SECTION 3

INVESTIGATION OF THE BASELINE CASE USING THE MODEL

3.1 DEFINITION OF THE BASELINE CASE

In the baseline case, the conceptual indirect liquefaction plant processes 30,000 tons per day of moisture-free (MF) Illinois No. 6 coal, whose analysis is given in table 3-1.[16] The as-received coal is dried to 5 percent moisture using nitrogen heated by medium-pressure steam and fed to 12 Shell gasifiers, each processing 2625 tons per day of the 5 percent moisture feed coal. The coal is fed by HP transport gas (carbon dioxide in this case) into the gasifiers where the coal is reacted with 99 percent purity oxygen at 2700°F and 400 psig pressure. Overall carbon conversion of 99 percent is achieved. The exit raw gas is cooled with recycle gas as was described in section 2.2.1. so as to be below the ash deformation temperature to prevent fouling of the waste heat boiler steam tubes. The raw gas is processed as described in figure 2-2 to produce a clean synthesis gas with a hydrogen to carbon monoxide molar ratio of 0.67 and a total sulfur content of 0.06 ppm by volume.

In the Fischer-Tropsch synthesis area, slurry-phase reactors are used. 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. These are the same reactor dimensions used by Mobil in their 1985 report.[10] The base case catalyst activity is that found by Mobil in their low-wax case run 256-3,[14] equivalent to a 90 percent synthesis gas conversion at a space velocity of 2.3 normal cubic meters/kg iron hour. In the base case the conversion per pass is 90 percent. Catalyst loading is 18.5 percent, and the superficial gas velocity is 9.5 centimeters per second. Catalyst life is 60 days. Catalyst density is 324 pounds per cubic foot, and reactor wax density is 58 pounds per cubic foot. For heat transfer considerations, an overall heat transfer coefficient of 0.376 kJ/sec m^2 deg K (70 Btu/hour sq ft °F) was used as determined by Farley and Ray.[11] This results in approximately 15 percent of the reactor volume being occupied by steam tubes. The Bach and Pilhofer[12] correlation was used to relate gas hold-up to superficial gas velocity. Under these conditions an average gas hold-up of approximately 20 percent is estimated. Reaction conditions of 17 bar pressure and 243°C were used for the F-T synthesis.

The F-T selectivity was chosen to produce approximately 50 percent wax. These conditions result in 59 reactors being required to process the clean synthesis gas. This is the number of reactors required to process the entire synthesis gas stream after reforming and recycling the C_1 and C_2 hydrocarbon gases and unconverted synthesis gas. Overall synthesis gas

Table 3-1
Properties of Illinois No. 6 Coal Used in Baseline Case

<u>Proximate Analysis (As Received wt%)</u>	
Moisture	12.0
Ash	8.8
Volatiles	31.4
Fixed Carbon	47.8
<u>Ultimate Analysis</u> (%wt m.a.f.)	
Carbon	77.26
Hydrogen	5.92
Oxygen	11.14
Nitrogen	1.39
Sulfur	4.29
Heating Value As Received HHV Basis	11,241 Btu/lb
Ash Fusion Temperature Reducing (°F)	
Initial Deformation	1950
Softening	2030

conversion is 100 percent after hydrogen and bleed gas streams have been removed during recycle.

The baseline plant recycles the unconverted synthesis gas and autothermally reforms the C_1 and C_2 hydrocarbons as shown in the schematic in figure 2-3. Hydrocarbon gases higher than C_2 are recovered in the hydrocarbon recovery unit. The F-T catalyst is water-gas shift active, and internal water-gas shift occurs in the slurry reactor producing large quantities of carbon dioxide. This is removed by a Benfield unit before the C_3^+ gases are recovered. Hydrogen for refining is recovered in the hydrogen recovery unit before the remaining gas is reformed. The reformed gas now containing carbon monoxide and hydrogen is mixed with the fresh feed gas and sent to the slurry reactors; therefore, the baseline plant does not produce SNG or ethylene.

The raw F-T products are separated and sent to the refinery. The C_3/C_4 fraction contains 75 percent olefins, which approximately matches the Mobil test data. The wax is withdrawn from the slurry reactors, filtered and hydrocracked to produce distillate. The baseline plant uses data from UOP on the hydrocracking of Mobil wax to determine the product yield and selectivity.[15] The other raw products are refined as shown in the schematic in figure 2-5. Final products from the plant are LPG, alcohols, gasoline and diesel.

The baseline plant is grassroots with the only inputs being coal, air, and water. All steam, electric power, fuel gas and other needed energy are internally generated. Oxygen is produced using high-pressure steam generated from the gasifier waste heat boilers. All unit operations in the baseline plant are balanced with respect to utility requirements. The plant produces a slight excess of electric power that is sold as a by-product. Other by-products include sulfur from the Claus sulfur recovery unit and ammonia from the Phosam-W ammonia recovery unit. The baseline plant configuration gasifies all of the plant input coal, and no additional coal is directly combusted in coal-fired boilers. This eliminates the need for coal-fired boilers and their supporting clean-up equipment.

3.2 BASELINE PLANT MASS AND ENERGY FLOWS

Figure 3-1 shows a simplified schematic of the major material flows in the baseline plant. Referring to figure 3-1, the gasification of 2,222,000 pounds per hour of moisture and ash free (MAF) coal produces a net raw synthesis gas having the composition shown at a rate of about 202,000 moles per hour of hydrogen and carbon monoxide. The gas flows and composition are shown after shift and cleaning. The F-T net raw product output is shown grouped into carbon number categories for convenience. The raw

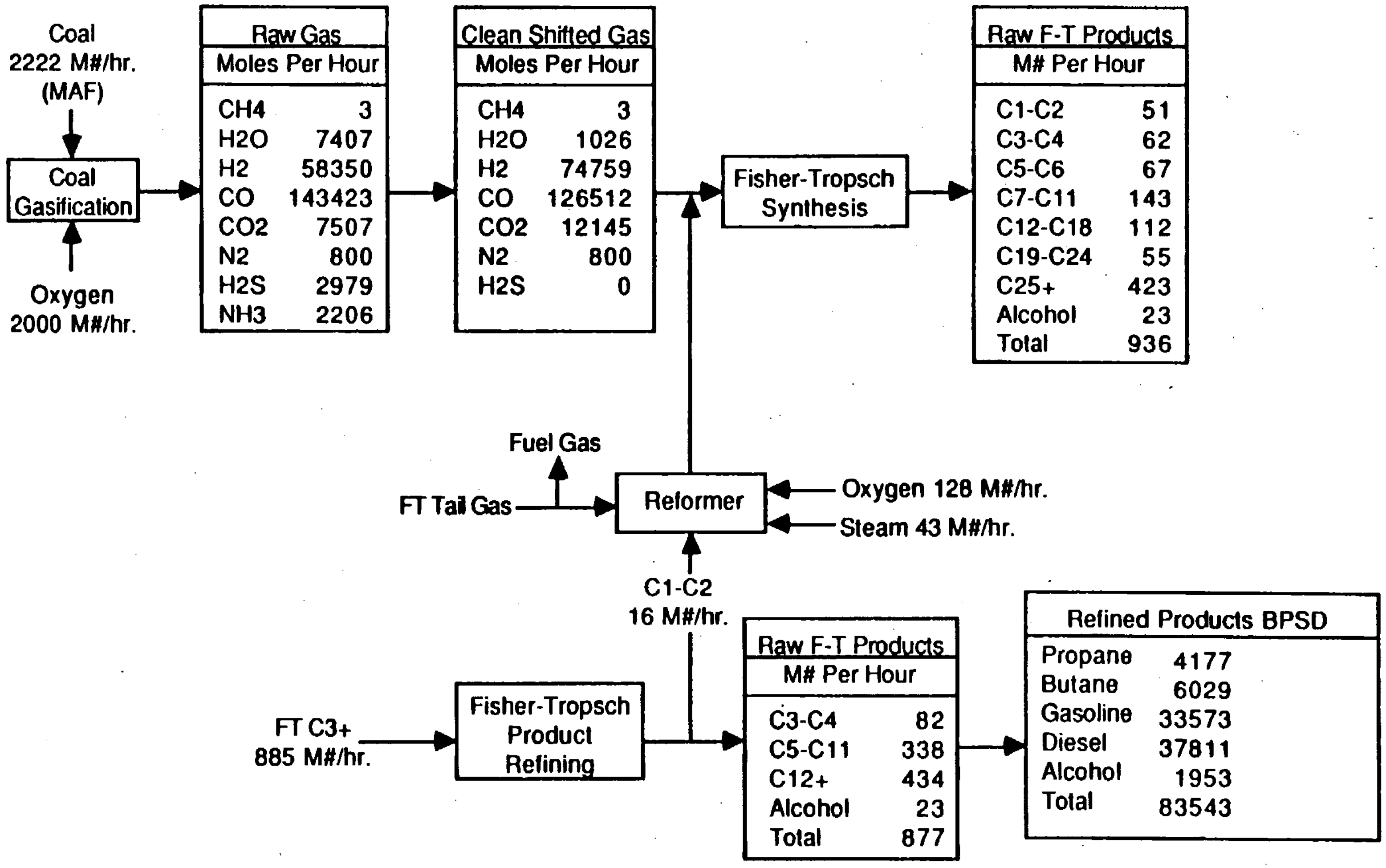

Figure 3-1
Summary of Materials Flows
(Base Case)

products are refined, and the wax is hydrocracked to produce the refined product slate shown in figure 3-1. The weights of products are converted to volumes on a barrel per stream day (BPSD) basis. Approximately 83,500 BPSD of total products are produced by the baseline plant.

The gasoline to diesel output ratio is shown to be about 0.9 to one. This is an arbitrary differentiation in many ways since there is overlap in the boiling range between what is called gasoline and diesel. In this baseline plant, the gasoline is defined as material in the carbon number range from C_5 to C_{11}. In earlier MITRE reports[1,2,4], the gasoline was defined in this manner, and for consistency the same definition is used. The diesel carbon range is defined as material from C_{12} to approximately C_{23}. In their report on wax hydrocracking,[15] UOP defines diesel as material between C_9 and C_{23}. Because of this, the products from their conceptual commercial plant are 70 percent diesel. The UOP diesel apparently meets the specifications, and it is probable that the low initial boiling point (IBP) resulting from the C_9 component offsets the heavy ends contribution. Clearly because of the high cetane number of the F-T diesel (about 75), this material should command a premium value as a blending feedstock compared to the F-T gasoline that has an intermediate octane number of 87, and therefore it would probably be more profitable to make as much "diesel" as possible. Careful blending of the products would be required so that the gasoline component will not have an end point of C_8.

Figure 3-2 shows a simplistic summary of the percentage of coal energy at various stages in the transformation of coal to products. The purpose of this figure is to illustrate the major energy losses in the plant. The gasification process produces a raw synthesis gas containing about 82 percent of the energy of the feed coal. The remainder of the coal energy is manifested as sensible heat in the exit gas, slag and wall losses. Since over 90 percent of this is contained in the exit gas sensible heat, the importance of waste heat recovery at this point is emphasized. The other main energy loss is in the F-T synthesis process, which, as can be seen, is highly exothermic. Figure 3-2 shows that only about 74 percent of the clean synthesis gas energy appears in the raw products. The remainder of the chemical energy is converted to sensible heat as a result of F-T synthesis and reforming of the light gases, and hydrogen is removed for use in product refining. The overall efficiency (HHV basis) to produce refined products is about 57 percent.

3.3 ECONOMICS OF THE BASELINE CASE

Table 3-2 summarizes the baseline plant construction costs. A construction cost of $2,830.5 million is required. Costs of the baseline units are scaled from the reference costs shown in table 2-3. Data on the cost of Shell gasifiers were taken from a recent EPRI report prepared by Florida

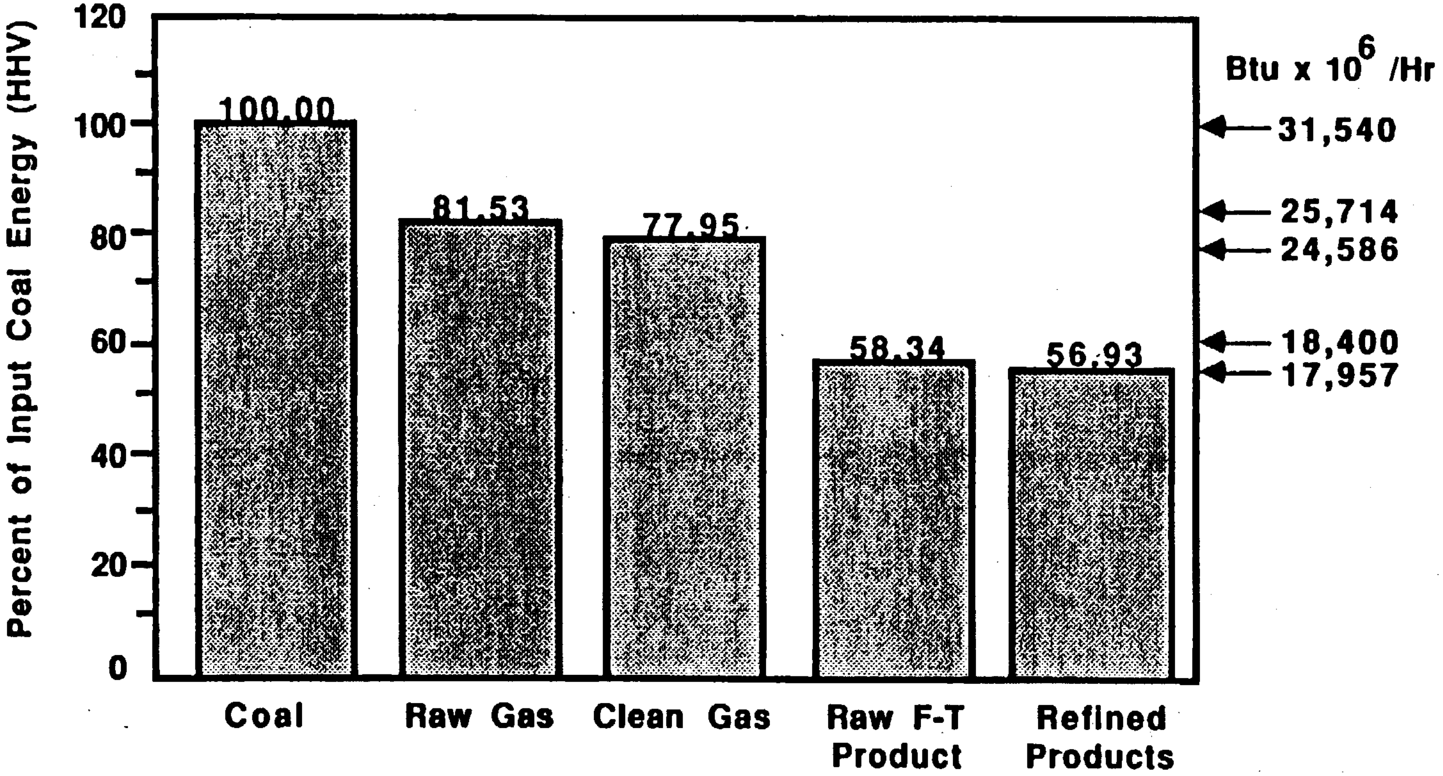

Figure 3-2
Percent of Coal Energy Remaining During Transformation
(Base Case)

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

					Scale Factor = 0.70	
Ref*	Unit#		Capacity (1000# or M)		Ratio to Ref.	Const. Cost (10^6,$1986)
Gas Preparation and Synthesis						
Mobil'85	250	F-T Synthesis	M	245	2.30	520.24
FPL	101	Shell Gasification	#	2,470	2.45	636.79
MRDC	102	Shift	M	66	1.83	32.52
Braun	103	COS Hydrolysis	M	239	3.21	21.60
Braun	104	Sulfur Polishing	M	215	3.19	19.91
Norton	105	AGR Selexol	M	231	10.15	93.68
Braun	106	Sulfur Recovery	M	2,979	1.04	50.69
UOP/SDC	109	Ammonia Recovery	M	609	0.39	14.43
MRDC	116	Autothermal Reformer	M	26	0.66	45.46
F-T Product Refining						
MRDC	262	Alcohol Recovery	#	174	0.363	9.02
MRDC	252	F-T Prod. Fractionation	#	384	1.688	34.86
MRDC	253	F-T Prod. Hydrotreater	#	327	2.641	21.71
MRDC	254	Hyd. Prod. Fractionation	#	812	6.577	23.67
MRDC	255	Cat Reformer	#	227	4.835	36.66
MRDC	256	C5/C6 Isomerization	#	117	3.159	19.76
MRDC	257	Catpoly Unit	#	62	1.176	7.65
MRDC	258	HF Alkylation	#	12	0.630	2.65
MRDC	259	Polygas Hydrotreating	#	22	1.147	4.40
MRDC	260	Lt. Ends Recovery	#	79	4.702	10.84
MRDC	261	H_2 Purification	#	14	1.361	5.58
MRDC	210	Hydrocarbon Recovery	M	32	1.050	33.46
MRDC	211	H_2 Recovery	#	8.29	2.180	25.31
GPH	213	Benfield CO_2 Removal	M	75	1.052	95.35
UOP	300	Wax Hydrocracking	#	478	1.656	37.32

Table 3-2
Construction Costs and Capacities for Units in Baseline Case (Concluded)

			Scale Factor = 0.70			
Ref*	Unit#		Capacity (1000# or M)		Ratio to Ref.	Const. Cost (10^6,$1986)
Offsite Operations						
UOP/SDC	221	Oxygen Plant	#	2,093	3.24	437.78
MRDC	227	Instrument/Plant Air	M		1.00	1.00
UOP/SDC	228	Coal Hand Drying	#	2879	1.02	188.51
UOP/SDC	230	Power Distribution	M	183	0.64	50.43
EPRI	231	BFW Preparation	M	259	0.47	5.06
MRDC	232	Cooling Water Prep.	M	6,049	1.93	1.32
UOP/SDC	233	CW Towers	M		1.93	37.58
MRDC	234	Power Gen.	M	223	3.66	45.47
MRDC	235	WW Treatment	M	2,016	0.96	42.55
MRDC	236	Blowdown	M	432	0.52	2.83
MRDC	237	Storage	M	877	4.29	39.73
MRDC	238	Intercon. Piping	M	3	1.02	34.46
MRDC	270	Gasoline Blending	M	338	2.40	6.15
MRDC	271	F-T Cat. Preparation	#	2	0.82	40.25
UOP/SDC	600	Infrastructure	M		1.02	79.65
MRDC	700	Miscellaneous	M		0.00	14.15 (.5% TIC)
TOTALS						2830.50

* 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

Power and Light Company with input from Shell Oil Company.[17] Table 3-3 shows the total capital required. For this baseline plant $4,405 million is required. The methodology used to compute this has been described in Table 2-4. Table 3-4 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 3-5 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 3-6 shows the calculated required selling prices (RSP) for refined products. These are calculated from the annual revenue requirements shown at the foot 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, and this sensitivity could be investigated in the future. 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.

Table 3-3
Capital Requirements
(Baseline Plant $M1986)

Construction Cost	$2,830,502
Engineering Design & Project Contingency	707,625
TOTAL PLANT INVESTMENT (TPI)	$3,538,127
Allowance for Funds used During Construction	597,944
TOTAL DEPRECIABLE CAPITAL	$4,136,071
Start-up Costs	$ 104,360
Working Capital	130,451
Initial Charge of Catalyst & Chemicals	33,716
TOTAL NON-DEPRECIABLE CAPITAL	$ 268,527
TOTAL CAPITAL REQUIRED	$4,404,598

Table 3-4
Calculation of Gross and Net Operating Cost
($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 - $0.04/kW	11,833
TOTAL BY-PRODUCT CREDITS	$ 71,714
TOTAL NET ANNUAL OPERATING COST	$450,089

Table 3-5
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 3-6

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**

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*CRF = Capital Recovery Factor.

SECTION 4

RECOMMENDATIONS FOR FUTURE RESEARCH AND DEVELOPMENT

To develop a detailed integrated model such as the one described in this report, it is necessary either to simulate process operations from theory or to use actual scaled test data. In the development of this general model and the baseline case, scaled test data, modified test data and theoretical simulation have all been used as input to model the total integrated facility. In the modeling process several assumptions have to be made because of data gaps and uncertainties. These assumptions can form the basis for additional research to determine if they can be verified and thus validate the results of the model. The model can also be used to investigate the impact of projected advances in specific aspects of the technology. These "what if" sensitivities can be readily performed to assess their potential impact on the economics of the technology. If the sensitivity is favorable to the overall economics, then making it a technical reality can become a research objective.

The conceptual 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 small 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 the technical performances of some of the units, 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 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.

The recommendations for future research and development (R&D) given here relate primarily to the investigation of the assumptions made in the model and the uncertainties in data. In addition, there are recommendations that relate to the optimization of the integrated system. Table 4-1 lists the recommendations and divides them into categories.

Table 4-1
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-phase Fischer-Tropsch reactors.
   - Develop reproducible F-T catalyst based on precipitated iron or other.
   - Develop sulfur-tolerant F-T catalyst.
   - Characterize catalyst for a 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 4-1
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.

The area of the plant that has the most uncertainty associated with it is the slurry-phase Fischer-Tropsch synthesis. Thus, this area has the greatest technical risk for commercialization. A large number of the other plant areas consist of commercially available technology, and the associated risk is correspondingly small. Coal handling and preparation, for example, is commercially available, as are the unit operations in the gas cleaning train. Shell gasification is not commercially available, but the 150-200 ton per day pilot plant experiences both in the United States and Germany have come far to demonstrate its commercial potential.

The majority of the refining operations used to upgrade the raw F-T product are commercially available and used in the petroleum industry. Even the use of these technologies on the very chemically different F-T feedstock is currently commercial practice at SASOL in South Africa. Hydrocracking the F-T wax has only been demonstrated on a bench-scale, but the apparent ease of this operation, the suitability of the feedstock and the high quality of the products augur well for ready commercialization. Increasing the octane value of F-T naphtha is a continuing problem and necessitates severe reforming as is done at SASOL. Paraffins are not the ideal feed to platformers, but they can be handled. The assumptions in the model concerning the reformer performance were copied from the MRDC report and have essentially been verified experimentally by UOP.

Since the major source of uncertainty pertains to the Fischer-Tropsch area, the recommendations focus on both the slurry-phase reactor and the catalysts to be used in them. Most research investigations on slurry-phase reactors that actually perform synthesis under reaction conditions have been in small diameter units, typically 2 inches internal diameter. The unit at Mobil had this diameter but it was of commercial height so that gas residence times in the catalyst slurry were simulated. In order to obtain the necessary information on slurry reactors that will allow accurate scale-up predictions it is recommended that a slurry bench-scale unit be built and operated. The unit should be large enough in diameter so that wall effects and slugging will not dominate the hydrodynamics and of the correct height to simulate commercial-scale operation. The unit should incorporate the necessary hardware to investigate slurry addition and withdrawal and should be fitted with heat transfer surfaces to investigate heat transfer coefficients. Ancilliary equipment to investigate the separation of wax and residual catalyst particles should also be part of this unit. A unit of this size will allow the hydrodynamics of slurry F-T reactors to be investigated in a precise manner. The complex interrelationships between superficial gas velocity, gas hold-up, catalyst loading and the physical properties of the solids, liquids, and gases can be determined so that a greater level of confidence in performance and scaling of these reactors can be obtained. The importance, or lack thereof, of mass transfer in slurry reactors could also be investigated in the bench-scale unit.

The key to Fischer-Tropsch synthesis is the catalyst that produces the hydrocarbons from the synthesis gas. Much F-T work has been done using iron-based ammonia catalysts, and several investigators have prepared precipitated iron and/or cobalt catalysts. However, the catalysts that have been prepared in small quantities often cannot be replicated with respect to their performance. It is recommended that a more systematic approach to the development of slurry-phase F-T catalysts be undertaken. For slurry applications special characteristics are preferred. These are high density, high physical stability (attrition resistant), non-agglomerating tendency, water-gas shift capability, and high activity. Supported or fused type catalysts may be preferable to precipitated catalysts in slurry applications. Development of reproducible methods of preparing batches of catalysts would be an invaluable contribution to the research program and would provide sufficient catalyst for use in the slurry-phase bench-scale unit. Standardized in situ activation procedures for the catalysts should be part of the development program. Parallel to this process oriented catalyst program, detailed catalyst characterization should be performed so that a more fundamental understanding of the observed effects may be obtained. Catalyst characterization should include both bulk and surface properties at all stages of catalyst preparation from calcination and activation to actual synthesis.

Investigating the relationships between the hydrodynamic and kinetic constraints of the slurry-phase system would be possible after implementing the above recommendations. These investigations are listed in item 3 of table 4-1. A mathematical understanding of these interactions will enable precise reactor volume requirements to be calculated for given conversions and catalyst activities. This will allow commercial scaling needs and potential to be established. Another important effect is that of pressure. If the slurry F-T reactors could be operated at higher pressures, less reactors would be required, and thus the plant capital cost and hence product costs would be reduced.

Item 4 in table 4-1 addresses the recommendations for additional systems studies. Investigation of once-through F-T with coproduction of electric power is an interesting concept that may have favorable economic potential. This will depend on several factors including the selling price of power and how well the system is optimized. Other system studies that should be investigated include optimizing the configuration for high wax production by assessing whether fixed-bed Arge or slurry F-T reactors are preferred. This would necessitate a better estimate of reactor costs for slurry-phase and fixed-bed reactors than is currently available.

The indirect liquefaction model described in this report will be extended, in future work, to include the capability of examining the once-through F-T configuration with electric power generation. In addition, the impact of higher temperature F-T synthesis to provide better quality waste heat could be investigated for varying assumptions of product selectivity change. Fixed-bed Arge and liquid-phase methanol synthesis reactors could be substituted for the slurry F-T units when sufficient operating and cost data are made available.

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