial-scale unit would increase several percent over that obtained in the PDU.[6] This increase is the result of several factors including a smaller wall heat loss in the commercial unit, reduced carrier gas flow and reduced oxygen consumption. Shell has demonstrated several of these efficiency gains from the results of their 150 metric tons per day unit in Harburg, FRG,[7] and since then have run many coals in their 200 T/D facility in Deerpark, Texas. Recent data from these Shell pilot plant tests have demonstrated 99^+ percent carbon conversion and thermal efficiencies in the range of 81-82 percent.[8]

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 thermodynamic equilibrium or on a specified approach to thermodynamic equilibrium. Carbon utilization and external thermal losses may be varied by input. This theoretical model produces results that are a very close match of test data for the entrained Shell gasifier performance.

The model can utilize carbon dioxide, nitrogen or synthesis gas as the high-pressure coal transport gas. Nitrogen was used in the Shell PDU gasification tests. 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 raw gas output. Shell suggests that product synthesis gas could also be used as high-pressure (HP) transport gas.[6]

In the integrated model, the exit gas at approximately 2700°F is cooled with recycle product gas to solidify molten ash particles in the exit to prevent molten slag from fouling the heat exchangers in the waste heat boilers. The model calculates the recycle required to achieve a temperature (controlled by input) that is below the ash deformation temperature of the feed coal. Figure 2-2 shows details of the clean synthesis gas production.

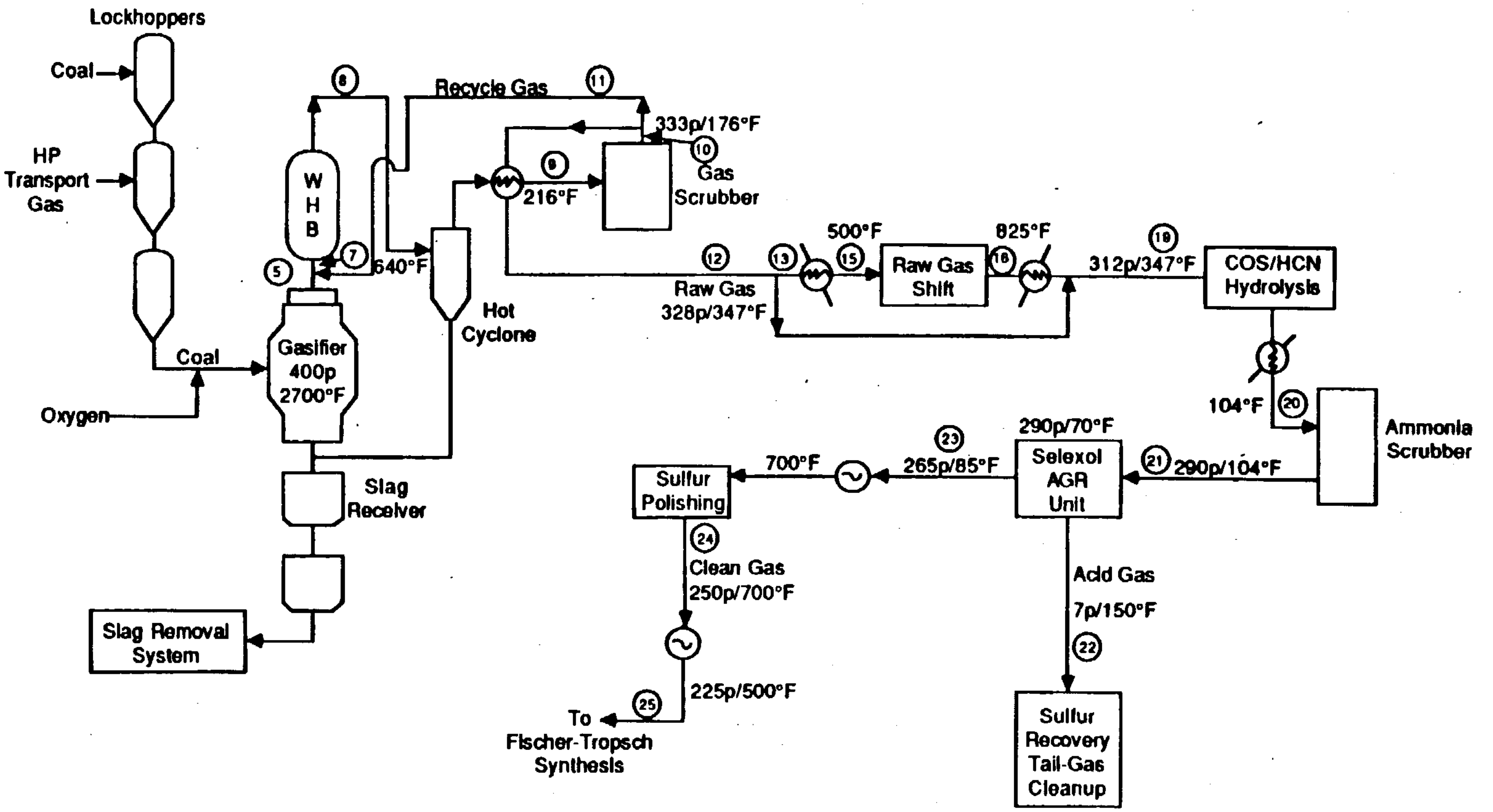
Stream 11 is the recycle gas stream needed to solidify the ash. The hot exit and recycle gas enter the waste heat boiler (WHB) that has both radiant and convective sections. High-pressure steam at approximately 1500 psig, 950°F is generated in the WHB. Most of this HP steam is utilized in the air separation/oxygen production facility. The overall heat and steam balance for the plant is discussed in Section 2.2.4.

Molten slag is removed through slag hoppers at the base of the gasifier, and overhead slag is cycloned and water scrubbed from the raw gas and returned to the underflow.

As shown in figure 2-2, the raw gas after gas scrubbing is split into two streams. One stream is shifted so that the recombined hydrogen to carbon monoxide molar ratio has the desired value. The model calculates the proportion of gas to be shifted, the amount of shift and the necessary steam to accomplish the shift for any required final hydrogen to carbon monoxide molar ratio. The amount of gas shifted, and the amount of shift are optimized to minimize steam consumption subject to the constraint that there be no less than 10 percent moisture in the shifted stream to avoid the potential for carbon formation.

Following shift, the gas enters carbonyl sulfide (COS) hydrolysis where the COS and the hydrogen cyanide (HCN) are hydrolyzed to H_2S and NH_3 respectively. COS hydrolysis is considered necessary since the Selexol physical absorption acid gas removal process absorbs H_2S much more readily than COS.[9] The hydrolysis reactions are not elementally modeled since the COS and HCN are only present in trace quantities. The hydrolysis unit is included in the integrated model so that unit size and stream heating and cooling requirements can be determined.

After another scrubber for NH_3 removal, the gas is sent to the Selexol process where the H_2S is reduced to about 1 ppm.[9] The sulfur in the acid gas is recovered using the Claus process.[9] Claus tailgas is cleaned using a Shell Claus Offgas Treating (SCOT) unit.[9] To remove the residual sulfur, the gas is sent to a zinc oxide polishing reactor.[9] Exit gas will contain about 0.06 ppm total sulfur, which is the sulfur level recommended for F-T synthesis.[5] Since optimum cleaning processes occur at different temperatures, the gas is alternately heated and cooled during the cleaning steps. The model conceptually simulates the heating and cooling requirements for the gas during the cleaning procedure. Clean product gas (stream 25) is then sent to the slurry-phase F-T units.



O Stream numbers corresponding to computer spreadsheet.
p- psig

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

2.2.2 The F-T Synthesis Section of the Model

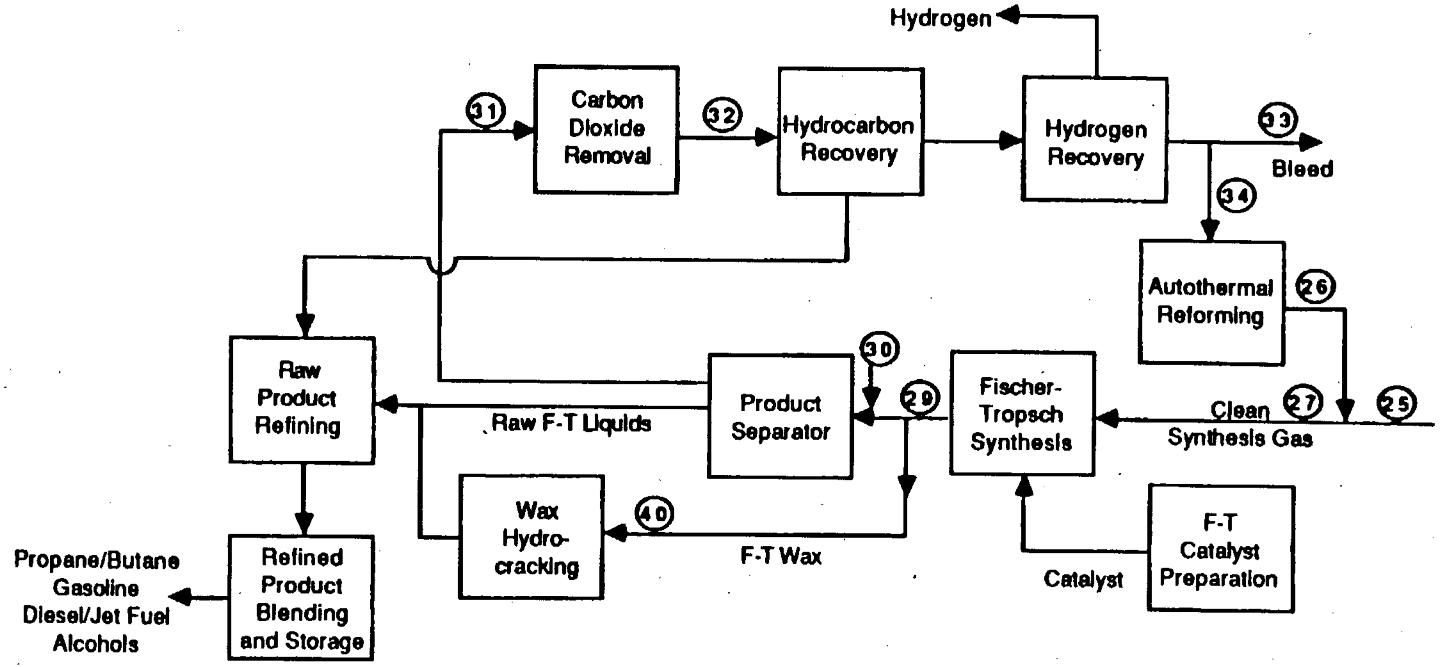
Figure 2-3 shows details of the F-T synthesis and recycle loop that is simulated in section two of the integrated model. The clean synthesis gas is passed to the slurry-phase F-T reactors (described below) where conversion to hydrocarbons and oxygenates occurs. The vapor phase effluent goes to product separation where essentially the C_5^+ material is dropped out and sent to the raw product refining section. The C_5^- material remains in the vapor state and this stream contains in addition the unconverted synthesis gas and carbon dioxide produced in the reaction. After passing through carbon dioxide removal, the C_3 and C_4 hydrocarbons are recovered in the hydrocarbon recovery unit. These recovered C_3 and C_4 hydrocarbons are sent to the refinery. In the hydrogen recovery unit the hydrogen required for the refining section is separated from the recycle gas using membrane separation. The computer model calculates the quantity of hydrogen required and sends the correct amount to all refining units needing hydrogen. The effluent gas from the hydrogen recovery unit still contains unconverted synthesis gas, methane, ethane and ethylene. When the conceptual plant is not designed to coproduce substitute natural gas (SNG), ethane or ethylene, the C_1 and C_2 hydrocarbons are autothermally reformed back to carbon monoxide and hydrogen with oxygen and steam. Before the recycle gas enters the reformer, a portion of the stream is bled to control nitrogen build-up and to provide plant fuel gas requirements. The computer model simulates this reforming process and calculates steam, oxygen and fuel gas requirements. The model also calculates the exit gas composition and feeds this information to the shift reactor units so that the combination of recycle gas and fresh feed (streams 25 and 26) have the correct hydrogen-to-carbon monoxide ratio for input to the F-T units. The model calculates compressor power requirements for the recycle loop and computes the steam required to drive the compressors.

Test results from the Mobil 2-inch reactor[10,14] have been used as the basis for MITRE estimates of the product selectivities. Mobil reported distributions with wax production ranging from 9.5 percent to 77 percent of the total product yield. The distributions had the following characteristics:

1. The production of C_2-C_{18} hydrocarbons closely approximates a theoretical Schulz-Flory distribution.

2. The product distribution of the wax (e.g., C_{19}^+) portion of the output is characterized by a probability of chain growth considerably higher than the C_1-C_{18} portion.

3. The production of methane is uniformly higher than would be predicted from theory at the theoretical chain growth probability (alpha) that matches the balance of the C_1-C_{18} distribution.



○ Stream numbers correspond to computer spreadsheet

Figure 2-3
Fischer-Tropsch Recycle Loop Details

4. Oxygenates are produced in an amount approximately equal to 5 percent of the C_1-C_{18} hydrocarbon make.

The algorithms developed by MITRE to approximate the Mobil distributions are based on theoretical distributions for the alphas indicated by the wax and non-wax portions of the output. The high C_1 output is estimated by setting C_1 output to be equal to the theoretical C_2 output on a weight percent basis. The C_1-C_{18} distribution is then scaled down by 5 percent to account for the estimated production of oxygenates. The theoretical production of C_{19}^+ material is scaled down until the production of C_{19} material is the same as would have been predicted by the non-wax alpha.

Figures 2-4, 2-5, and 2-6 show MITRE estimates compared to Mobil test results for distributions having wax makes of 9.5 percent, 46 percent, and 77 percent, respectively. Figure 2-7 shows the values of alpha required to match the Mobil distributions plotted as a function of weight percent wax make. Distributions for any wax make can thus be approximated from the MITRE algorithm by selecting appropriate alphas from the curve.

Figure 2-8 details 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.[10] These reactors are 14.5 feet in diameter and 35 feet in height with an upper disengaging section 16 feet in diameter and 14 feet 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 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.

F-T catalyst life is an input variable. Fresh catalyst slurry is introduced to the reactor when required to keep the average catalyst activity of the inventory to the required level. This catalyst is slurried and prepared in catalyst pretreatment vessels as described in the Mobil report of 1985.[10] Spent catalyst is withdrawn from the bottom of the reactor, centrifuged to remove wax and discarded. Continuous withdrawal and addition of activated catalyst slurry has never been demonstrated on a pilot scale for slurry reactors. Thus, this area of the model is speculative in the implied assumptions that these procedures are possible. Also, effective removal of the finely divided catalyst particles from the

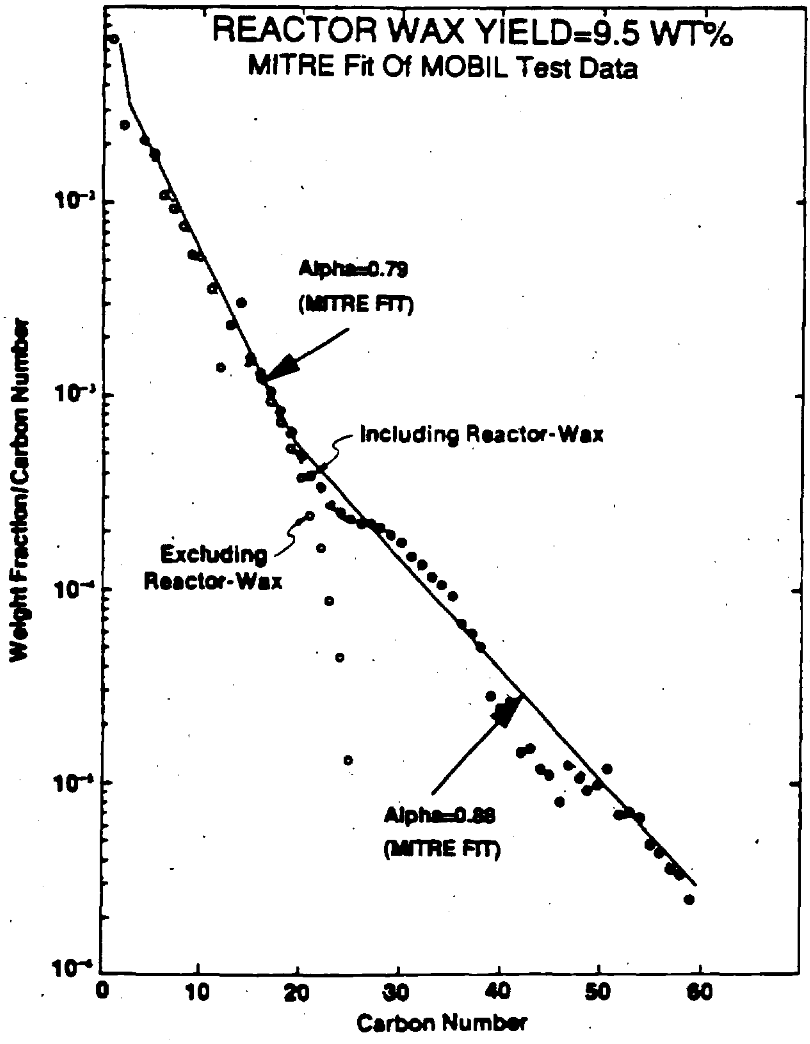


Figure 2-4
MITRE Fit of Experimental Test
Schulz-Flory Distribution Mobil Run C7-256-3,
9.5 wt% Wax

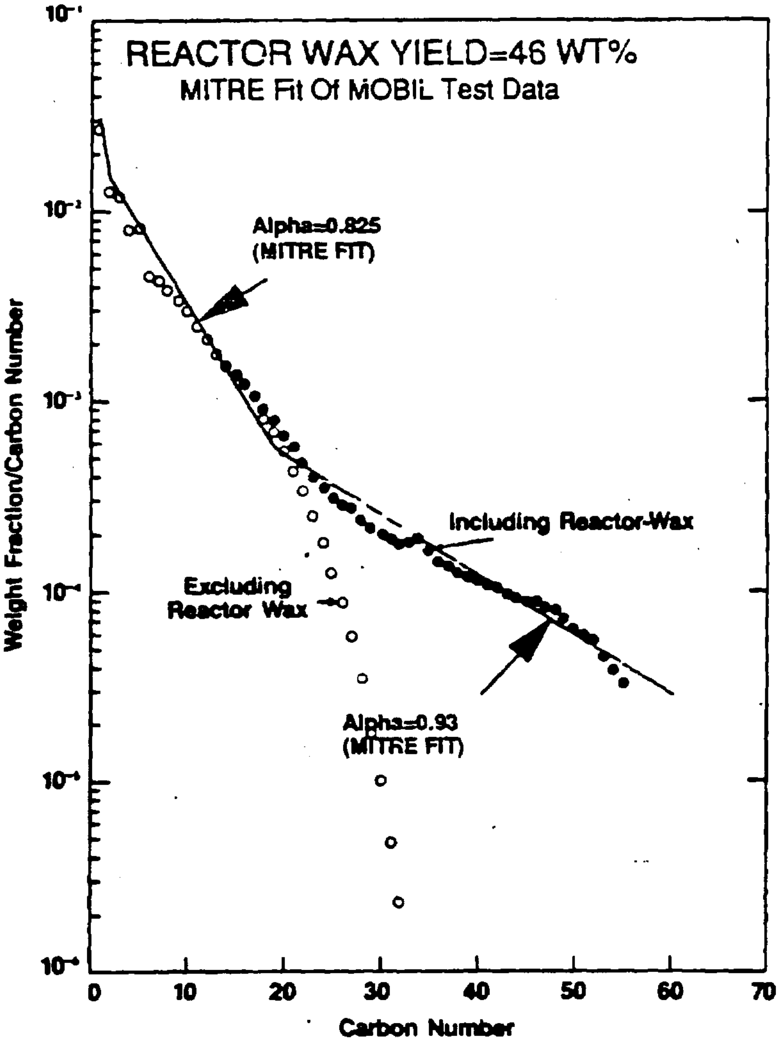


Figure 2-5
MITRE Fit of Experimental Test
Schulz-Flory Distribution Mobil Run C7-256-4,
46 wt% Wax

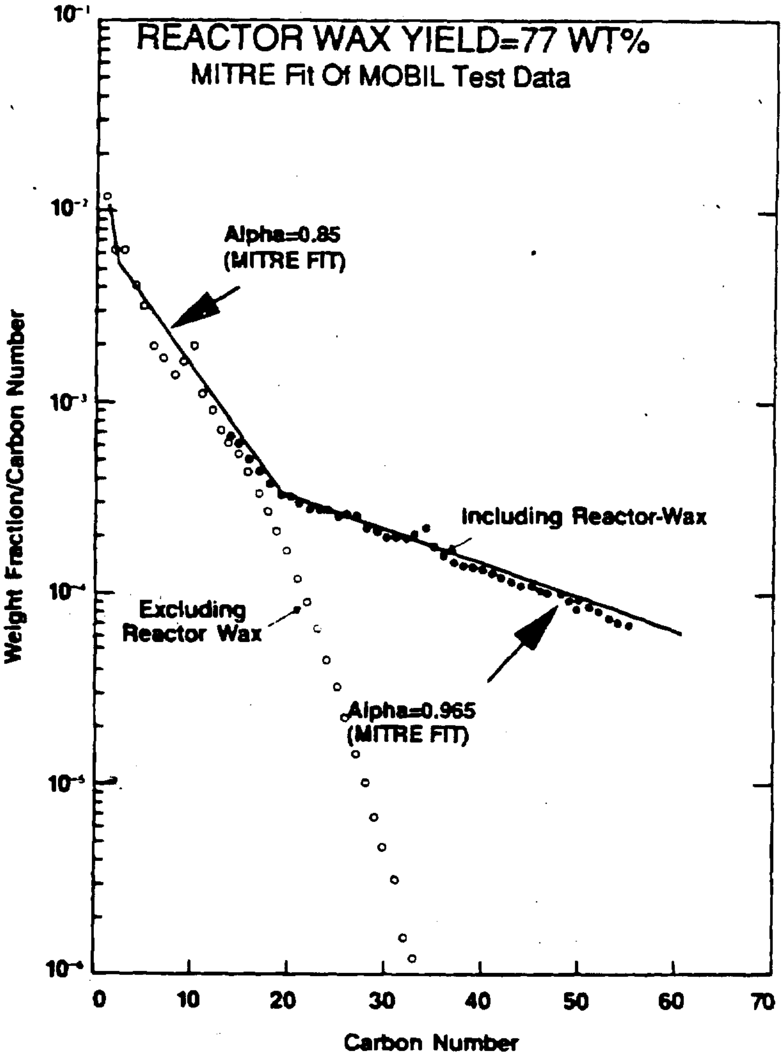


Figure 2-6
MITRE Fit of Experimental Test
Schulz-Flory Distribution Mobil Run C7-256-5,
77 wt% Wax

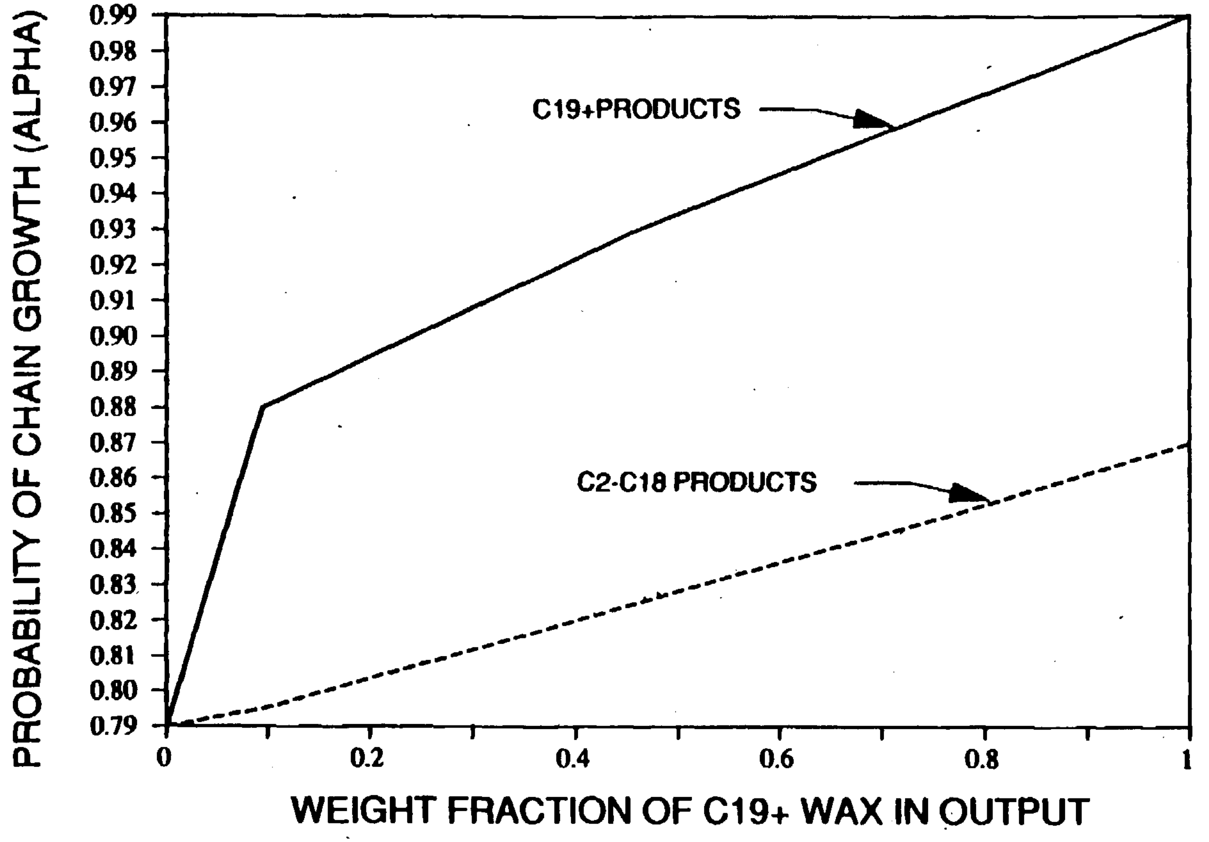


Figure 2-7
Values of Alpha Required to Match
Mobil Distributions

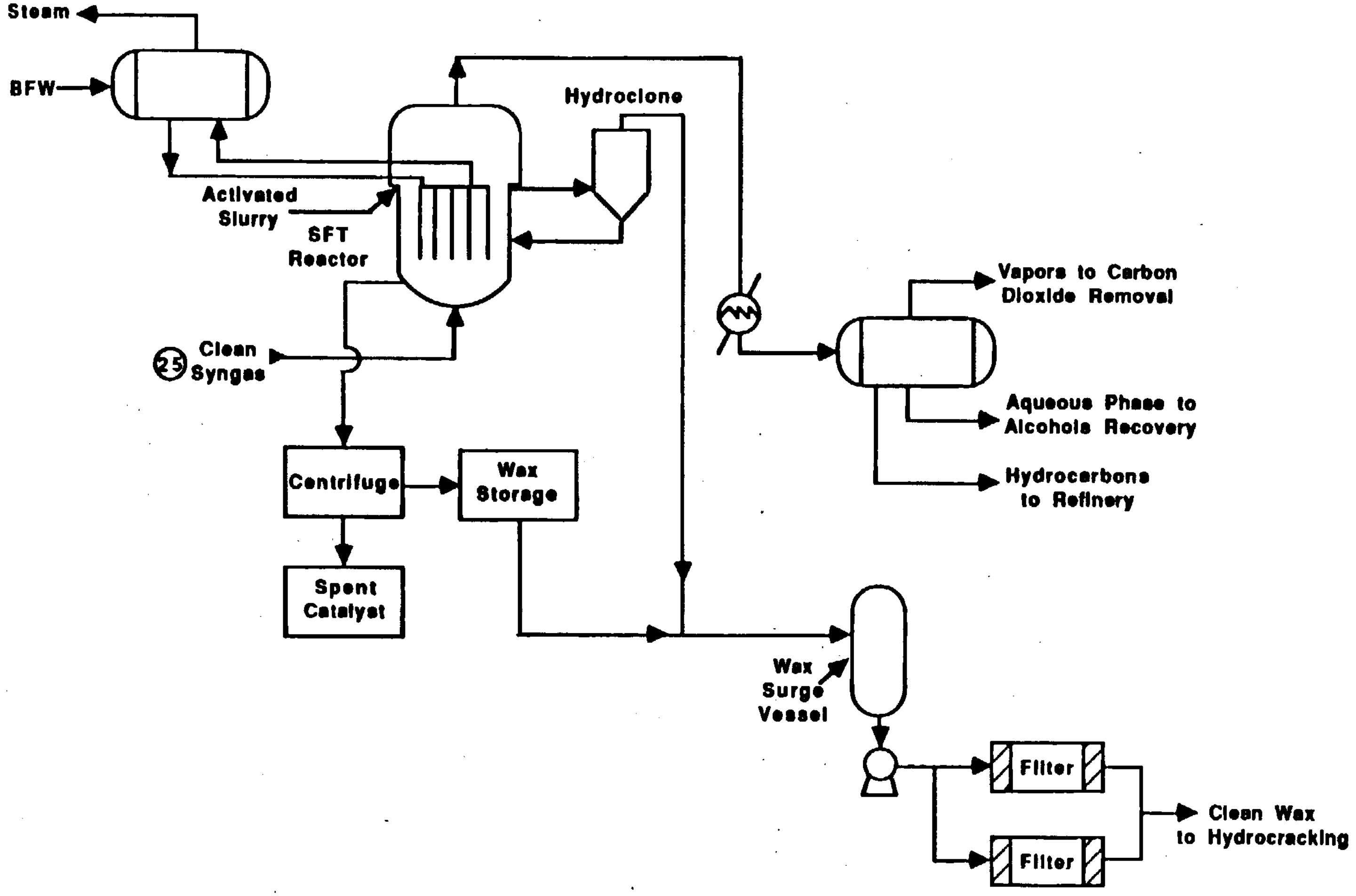


Figure 2-8
Detail of Slurry Fischer-Tropsch Reactor System

wax has not been proven, but the model assumes this is possible so that the clean wax may be hydrocracked in a fixed-bed UOP Unibon unit.

Slurry reactors are complex because, in addition to the usual chemical kinetic and mass diffusion constraints, the reactor hydrodynamics also impart a constraint. For the reaction kinetics part of the simulation, it is assumed that the F-T catalyst has a certain activity that is defined by a pseudo-first-order rate constant A. This rate constant relates the conversion per pass of the synthesis gas (C) to the space velocity (SV) by the following equation:

$A = (SV/P)*\log(1/(1-C))$

where SV is the space velocity in normal liters of gas per gram catalyst-hour

P is the total pressure in bar

C is the per pass conversion.

This equation was used by Farley and Ray[11] to assess the catalytic activity of their F-T slurry during operations of their slurry-phase unit. Using the above relationship, it is possible to relate the space velocity to the per pass conversion for any catalyst whose activity rate constant A is known.

The hydrodynamic performance of the reactors was simulated by assuming a relationship between the superficial gas velocity (U_S) and the average gas hold-up (h_G). The relationship used, that of Bach and Pilhofer, is suggested by Bukur[12] at Texas A&M University. Bukur has found it to correlate well with much of the data for slurry F-T reactors. Other correlations may be used if desired. The mathematical equation that describes this relationship is used in the model to calculate the gas hold-up that results from varying superficial gas velocities of feed synthesis gas. Kölbel and Ralek,[13] in their treatise on the Fischer-Tropsch synthesis in the liquid phase, show an operational range diagram for a bubble column reactor with suspended solid matter of average particle size 30 microns and solid to liquid density 2:1. In this diagram there is an upper boundary curve shown, above which the formation of large bubbles occurs with a substantially reduced interfacial surface area. Kölbel and Ralek state that the actual curve is dependent on the material properties and the reactor geometry. The data used in this report are taken from operations of the 2-inch diameter reactor of Mobil.[10,14] 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 shown in the Kölbel and Ralek operational range diagram.

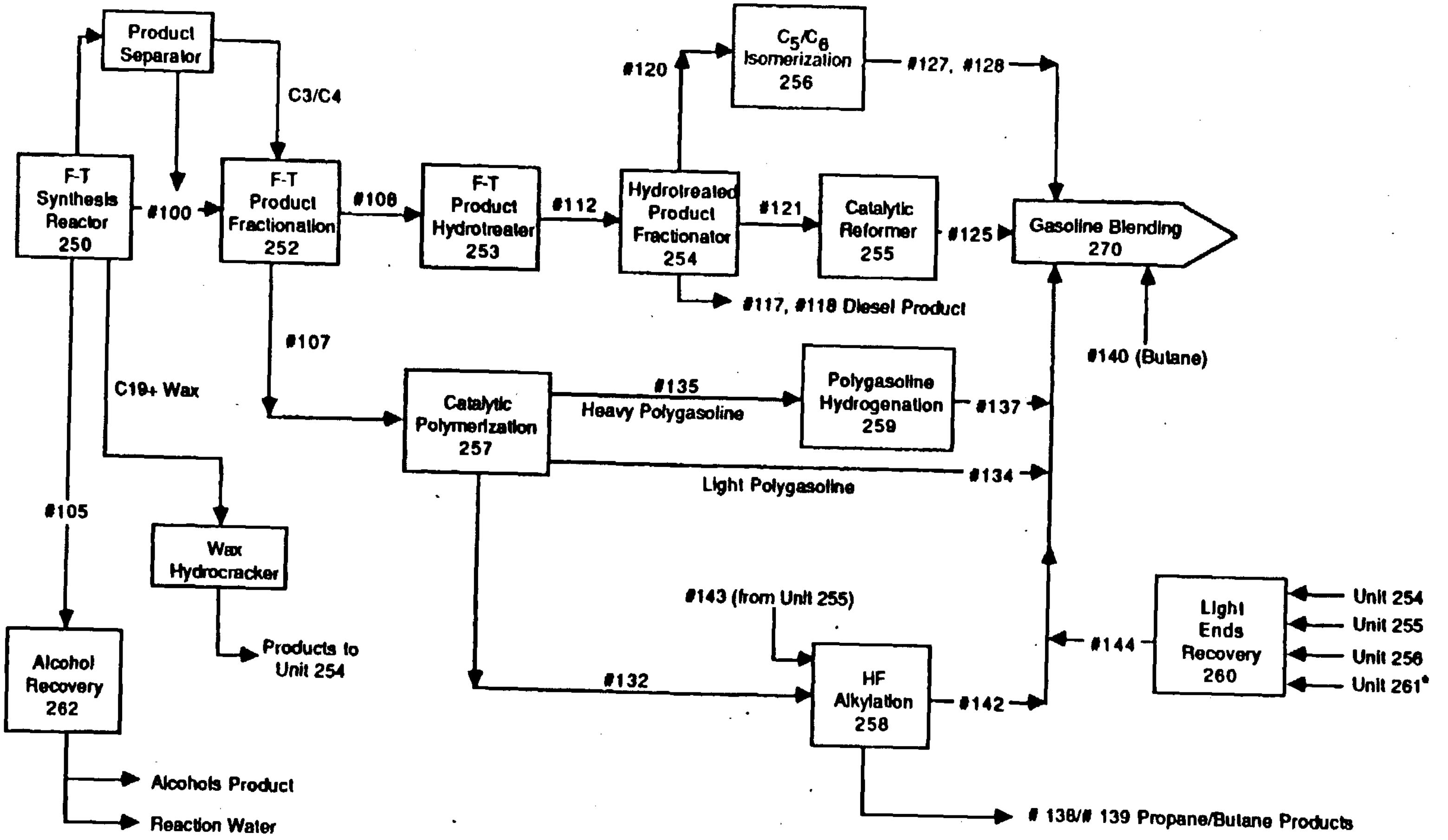
The model calculates the number of reactors required to process a certain volume of synthesis gas at certain temperature and pressure for a given catalyst loading (weight percent of catalyst in the slurry), and for certain reactor wax and catalyst densities. The kinetic information in the program calculates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

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. The results in this report assume a heat transfer coefficient of 70 Btu/hour sq ft deg F as suggested by Farley and Ray.[11] However, the value of this heat transfer coefficient is an input variable in the model and can be changed as better data are obtained. The log mean temperature difference is determined by the reactor temperature, and the cooling fluid inlet and outlet temperatures. The model calculates the heat released in the reaction, the log of the mean temperature difference, and hence the area of heat transfer required for an input overall heat transfer coefficient. Using standard pipe parameters, this area is translated into the volume of piping needed, and hence the percent of total reactor volume occupied is calculated. This volume percentage is then used in the model to adjust the number of reactors to include the heat transfer equipment.

2.2.3 The Refining Section of the Model

The purpose of the refining section is to produce liquefied petroleum gas (LPG), gasoline and diesel fuel from the raw F-T product. This product is predominantly paraffinic compounds containing a large percentage of olefins together with some oxygenates. The carbon range can be from C_1 to C_{500} or higher depending on the nature of the wax produced. Since C_1 and C_2 are autothermally reformed, the raw product delivered to the refinery consists of C_3 and C_4 paraffins and olefins, a C_5 to C_{11} raw naphtha range material, a C_{12} to C_{18} diesel range material, a C_{19}^+ wax material and a range of oxygenates. This complex refining scheme includes processes for polymerizing the C_3/C_4 olefins into naphtha range material, increasing the octane number of the naphtha, hydrocracking the wax to distillate and recovering the oxygenates.

Figure 2-9 shows a schematic of the refining section of the model. The stream numbers in the figure correspond to the computer spreadsheet print out. Stream 100 consists of the raw F-T output except for the C_3 and C_4 material, the alcohols, reaction water and wax. This stream is fed to unit 252, the F-T product fractionation unit where the raw product is separated into streams 107 and 108. Stream 107 containing essentially all



* Unit 261 Hydrogen Purification not shown.
\# Corresponds to stream numbers in computer spreadsheet.

Figure 2-9
Raw Fischer-Tropsch Product Refining

of the C_3 and C_4 hydrocarbons is sent to the catalytic polymerization unit 257. In this unit the C_3 and C_4 olefins react over an acid catalyst to form C_6^+ naphtha range material. The paraffins are inert in this unit and pass through unchanged. The model simulates the catalytic polymerization reactions that occur to produce light and heavy polygasoline. The light polygasoline is sent directly to gasoline blending, and the heavy polygasoline is hydrogenated to saturate olefins before blending. The unconverted C_3 and C_4 olefins, together with the propane and butane, are sent to alkylation unit 258. Here the residual olefins react with isobutane from the platformer (unit 255) to yield additional naphtha range material. The alkylate (stream 142) is then blended into the gasoline. The model simulates the alkylation reactions based on molar stoichiometry. The butanes and propanes are sold as product LPG, except for a small quantity of butane that is blended into the gasoline.

Stream 108 consists essentially of the C_5^+ hydrocarbons (excluding wax) that must be hydrotreated to reduce the olefin content and remove residual oxygen. This stream is sent to the product hydrotreater unit 253, and the output is then fractionated in unit 254. The model simulates the hydrotreatment and calculates the required hydrogen that is recovered from the recycle gas stream by the hydrogen recovery unit. In order to increase the octane, the C_5 and C_6 paraffins are sent to isomerization unit 256, and the C_7 to C_{11} raw naphtha stream is sent to the catalytic reformer. The outputs from these units are blended into the final gasoline. The model calculates reformate and isomerate yields from yield data in the MRDC report.[3] The hydrotreated C_{12} to C_{18} stream from unit 254 is the diesel product.

The wax produced in the F-T reaction is filtered and sent to the UOP Unibon hydrocracker where it is cracked to produce gases, naphtha and distillate. The model calculates the hydrogen required and the products produced based on an input feed cracking selectivity. Experimental results from hydrocracking several waxes have been obtained by UOP[14] and their conclusion is that F-T wax is an excellent feedstock for this process and can readily be cracked to produce high quality diesel blending stock.

The alcohols and other oxygenates are separated from the reaction water in the alcohol recovery unit and can be sold as products or can be blended into the gasoline to enhance the octane.

2.2.4 Waste Heat Recovery and Steam Generation

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.

The overall sensible heat balance is summarized in table 2-1. Negative numbers represent heating requirements. The major heat sources are the gasifier exit stream and the F-T synthesis reactors.

The steam generation system is designed to produce high-pressure (HP) steam at about 1500 psia, and medium-pressure (MP) steam. The MP steam pressure is selected to be compatible with F-T reactor temperature, which is the major source of heat available for MP steam saturation. A difference of 15-20°F between steam saturation temperature and reactor temperature is desired. In the base case described in this report, the reactor temperature is 493°F. A MP steam pressure of 550 psia having a saturation temperature of 476°F is selected for the base case.

The steam generation system is shown schematically in figure 2-10. Miscellaneous heat sources having a driving temperature below 500°F are used to heat BFW. The HP steam is saturated and superheated to 950°F in the gasifier waste heat boiler. HP steam is used to meet power requirements in the oxygen plant.

MP steam is saturated in the F-T heat recovery system. MP steam not required for process purposes is superheated to 900°F in the waste heat boiler. All superheated MP steam is used to drive turbines for electric power generation. Turbine bleeds at 200 and 50 psia are used to supply low-pressure steam to meet process requirements.

The quantity of MP steam made is determined by the reaction heat available for MP steam saturation. The quantity of HP steam produced is limited to the quantity that can be produced and finished in the gasifier WHB after MP superheat requirements are met. This strategy is believed to result in near optimum use of the waste heat available from all sources.

2.2.5 The Off-Sites Section of the Model

Table 2-2 lists the off-site units that are an integral part of the model. The off-sites support the on-site process units and are briefly described below.

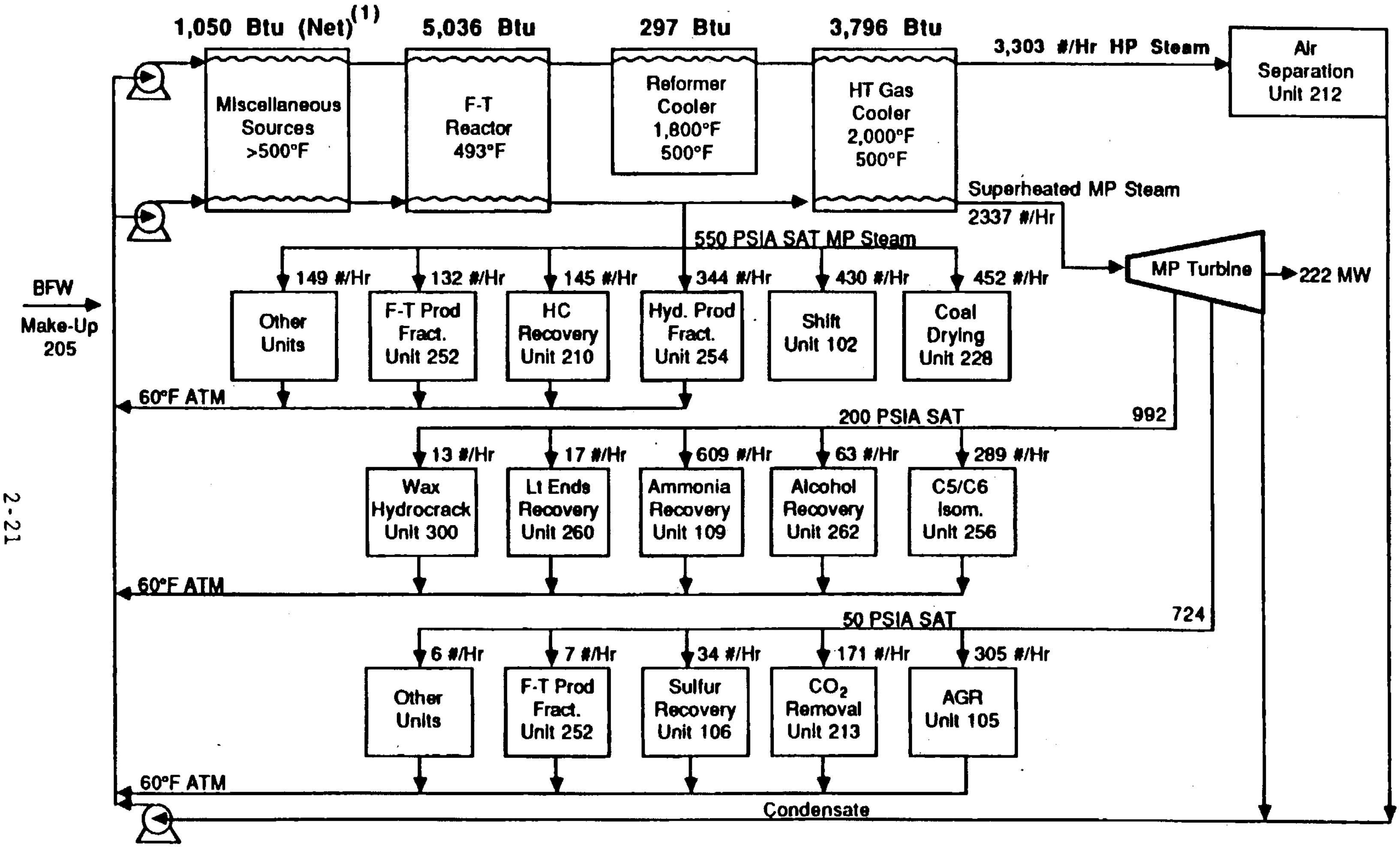
The oxygen plant or air separation unit (unit 221) provides the oxygen required for the gasifiers, and also provides plant nitrogen requirements for coal drying and other uses. The plant consists of steam driven turbines that are powered by the high-pressure steam generated in the gasifier waste heat boilers. The model calculates the steam requirements for the oxygen needed.

The coal handling and drying unit 228 consists of coal receiving, storage, crushing, drying, and pulverizing. The coal is dried with hot nitrogen

Table 2-1
Overall Sensible Heat Balance

Heat Source	10^6 Btu	Temp Range °F		Above 496	Above 600
Gasifier Cooler (HT)	3,796	2,000	500	3,796	3,543
Gasifier Cooler (LT)	641	500	216	8	0
Shift Heater/Cooler	(21)	176	357	0	0
Shift Boiler	175	825	500	180	121
Polish Heater/Cooler	(69)	85	700	0	0
Reactor Exotherm	5,036	496		0	0
Reactor Cooler	387	496	250	0	0
Reformer Heater	(63)	100	500	0	0
Reformer Cooler	297	1,800	496	297	274
Turbine Exhaust	0	970	280	0	0
TOTAL	**10,180**			**4,281**	**3,938**
Steam Generation Summary	High PR	MP Steam	MED PR	200psi	50psi
Pressure	1,500	550	550	200	50
Temperature	900	900	478(SAT)	382(SAT)	281(SAT)
Enthalpy	1,429	1,464	1,204	1,198	1,174
BFW = 100°F	1000#	1000#	1000#	1000#	1000#
Power Generation		2,337			
Oxygen Separation	3,303	0			
Shift/Reformer			473		
Other 0	0	1,180	992	724	
TOTAL	**3,303**	**2,337**	**1,653**	**992**	**724**

Sources:	**10^6Btu**		**Uses:**		**10^6Btu**
Deg F=< 496	862		Saturated Process Steam		2,603
@F= 496	5,036		HP Steam		4,390
Deg F=> 496	4,281		MP Superheated Steam		3,188
Deg F=> 598	3,938				
TOTAL	**10,180**		**TOTAL**		**10,180**
Total Steam M#/hr	8,017				
Power Generation:	MW		600 F+ Available		3,938
HP Turbine	0		600 F+ Required		3,290
MP Turbine	222				MW
			Steam	**Total**	**Net**
Total MW Produced =			222.11	222	39
MW Required =			183		



(1) Net of miscellaneous gas-to-gas reheat requirements.

Figure 2-10
Steam Balance Summary
(10^6 Btu and 1,000 #/Hr)

Table 2-2
Off-Site Units

UNIT #	DESCRIPTION
221	Oxygen Plant
227	Instrument/Plant Air
228	Coal Handling and Drying
229	Ash Handling
230	Electrical Distribution
231	Boiler Feed Water (BFW) Preparation
232	Cooling Water (CW) Preparation
233	Cooling Water Towers
234	Power Generation
235	Wastewater Treatment
236	Blowdown
237	Storage
238	Interconnecting Piping
241	Refrigeration
270	Gasoline Blending
271	Fischer-Tropsch Catalyst Preparation
600	Infrastructure*
700	Miscellaneous

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*Includes the following: Buildings, laboratory, maintenance shops
Storm and fire water systems
Loading/unloading facilities
Site preparation (including parking lots, fencing, lighting security, sewers).

during the pulverization process. The nitrogen is heated with medium-pressure saturated steam, a configuration used by Fluor in their study of Shell gasification/combined cycle for EPRI.[16] The model calculates nitrogen and steam requirements for drying input quantities of coal to any residual moisture content.

The cooling water system includes cooling water preparation (unit 232) and the cooling towers (unit 233). Cooling water duty for the entire plant is calculated by the model based on requirements for steam condensation and other uses. The boiler feed water system consists of the BFW preparation unit and the deaerator (unit 231) that purifies and recycles water for use in the plant operations. The model calculates BFW requirements based on estimated uses and blowdown losses during recycle. The wastewater facility treats the various process wastewaters from the plant complex using activated biological treatment. The model calculates the quantities of wastewater produced. It is assumed that the treated water is used as cooling water make up.

All plant power needs are generated by the power generation unit 234, and the power is distributed to users by the electrical distribution system (unit 230). In the baseline model, the power is produced using steam turbines. Power requirements for all unit operations are calculated in the model, and excess power is sold as a by-product.

The Fischer-Tropsch catalyst preparation unit (unit 271) prepares the iron catalysts for the synthesis reactors using magnetite as raw material. The model calculates the catalyst make up required for an input average catalyst life.

Other off-site units in the model include storage facilities for products and chemicals, refrigeration for hydrocarbon recovery and acid gas removal units, gasoline blending to produce the final gasoline mix from the component streams, interconnecting piping, and miscellaneous units such as water ponds, additional tankage, etc. The associated infrastructure (unit 600) includes site preparation, buildings, and fire and storm water systems.

2.2.6 The Economic Section of the Model

The construction cost for the conceptual commercial plant that is simulated in the model is estimated in the following manner. Individual unit costs are used based on data from several open literature sources. These reference costs are for units of varying capacities and are costed in different year dollars. These reference construction costs and capacities, scaled by the model for the required capacity and the reference year dollar costs, are all brought to the same year basis using the Nelson-Farrar cost indices. Table 2-3 shows the plant units together with their reference capacities and construction costs. Also shown in the table are the open literature data sources for the costs.

The plant capital requirements are then computed by the model from the estimated construction cost as follows. Engineering design and project contingency is estimated at 25 percent of the construction cost. The sum of these gives the total plant investment (TPI). The allowance for funds used during construction is 16.9 percent of the TPI. The sum of TPI and the funds used during construction constitute the total depreciable capital. The non-depreciable capital is calculated as the sum of the start-up costs, working capital, and initial charge for catalysts and plant chemicals. The start-up costs are 20 percent of the gross annual operating costs (GAOC), and the working capital is 25 percent of the GAOC. The total plant capital cost is then the sum of the depreciable and non-depreciable capital. Table 2-4 illustrates how the total capital required is computed.

The GAOC is calculated in the model in the following manner. Costs of coal, catalyst, chemicals, and water requirements are calculated based on unit input costs. Process operating labor is estimated based on plant manpower needs for the different plant areas. These manpower needs are based on those estimated by Mobil for their conceptual plant.[3] Overhead, general and administrative costs are 60 percent of labor. Maintenance is 3.5 percent of the TPI, and local taxes and insurance is 2 percent of TPI. Solids disposal is calculated based on a cost of $6 per ton. By-product credits from the sale of ammonia, sulfur, and excess electric power are subtracted from the total GAOC to give the net annual operating cost.

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.

2.2.7 Sensitivities That Can Be Investigated with the Model

The integrated simulation model is very flexible in its ability to investigate a large variety of sensitivities. Since the objective of the development of the model is to provide research guidance and a quantitative

Table 2-3
Reference Construction Costs and Capacities for Units in Model (Continued on next page)

Ref*	Unit#	Description	Con.Cost $MM	Year	Base Yr Cost $MM (1986)	Capacity Moles/Hr	Capacity Lb/Hr
Gas Preparation and Synthesis:							
Mobil'85	250	F-T Synthesis	287.00	1985	290.58	106,782	2,111,070
FPL	101	Shell Gasification	350.70	1987	340.50	(5%M** Coal)	1,010,100
MRDC	102	Shift	13.00	1977	21.33	36,303	737,400
Braun	103	COS Hydrolysis	5.40	1976	9.54	74,472	
Braun	104	Sulfur Polishing	5.00	1976	8.83	67,512	
Norton	105	AGR Selexol	10.80	1978	18.50	22,800	
Braun	106	Sulfur Recov., Claus/Scot	28.00	1976	49.47	2,877	
UOP/SDC	109	Ammonia Recov. Phosam W	23.00	1981	27.73	86,000	1,548,860
MRDC	116	Autothermal Reforming	36.50	1977	60.83	40,111	606,637
F-T Product Refining:							
MRDC	262	Alcohol Recovery	11.00	1977	18.33	25,560	479,848
MRDC	252	F-T Prod. Fractionation	14.50	1977	24.17	4,322	227,500
MRDC	253	F-T Product Hydrotreater	6.60	1977	11.00	1,100	123,922
MRDC	254	Hyd. Prod. Fractionator	3.80	1977	6.33	1,212	123,400
MRDC	255	Cat Reformer	7.30	1977	12.17	397	46,972
MRDC	256	C_5/C_6 Isomerization	5.30	1977	8.83	474	37,128
MRDC	257	Cat Poly Unit	4.10	1977	6.83	1,093	52,589
MRDC	258	HF Alkylation	2.20	1977	3.67	376	18,729
MRDC	259	Polygas Hydrotreater	2.40	1977	4.00	135	19,482
MRDC	260	Lt Ends Recovery	2.20	1977	3.67	408	16,788
MRDC	261	H_2 Purification	2.70	1977	4.50	860	10,421
MRDC	210	Hydrocarbon Recovery	19.40	1977	32.33	30,409	533,527
MRDC	211	H_2 Recovery	8.80	1977	14.67	1,887	3,804
GPH	213	Benfield CO_2 Removal	92.00	1986	92.00	71,000	
UOP	300	Unibon Wax Hydrocracking	27.00	1987	26.21		288,649

Table 2-3
Reference Construction Costs and Capacities for Units in Model (Concluded)

Ref*	Unit#	Description	Con.Cost $MM	Year	Base Yr Cost $MM (1986)	Capacity Moles/Hr	Capacity Lb/Hr
Offsite Units:							
UOP/SDC	221	Oxygen Plant	160	1981	192.17	20,175	645,656
MRDC	227	Instrument/Plant Air	1	1977	1.00		
UOP/SDC	228	Coal Hand Drying	154	1981	185.98		2,823,734
UOP/SDC	230	Power Distribution	57	1981	68.67	285 (MW)	
EPRI	231	BFW Preparation	7	1981	8.53		547,000
MRDC	232	Cooling Water Prep.	0.50	1977	0.83		3,141,600
UOP/SDC	233	CW Towers	20	1981	23.76	334,000 (GPM)	
MRDC	234	Power Generation	11	1977	18.33	61 (MW)	
MRDC	235	WW Treatment	26	1977	43.83		2,103,600
MRDC	236	Blowdown	3	1977	4.50		837,900
MRDC	237	Storage	9	1977	14.33		204,300
MRDC	238	Intercon. Piping	20	1977	34.00	849,123 (lb/hr Coal)	
MRDC	241	Refrigeration	2	1987	1.46	90 (10^6 Btu/hr)	
MRDC	270	Gasoline Blending	2	1977	3.33		140,900
MRDC	271	F-T Cat. Preparation	28	1977	46.17		2,480
UOP/SDC	600	Infrastructure/Misc.	65	1981	78.58	(Scaled on Coal thru)	
MRDC	700	Misc	30	1977	50.00	106,782 (Syngas Feed)	

* Mobil 85 - Ref. 10
FPL - Ref. 17
MRDC - Ref. 3
Braun - Ref. 9
Norton - Norton Sales Tech. Info. Brochure
UOP/SDC - Ref. 18
GPH - Gas Processing Handbook 1986
UOP - Ref. 15
EPRI - Ref. 16
** M=Moisture

Table 2-4
Calculation of Plant Capital Requirements

1.	Construction Cost	
2.	Engineering Design & Project Contingency	25% of 1
3.	TOTAL PLANT INVESTMENT (TPI)	Sum of 1 and 2
4.	Allowance for Funds Used During Construction	16.9% of 3
5.	TOTAL DEPRECIABLE CAPITAL	Sum of 3 and 4
6.	Start-up Costs	20% of GAOC*
7.	Working Capital	25% of GAOC
8.	Initial Charge of Catalyst & Chemicals	Calculated
9.	TOTAL NON-DEPRECIABLE CAPITAL	Sum of 6, 7, and 8
10.	TOTAL CAPITAL REQUIRED	Sum of 5 and 9

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*GAOC = Gross Annual Operating Cost.

measure of research success, it is necessary to analyze the impact of changing parameters.

Table 2-5 lists the sensitivities that can be currently investigated using the model. The gasification section of the model allows characteristics of coal input to the Shell gasification area to be changed. The overall feed rate of coal can be changed, hence the plant size. Since the model simulates the gasification performance from thermodynamics, the carbon conversion and heat loss from the gasifier are also a variable. Thus gasification performance of coals not tested can be simulated by entering the appropriate coal characteristics. The model also allows the high-pressure coal transport gas to be changed from carbon dioxide to nitrogen or synthesis gas. Synthesis gas hydrogen-to-carbon monoxide molar ratio can be changed by changing or eliminating shift. The unit operations for raw gas cleaning can be eliminated or bypassed to the extent required.

In the F-T section of the plant, the raw F-T selectivity can be altered so that high wax, low wax, or any other selectivity case can be investigated. In the model, the selectivity is governed by the Schulz-Flory distribution that can be altered as required. In addition, the percent olefins and oxygenates for the different carbon numbers can also be changed. The impact of varying the Fischer-Tropsch catalyst activity can also be investigated by entering different rate constant values into the model. The catalyst life can also be changed as required.

The model allows several parametric changes to be made in the F-T slurry reactor itself. These include the reactor size, the amount of catalyst in the slurry (catalyst loading), the relationship between gas hold-up and superficial gas velocity, the reactor pressure and temperature, and the overall heat transfer coefficient.

In the raw F-T product refining section, unit refining operations can be eliminated, and when data are available new ones can be added. The wax hydrocracking selectivity can also be modified and the hydrocracker distillate could be recycled to reduce the diesel end point.

In the overall configuration, the plant can be operated in a recycle mode, where all the C_1 and C_2 gases are reformed back to synthesis gas or in the once-through mode where there is no recycle back to the synthesis reactors. This latter configuration will be analyzed in conjunction with a combined cycle electric power generation facility to investigate the potential for such an arrangement.

The model also allows many economic sensitivities to be investigated. These include changing of the financial assumptions in the DCF analysis, and also changing the cost of feedstocks and unit construction costs in the conceptual plant as better data become available.

Table 2-5
Sensitivities That Can Be Investigated Using the Model

Synthesis Gas Preparation:

- coal feed stock characteristics
- coal feed rate
- carbon conversion
- transport gas
- hydrogen-to-carbon monoxide ratio
- bypass gas cleaning operations

Fischer-Tropsch Section:

- raw F-T selectivity including paraffin to olefin ratio and oxygenates
- F-T catalyst activity
- size of slurry F-T reactor
- catalyst loading
- catalyst life
- relationship for gas hold-up and superficial gas velocity
- heat transfer coefficient
- reactor pressure

Refining Section:

- bypass or eliminate refinery operations
- wax hydrocarbon selectivity

Overall System:

- option to recycle unconverted gas or use once-through
- option to automatically reform C_1 and C_2 gases

Economic Sensitivities:

- unit operation construction costs and feedstock costs
- financial parameters