BASELINE DESIGN/ECONOMICS FOR ADVANCED FISCHER-TROPSCH TECHNOLOGY. QUARTERLY REPORT, JANUARY--MARCH 1992

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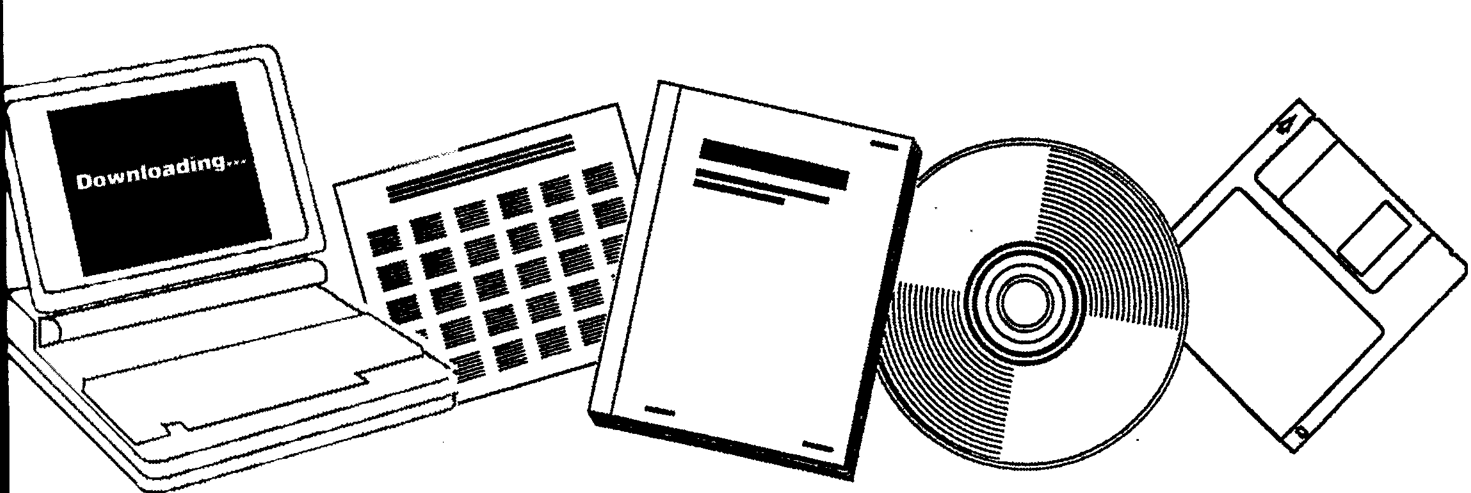

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Baseline Design/Economics for Advanced Fischer-Tropsch Technology

Contract No. DE-AC22-91PC90027

Quarterly Report

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Section 1

Introduction

Effective September 26, 1991, Bechtel, with Amoco as the main subcontractor, initiated a study to develop a computer model and baseline design for advanced Fischer-Tropsch (F-T) technology for the U.S. Department of Energy's (DOE's) Pittsburgh Energy Technology Center (PETC). The 24-month study, with an approved budget of $2.3 million, is under DOE Contract Number DE-AC22-91PC90027.

The objectives of the study are to:

- Develop a baseline design for indirect liquefaction using advanced F-T technology.
- Prepare the capital and operating costs for the baseline design.
- Develop a process flow sheet simulation (PFS) model.

The baseline design, the economic analysis, and the computer model will be the major research planning tools that PETC will use to plan, guide, and evaluate its ongoing and future research and commercialization programs relating to indirect coal liquefaction for the manufacture of synthetic liquid fuels from coal.

This report is Bechtel's second quarterly technical progress report and covers the period of December 23, 1991 through March 15, 1992, which is the reporting period covered by the three monthly status reports already published.

This report consists of four sections:

- Introduction
- Summary
- Study Progress by Task
- Key Personnel Staffing Report

Section 2

Summary

This report summarizes the activities completed during the period December 23, 1992 through March 15, 1992 for the tasks scheduled for the period, i.e., Tasks 1, 3, and 7.

In Task 1, Baseline Design and Alternates, the following activities related to the tradeoff studies were completed:

- Approach and basis
- Oxygen purity
- F-T reactor pressure
- Wax yield
- Autothermal reformer
- Hydrocarbons (C_3/C_4s) recovery
- Hydrogen recovery

The recommended purity of oxygen feed to the Shell gasifier was determined to be 99.5 mol%. Bechtel recommends that the pressure level for the F-T reactor should be a natural design pressure without recompression of the clean syngas from the Shell gasification unit. The preferred wax yield for the baseline design case was determined to be 50 wt%. An autothermal reformer should be incorporated into the F-T recycle loop because it offers economical benefits and operational flexibility. Deep refrigeration (-130°F) and hydrogen recovery by PSA-only (with 6000 mols/hr water injection) provide the most economical route to recover C_3s, C_4s, and hydrogen from the F-T recycle loop. Various options for the CO_2 removal are still under investigation.

In Task 3, Engineering Design Criteria, activities were initiated to support the process tradeoff studies in Task 1 and to develop the environmental strategy for the Illinois site. The work completed to date consists of the development of the F-T reactor yield correlation from the Mobil data and a brief review of the environmental strategy prepared for the same site in the direct liquefaction baseline study. Some work has also been done in establishing site-related criteria, in establishing the maximum vessel diameter for train sizing and in coping with the low H_2/CO ratio from the Shell gasifier.

In Task 7, Project Management and Administration, the following activities were completed:

- The subcontract agreement between Amoco and Bechtel was negotiated.
- A first technical progress meeting was held at the Bechtel office in February. Conference notes were prepared and distributed.
- The final Project Management Plan was approved by PETC and issued in March 1992.

Study Progress by Task

Section 3

Study Progress by Task

This study has been divided into seven major tasks:

- Task 1: Establish the baseline design and alternates.
- Task 2: Evaluate baseline economics.
- Task 3: Develop engineering design criteria.
- Task 4: Develop a process flowsheet simulation (PFS) model.
- Task 5: Perform sensitivity studies using the PFS model.
- Task 6: Document the PFS model and develop a DOE training session on its use.
- Task 7: Perform project management, technical coordination, and other miscellaneous support functions.

During the reporting period (December 23, 1991 through March 15, 1992), several activities were completed in Tasks 1, 3, and 7. These accomplishments are described below.

3.1 TASK 1 – BASELINE DESIGN AND ALTERNATES

The baseline design is for a F-T synthesis facility, using slurry reactors operating in the high-wax mode, to produce LPG, diesel, gasoline, and distillate from synthesis gas that was produced in Shell gasifiers from 20,000 tons per day (tpd) of bituminous Illinois coal. An alternate case will be performed to assess the impact of subbituminous western coal on the baseline design. Work during the reporting period was focused on tradeoff studies to determine the basis for design of the F-T recycle loop for the baseline case.

3.1.1 Tradeoff Study Approach and Basis

The major objectives of the tradeoff studies are to select the most cost-effective F-T recycle loop configuration for the baseline design through the evaluation of various process alternates and to investigate alternate process units and variables with the greatest impacts on the baseline design. As shown in Figure 3-1, the F-T recycle loop consists of these major process units: F-T synthesis, carbon dioxide removal, recycle gas compression and dehydration, hydrocarbons recovery, hydrogen recovery, and autothermal reforming.

The process units and process variables studied include:

- Oxygen purity for the Shell gasifiers
- F-T reactor pressure
- Wax yield (F-T reactor temperature)
- Autothermal reforming

- Hydrocarbons (C_3/C_4s) recovery
- H_2 rec[illegible]
- CO [illegible] val

Different [illegible] s alternates were first evaluated by direct comparison of the capital and operating costs. T[illegible] n [illegible] pacts on other process units were also investigated and quantified, if necessary. Capital [illegible] mates, spreadsheet balances, and HYSIM process models prepared during the Slurry [illegible] Design Studies sponsored by DOE/PETC (DOE Contract No. DE-AC22-89PC89867) were updated and revised for these tradeoff studies. To minimize the work scope of the tradeoff studies, capital and operating cost estimates for the process units were used for comparison purposes for those specific tradeoff cases and included only the affected equipment.

The process basis and assumptions are also varied within each tradeoff case in order to provide a better comparison among different options. Some of the common bases and assumptions are: (1) the F-T product yields and loop material balances are calculated by a new spreadsheet simulation program or ASPEN/SP models using the triple alpha theory (to be discussed in Task 3); (2) more detailed heat and material balances around the F-T recycle loop are generated using the HYSIM and ASPEN/SP models; (3) the F-T plant capacity is based on 20,000 stpd of washed Illinois No. 6 coal with 5 wt% moisture to the gasifiers; (4) the wax yield is assumed to be 50 wt%; and (5) autothermal reforming is incorporated in the F-T recycle loop. Deviations in wax yield and inclusion or exclusion of autothermal reforming [illegible] examined in relation to this base. While once-through operation is an interesting possible [illegible] for future study, it was deemed outside the scope of these studies since it would undoubtedly [illegible] the production of excess power. Target syngas conversion for the tradeoff studies was 80%.

The basis for the operating cost and product values are listed in Table 3-1. The electric power cost of 5.1¢/kWh is based on the market price for purchased power. The power cost is consistent with the cost determined in a separate DOE/PETC sponsored study (Direct Coal Liquefaction Baseline Design and System Analysis, DOE Contract No. DE-AC22-90PC89857) for the same plant location.

The product values are based on their typical market value at this time. They do not yet include any premium or debit for octane and cetane values for the coal derived liquid. A simple payout of 4 years is used as an economic criterion for justification for inclusion of a process unit.

3.1.2 Oxygen Purity

Use of oxygen in different purities in the Shell gasification process and autothermal reformer has a direct effect on the physical size of various process units in the F-T recycle loop. Thus, the capital and operating costs of the process units in the F-T recycle loop have to be considered as well as those for the air separation plant.

Two oxygen purities (95 versus 99.5 mol%) were considered for this tradeoff study. The basis for the F-T recycle loop design was the membrane/PSA option for hydrogen recovery, even though it was not the final choice. The PSA-only option for hydrogen recovery was not considered for this tradeoff case because the hydrogen content in the recycle gas stream is below the practical limit of the PSA when the oxygen purity is at 95 mol%.

The heat and material balance for major unit operations in the F-T recycle loop were computed using a spreadsheet program developed for this purpose which uses separation factors from the HYSIM and ASPEN-SP models. Design Study was revised for the 95 and 99.5 mol% oxygen purity cases. Table 3-2 summarizes the basis and the flow rates of the process units that are impacted most by the change in the oxygen purity. As shown, the recycle gas flow rate is reduced from 578 to 315 MMscfd as the oxygen purity is increased from 95 to 99.5 mol% purity, respectively. Since the purge rate is set by the constant fuel demand from the F-T plant (585 MM Btu/hr), the purge gas stream for the low oxygen purity case is increased from 5,000 to 13,680 moles/hr owing to its lower heating value.

Table 3-3 summarizes the capital and operating costs of the air separation plant and the affected process units in the F-T recycle loop for the two different oxygen purity cases. As expected, the capital cost and operating costs for the air separation plant are higher for the 99.5 mol% oxygen purity case. However, these increases are more than offset by the decreases of the capital and operating costs for the other process units. The 99.5 mol% oxygen case shows a $16 million lower capital cost and $12.4 million per year lower annual operating cost than the 95 mol% case.

Results of this tradeoff case indicate that 99.5 mol% oxygen purity should be used for the baseline design case.

3.1.3 F-T Reactor Pressure and Temperature

To optimize pressure and temperature it is first necessary to determine the effect of these parameters on reactor sizing and wax yield. Bechtel has reanalyzed Mobil's first stage data for pressure and temperature effects by selecting lined-out periods throughout the pilot plant operations (Kuo, 1983, DE-AC22-80PC30022 and Kuo, 1985, DE-AC22-83PC60019). These are listed in Table 3-4. Operating pressure varies from 1.48 to 2.52 MPa and temperature from 244°C to 275°C.

A plot of wax yield in wt% versus reactor temperature is shown in Figure 3-2. A straight line against temperature is shown, but this is heavily influenced by the point at 275 °C. If this point is discarded, the line would be downward curving and would correspond rather closely to a similar correlation developed by MITRE. The way the curve is drawn in Figure 3-2 puts the low wax mode operation in the best possible light. The points are keyed to pressure, and no discernible effect of pressure on wax yield is found. The cost tradeoffs when wax yield is varied are discussed in Section 3.1.4.

The effect of operating pressure on overall syngas conversion is evaluated in Figure 3-3 using a pressure-corrected semiempirical factor, kP/SV. Theoretically, doubling the operating pressure, P, will double the allowable space velocity, SV, for a given conversion level. The reactor model developed in the Slurry Reactor Design Studies (DOE Contract DE-AC22-89PC89867) establishes that mass transfer contributes only about 10% of the total resistance and thus the logarithm of (100 - syngas conversion) should be nearly proportional to the reaction rate constant, k, determined in that study [$k=3.3*10^9\exp(-130/RT)$], divided by the space velocity. It is apparent from Figure 3-3, which uses all of the data from Table 3-4, that a single line is not obtained and most of the high pressure data are at much lower than expected conversion.

Mobil did two pressure scans early in its test program, and the results are presented in Table 3-5. These data show close to the theoretical pressure effect; i.e., when pressure is raised while maintaining the same superficial velocity, conversion stays almost constant. It is known that Table 3-4 contains data for extended operations where the catalyst activity had fallen. Some of the high pressure data are also at very low superficial velocity and the hydrodynamics may have been poor, leading to an abnormally high mass transfer contribution. These data are shaded in Table 3-4. When these data are eliminated from Figure 3-3 and the Table 3-5 data are added, a reasonable correlation is obtained.

On closer inspection, however, it is found that the data fit is slightly improved if the activation energy is reduced from 130 to 100 MJ/kg mol. This is also more in line with the F-T literature. The final correlation with the revised data set is shown in Figure 3-4. The reaction rate constant is now given by $k=3.65*10^6\exp(-100/RT)$. The fit is reasonable, although the two high pressure runs 256-6 and 256-7 are still at too low a conversion level. Mobil realized that this was happening and abandoned efforts to run at high pressure in their later pilot plant operations.

Since the effect of pressure is still uncertain (one set of data confirms theory, another does not), a tradeoff study would be meaningless. Bechtel recommends that a natural design pressure, achievable without recompression of the clean gas from the gasifier, be used for the baseline design. This would be about 2 MPa, right in the middle of the range studied by Mobil. A compression stage will be included in the process simulation model, and it will then be possible to optimize the system using whatever pressure effect the user wishes to build into the model.

For the purpose of the tradeoff studies, reactor capacity and reactor depth have been estimated for various wax yields for a 4.8-meter-diameter reactor, using Bechtel's reactor model 2, wax yield correlation as shown in Figure 3-2 and the reaction rate constant $k=2.5*10^6\exp(-100/RT)$, at an inlet superficial velocity of 10 cm/s and a slurry concentration of 22.5 wt%. As a degree of conservatism, this rate constant is 70% of that in Figure 3-4. The results are summarized below:

Wt% Wax	Temp., °C	Press., MPa	Depth, m	Cap., Nm^3/h
10	270.8	1.48	6.87	41910
10	270.8	2.60	6.87	67380
50	253.1	1.48	15.0	46422
50	253.1	2.60	15.0	78090
76	241.7	1.48	26.35	48690
76	241.7	2.60	26.35	83333

The pressure effect shown above is the theoretical effect. The reactor size remains constant, while capacity increases in direct proportion to pressure. Fewer reactors are required at higher pressure but the reactor weight will increase, almost in direct proportion to pressure, since the wall thickness must be increased. Under this assumption, therefore, the economics of pressure will depend more on its effect on the recycle loop than on the reactors themselves.

For future design purposes, Bechtel has reanalyzed multiple sets of Mobil data over the pressure range in question using the plug flow model described in the Slurry Reactor Design Studies (the high L/D Mobil pilot plant reactor should approximate plug flow). The frequency factor term was varied until the predicted conversion level agreed with the data. The results were as follows:

Run Number	P	T	SV	Syngas Conv.	Freq. Factor
256-1-2	1.136	260	9.12	53.6	$4.4*10^6$
256-3-4	1.480	258	2.40	86.3	$2.3*10^6$
256-3-49	1.487	262	2.09	85.4	$1.62*10^6$
256-4-25	2.515	256	2.92	40.6	$0.65*10^6$
256-5-5	1.473	244	2.26	55.2	$2.2*10^6$
256-6-5	2.184	249	3.99	43.2	$1.62*10^6$
256-11-7	1.487	258	2.30	83.2	$1.8*10^6$
256-13-8	1.48	249	2.34	82.5	$1.8*10^6$

The average of the above frequency factors is $2.05*10^6$, giving a design reaction rate constant of $k=2.05*10^6\exp(-100/RT)$.

3.1.4 Wax Yield

The main objective of this tradeoff case is to establish a wax yield basis for the baseline design case. The F-T reactor yield model developed in Task 3 of this Study was used to investigate the effect of wax yield on the overall F-T plant configuration. The Excel spreadsheet program mentioned previously was used to develop the material balance for the F-T recycle loop. The final liquid product yields were estimated with the same upgrading configuration as in the previous Slurry Reactor Design Study. Three different wax yields – 76 wt%, 50 wt%, and 9.6 wt% – were selected for this tradeoff case.

Table 3-6 summarizes the product yields and key process flows within the F-T recycle loop. The gasoline-to-distillate ratio decreases for increased wax yield but the combined yield of gasoline and diesel increases. The production of C_3/C_4s essentially remains constant for different wax yields.

The estimated plant capital costs and operating costs for the three wax yield cases are summarized in Tables 3-7 and 3-8, respectively. The total capital cost increases as the wax yield decreases. The capital costs for the process units within the F-T recycle loop do not show a clear trend with the wax yield. The capital costs of the refining section decreases as the wax yield increases. Savings in reactor cost at low wax yield are counterbalanced by increases in cost of the autothermal reformer and oxygen plant.

The comparison of the annual operating cost is limited to the cost of power and steam because other annual operating costs are not significantly affected by the variation of wax yield. As shown in Table 3-8, the annual revenue is increased from $337.7 million to $385.2 million as the wax yield is varied from 9.6 to 76 wt%. The annual cost for power and steam shows an opposite trend with the same variation of wax yield. The net result is a decrease in revenue at low wax yield.

Although higher net revenue is generated in the highest wax yield case, Bechtel recommends that 50 wt% yield be selected for the baseline design because most Mobil data are in the range between 10 and 50 wt% wax yield. There were only three material balance runs, covering 6 days of operation, at 70% and higher wax yields. The operating temperature was 240°C to 245°C, and the Mobil pilot plant reactor had insufficient depth to achieve over about 55% syngas conversion.

3.1.5 Autothermal Reforming

The autothermal reformer is incorporated in the F-T recycle loop in order to minimize the buildup of light ends and increase the C_3+ product yield at the expense of purge gas. Since the reforming reaction to synthesis gas is endothermic, oxygen is added and a portion of the gas stream is burned to CO_2 and H_2O to balance the heat requirement. The reaction is catalytic partial oxidation, and prototypes exist at Sasol and in the autothermal reformer used in methanol production via combined reforming.

Table 3-9 provides a relative comparison of sizes and operating conditions for key process units with and without the autothermal reformer included in the F-T recycle loop. With the inclusion of an autothermal reformer, a portion of the light ends are effectively converted to synthesis gas or and do not build up in the loop, resulting in a reduction in the recycle rate (from 413 to 378.2 MMscfd). The number of F-T reactors required is reduced from 29 to 26 with the inclusion of the autothermal reformer.

Table 3-10 summarizes the comparisons of the capital costs, annual operating costs, and the annual revenue for the two cases: with and without the autothermal reformer. Although the total capital cost is $9.8 million higher for the autothermal reformer case, it is offset by the higher net revenue of $22.5 million generated. The simple payout is estimated to be 0.44 year.

The inclusion of the autothermal reformer in the recycle loop will also provide added operating flexibility. In case of failure of an upstream unit in the F-T recycle loop such as the hydrocarbons recovery unit, the additional recycled hydrocarbons can be converted to syngas in the autothermal reformer. Thus, complete plant shut down is avoid even though the plant may have to be operated at reduced capacity.

Venders of the autothermal reformer (Lurgi and Haldor Topsoe) confirmed that the presence of olefins in the autothermal reformer feed will not pose any operating problems. They also suggested that the reformer gas inlet temperature (not the oxygen temperature) can be as high as 1700°F as compared to the 1100°F used for this tradeoff case.

The autothermal reformer will be included in the baseline design because it offers economical benefits and operational flexibility. The inlet temperature of the reformer feed will be increased closer to 1700°F in order to reduce the oxygen consumption rate.

3.1.6 Hydrocarbons Recovery

Three different hydrocarbons recovery schemes were investigated: adsorption with refrigeration, deep (-130°F) refrigeration, and medium (-30°F) refrigeration. After a preliminary investigation, the adsorption/refrigeration scheme was dropped from further consideration because the required circulation rate of the lean oil adsorbent is very high and an unacceptable amount of adsorbent is lost through carryover by the vapor stream. The refrigeration method was selected as the basis for the hydrocarbons recovery tradeoff case. Both deep and medium refrigeration were studied in detail by a combination of HYSIM and spreadsheet simulations to develop the tradeoff cost information. The wax yield for both cases is 50 wt%.

The deep refrigeration case involves the use of propane/ethylene cascade refrigeration to reach a flash separation temperature of -130°F. About 85% of the propane/propylene and 98% of the butane/butylenes are recovered. The medium refrigeration case uses only propane as the refrigerant and flashes at a separation temperature of -30°F. The corresponding recoveries of C_3s and C_4s are 17% and 52%, respectively.

Table 3-11 summarizes the key process conditions for these two hydrocarbons recovery schemes. The number of F-T reactors is not affected by the hydrocarbons recovery scheme. As expected, the combined compressor power requirement for deep refrigeration is much higher than that for medium refrigeration (8773 versus 2127 bhp). Deep refrigeration also makes CO_2 removal and drying requirements more stringent. The deep refrigeration case used a molecular sieve drying scheme whereas the medium refrigeration case used glycol. Differences in CO_2 removal were considered marginal.

Since an autothermal reformer is included in the F-T recycle loop, hydrocarbons remaining after recovery are converted to synthesis gas. Since less C_3s and C_4s are recovered in the medium refrigeration case, the size of the autothermal reformer has to be increased accordingly. Since the autothermal reformer is not 100% efficient, more sellable products are obtained in the deep refrigeration case than in the medium refrigeration case. On the other hand, the distillate/gasoline ratio is decreased.

This difference in liquid product yield between the deep and medium refrigeration schemes affects the capital costs of the downstream F-T product upgrading units and the net overall product revenue. As indicated in Table 3-12, the deep refrigeration case results in a higher total capital cost in the upgrading section. This is due to higher capital costs for alkylation and cat polymerization units which are associated with C_3s and C_4s upgrading.

Tables 3-12 and 3-13 show the comparison of the capital cost and the net revenues for the two refrigeration cases, respectively. The total installed cost of the deep refrigeration case is $19.6 million higher than that of the medium refrigeration case. However, the net product revenue for the deep refrigeration case is $5.6 million higher than that of the medium refrigeration case. The simple payout is 3.6 years. Thus, deep refrigeration is narrowly preferred over medium refrigeration for hydrocarbons recovery within the F-T recycle loop.

The combined C_3/C_4 product yield is reduced from 16 to 7 to 3 wt% of the total F-T product per pass as the wax yield increases from 9.7 to 50 to 76 wt%, respectively. Thus, at high wax yield, the value of deep refrigeration will be reduced.

3.1.7 Hydrogen Recovery

General. The primary goal of this study is to assess the technical and economic viability of different approaches to generate the hydrogen required for the upgrading sections of the F-T plant. It is estimated that 31 MMscfd of hydrogen will be required to upgrade about 40,000 bpsd of liquid products. The hydrogen should contain less than 50 ppm of CO. The higher the purity of the hydrogen, the lower the treat gas circulation rate required in the hydrotreaters to achieve a given partial pressure. A target hydrogen purity of 99.6% was set.

A slip stream of the effluent stream from the hydrocarbons recovery unit is sent to the hydrogen recovery unit. A portion of the gas from the hydrogen recovery unit will be purged in order to meet the in-plant fuel gas demand and to remove excess inert gases from the F-T recycle loop. If there is still a deficit in fuel gas, additional recycle gas will be purged. If there is a surplus, it will be combined with the effluent stream of the hydrocarbons recovery unit and sent to the autothermal reformer. The amount of gas to be purged out of the recycle loop is determined by the following considerations: (1) to provide the required quantity of fuel gas for utility usage throughout the whole baseline plant, and (2) to minimize the inerts buildup in the recycle loop. In all cases, the flow rate of the purge stream is set by its heat content which is maintained constant at approximately 585 MMBtu/hr (LHV), a preliminary estimate of the fuel gas demand.

Four hydrogen recovery options were evaluated in the tradeoff study: membrane separation followed by methanation, membrane separation followed by PSA, water gas shift followed by PSA, and PSA-only.

Results from the early stage of the hydrogen recovery tradeoff study indicated that the hydrogen concentration in the F-T recycle loop affects significantly the selection of the hydrogen recovery scheme and its cost effectiveness. The amount of water injected to the F-T reactor was varied as a means to increase the hydrogen content without reducing the overall syngas conversion.

Three different water injection rates were investigated: 4,000, 5,000, and 6,000 mols/hr. (This is in addition to the roughly 6000 mols/hr of water vapor in the effluent recycle gas from the autothermal reformer.) The operating conditions of the remaining process units within the F-T recycle loop were not altered. Table 3-14 shows the basis and summarizes the results of this investigation. The hydrogen content in the effluent stream of the hydrocarbons recovery unit (feed stream to the hydrogen recovery unit) is increased from 23.6 mol% (without water injection) to 41.1 mol% with 6,000 moles per hour water injection. The 4000 mols/hr case was selected as the basis for the comparison of the three combination hydrogen recovery options. Later, when PSA-only was considered as a option, hydrogen purity was so important to the economics that the 6000 mols/hr case was considered.

Process Designs. The process designs for the four hydrogen recovery options are described below.

Membrane/Methanation. The block flow diagram for this option is shown in Figure 3-5. Three membrane separation stages are required in order to concentrate the hydrogen concentration from 33.6% to 99.6%. Each stage of the membrane separation unit operates at 195°F with a feed inlet pressure of 390 psia and the permeate leaving at 120 psia. In each stage, the hydrogen recovery is 80%. The permeate leaving the third stage contains 99.6 mol% of hydrogen and 2600 ppm of carbon monoxide. A methanation unit is used to reduce the carbon monoxide concentration to less than 50 ppm before the hydrogen stream is sent to the upgrading sections.

Approximately 50% of the total gas stream leaving the hydrocarbons recovery unit is diverted to the hydrogen recovery unit in order to obtain 31 MMscfd of hydrogen. A portion of the membrane residue gas stream is withdrawn to meet the in-plant fuel demand of 585 MM Btu/hr (LHV). Since the residue from membrane 1 contains the highest inert gas concentration, this stream is selected as the purge stream for in-plant fuel in order to minimize the amount of inert gases in the F-T recycle loop. The residues from the other respective membrane stages are returned to the F-T recycle loop as feed to the autothermal reformer.

Membrane/PSA. The block flow diagram for this option is shown in Figure 3-6. In this option, about 46% of the total gas stream leaving the hydrocarbons recovery unit is diverted to the hydrogen recovery unit. A single stage membrane separation unit is employed to concentrate the hydrogen content to the optimum concentration for PSA. The PSA is designed for 80% hydrogen recovery and sized to produce 31 MMscfd of 99.6% purity hydrogen.

Major process conditions and flow rates are also shown in Figure 3-6. The permeate stream has to be recompressed from 230 psia to 400 psia before it enters the PSA unit. A portion of the reject gas stream leaving the PSA unit is designated as purge stream and the remainder is compressed to 400 psia before it is returned to the F-T recycle loop. The flow rate of the purge stream is established so that it will meet the in-plant fuel demand of 585 MMBtu/hr (LHV).

Shift/PSA. The block flow diagram for this option is shown in Figure 3-7. The purpose of the shift unit is to increase the hydrogen purity in the PSA unit feed. Approximately 21% of the total gas stream leaving the hydrocarbons recovery unit is sent to the hydrogen recovery unit to generate 31 MMscfd of 99.6 mol% hydrogen. As shown in Figure 3-7, about 54,000 lb/hr of 900 psia/700°F steam is fed to the shift unit. The inlet temperature of the shift unit is about 400°F. In the shift reactor, approximately 60% of the CO is converted. The effluent stream is cooled to 100°F and flashed to condense excess water before it is sent to the PSA unit.

The reject stream from the PSA unit is combined with roughly 6.7% of the gas from the F-T recycle loop in order to meet the required in-plant fuel demand of 585 MMBtu/hr (LHV).

PSA-Only. Two subcases are investigated for this option because, in commercial practice, the PSA feed gas should contain greater than 40 mol% of hydrogen. When the water injection to the F-T reactor is maintained at 4,000 mols/hr, as in the previous three options for hydrogen recovery, the hydrogen content is about 33.6 mol%. Thus, a subcase with 41.1 mol% hydrogen in the PSA feed (at 6,000 mols/hr water injection rate) is also included in the analysis of this option

The block flow diagrams for these two subcases are shown in Figures 3-8 and 3-9. In both cases, the PSA units are operated at 80% hydrogen recovery and the PSA reject gas streams exceed the in-plant fuel demand. Thus, the excess gas from the PSA reject stream has to be recompressed and returned to the F-T recycle loop.

Discussion. The key process conditions and flow rates for the various hydrogen recovery options evaluated in this tradeoff case are summarized in Table 3-15. As expected, the PSA feed flow rate depends on the hydrogen content in the feed. The shift unit is a more effective means to concentrate the hydrogen in the PSA feed than the membrane separation.

The estimated capital and annual operating costs are summarized in Table 3-16. Within the accuracy of the cost estimate for the tradeoff study, the estimated total installed costs for the Case 3 (Shift/PSA) and Case 4B (PSA-only with 6,000 mols/hr water injection) are essentially the same.

However, the annual operating cost for Case 3 is $3.03 million higher than that of Case 4B. Therefore, Case 4B is chosen to be included in the baseline design case.

3.1.8 Carbon Dioxide Removal

CO_2 is a byproduct in the F-T reaction. It has to be removed from the F-T recycle loop in order to prevent buildup in the F-T reactor, to reduce the size of equipment in the F-T loop, and to avoid plugging problems by solid CO_2 in the cryogenic unit for hydrocarbons recovery. A portion of the CO_2 removed is recompressed for the coal drying unit and the coal feed system.

Three different types of CO_2 removal systems are being evaluated: chemical solvents, physical solvents, and adsorption systems. The amount of CO_2 removed is determined by (1) the tradeoff between the cost of the CO_2 removal unit and the cost savings from smaller equipment in the F-T loop, and (2) the acceptable amount of CO_2 in the downstream process unit, such as hydrocarbons recovery.

In the selection of an applicable CO_2 removal system, the potential interaction between the selected solvent with the light hydrocargon and CO in the recycle gas will have to be considered. Several process vendors have been asked to submit performance data for the baseline design. In-house process simulation will be used to determine the optimal CO_2 removal design.

3.2 TASK 3 – ENGINEERING DESIGN CRITERIA

In this reporting period, three major activities were initiated: design criteria for the F-T baseline design case, the F-T reactor yield correlation, and the environmental strategy for the Illinois site.

3.2.1 Design Criteria for the Baseline Design

F-T Reactor Design Basis – H_2/CO Ratio and Steam Addition. The Shell gasifier has been chosen for this design based on its high thermal efficiency and minimum oxygen demand. The gasifier in this design uses CO_2, rather than N_2, as its inert solids transfer medium. This is done to minimize buildup of nitrogen in the Fischer-Tropsch (F-T) recycle loop, a factor which has been shown to be highly detrimental in Bechtel's analysis of the effects of oxygen purity. The resulting clean gas composition, from Illinois No. 6 coal, has a H_2/CO ratio of 0.37. Using N_2 transfer gas in a Shell gasifier, a H_2/CO ratio of about 0.5 would be expected.

Almost all pilot plant operations on the slurry reactor have been performed on a feed gas having a H_2/CO ratio of about 0.7. There are two reasons for this: (1) when using this ratio gas with a catalyst active for water gas shift (WGS) the consumption ratio is also close to 0.7 and (2) this is the typical H_2/CO ratio from a slurry-feed gasifier. One of the consequences of using a Shell gasifier, therefore, is that the makeup gas to the F-T reactor has a lower H_2/CO ratio than has been considered conventional up to this point. One way of overcoming this deficiency is to bring in additional water vapor. A second solution would be to add a water gas shift step ahead of the F-T reactor. The latter is certainly a valid fallback design but adds cost. Bechtel has taken the position that it should be avoided unless later experimental work demonstrates that it is necessary.

In Bechtel's designs (both in this study and in the earlier studies under Contract DE-AC22-89PC89867), the stoichiometric effect of the low H_2/CO ratio is compensated for by adding water vapor to the reactor feed gas using a saturator. The F-T reactor material balance calculation assumes the same ΔT approach to WGS equilibrium and sufficient H_2O is added such that H_2 conversion and CO conversion are in the same ratio as in Mobil's pilot plant work. Typically, at an overall syngas conversion of 80%, H_2 conversion is about 73% and CO conversion is about 83%. The product still contains only about 1% water vapor and most of the oxygen atoms in the feed gas wind up as CO_2. Thus, the added steam has been converted almost entirely to CO_2 by virtue of water gas shift.

There are experimental data to show that this type of F-T operation is feasible but they are not of long duration. The simultaneous existence of the WGS reaction is well known, the only difference is that the added water must diffuse to the catalyst, whereas product water formed in situ does not. Some concern has been expressed that the low H_2/CO ratio might lead to carbon formation and catalyst deactivation and that the added steam could inhibit the F-T reaction.

Bechtel's position is that water vapor addition should directionally reduce carbon laydown tendency, just as it does in steam reforming. At present, there is insufficient data on operation at 0.37 H_2/CO ratio to indicate whether it is or is not feasible. Operation at 0.7 ratio appears feasible without water addition (though the catalyst does turn black) and lower ratios will be compensated for by water vapor addition. Obtaining such data should be a high priority for the DOE since it may be essential to taking full advantage of the high thermal efficiency of the Shell gasifier. It seems entirely possible that catalyst selection may be critical. The fallback position would be to introduce a separate water gas shift step ahead of the F-T reactor.

One of the presumed advantages of the slurry reactor is that it can be operated at low H_2/CO ratio, using makeup gas directly from the gasifier without shifting. In Bechtel's earlier report under contract DE-AC22-89PC89867, Dr. Akgerman provided a discussion of carbon formation in F-T reactors (Appendix A). His conclusion was that a slurry reactor has a significant advantage over a fixed-bed reactor in that the catalyst actually sees a higher H_2/CO ratio due to a combination of gas solubility and diffusion rates differences. Akgerman references work by Dry (of Sasol) who found carbon formation rate in a fixed-bed reactor to be related to the ratio $P_{CO}/P_{H_2}^2$. In a slurry reactor, the appropriate ratio is that of concentrations in the liquid phase, which should be much lower than $P_{CO}/P_{H_2}^2$. Akgerman's conclusion is that a slurry reactor at 0.7 ratio is no worse in carbon forming tendency than a fixed-bed reactor at 2.0 ratio. The addition of water vapor should improve the ratio by converting CO to CO_2 and H_2.

Akgerman attributes carbon formation to the Boudouard reaction:

$$2\,CO \rightarrow CO_2 + C_0$$

This reaction is known to be catalyzed by the same types of alkaline materials which are sometimes added to F-T catalysts to adjust selectivity. On the other hand, the F-T reaction is run under conditions where the outlet Boudouard ratio is conducive to carbon removal. Even though the H_2/CO ratio may be very low, the addition of steam produces an equivalent amount of CO_2 which, as seen by the above equation, will prevent carbon formation. If carbon is produced, it must be due to localized concentration gradients.

Bechtel does not expect that the addition of water vapor will inhibit the F-T reaction since, as discussed above, water rapidly reacts and forms CO_2. It is true that Satterfield's rate expression for iron F-T catalysts involves an inhibiting effect due to water which comes into play at conversions over 60% when water is a byproduct. This is probably the reason why low H_2/CO ratio operations, where CO_2, rather than H_2O, is the byproduct, can be run at a comparatively low temperature.

The situation in a large slurry reactor should be improved by liquid backmixing, which makes the liquid uniform in composition, and this composition should be high in CO_2.

Maximum Size Considerations for Vessels.

Background. In the previous Slurry Reactor Design Studies (DE-AC22-89PC89867), the F-T reactors were limited to a maximum internal diameter (ID) of 4.8 meters (15.75 feet), the maximum size for commercially installed Lurgi methanol reactors of the tubular fixed-bed type. The slurry reactors planned for this study should have similar mechanical limitations because of the internal tubesheets used to hold the cooling tubes. There is reason to believe that larger reactors than this may be mechanically feasible. A brief study has now been conducted to learn whether larger reactors would be feasible for the baseline design, given the question of transportation of large shop fabricated reactors to the site and the possibility of field fabrication. Further inquiries will be made during the mechanical design phase of the study.

Mechanical Size Limitations. Pictures of the large fixed-bed reactors built by Belleli for Shell's Middle Distillates Synthesis (F-T) plant in Malaysia were recently published in the *Oil and Gas Journal* (1/13/92). Judging by the size of a man in the photo, Shell's reactors may be 10 meters in diameter and about 18 meters tan-tan length, with hemispherical heads. In private discussions at the 1989 World Methanol Conference, Lurgi indicated that it is prepared to use 7-meter-diameter reactors in new methanol plants.

Such reactors have the catalyst in tubes suspended between upper and lower tubesheets with steam generation on the outside of the tubes. The vessel walls must withstand a steam pressure of about

500 psi. The tubesheets must withstand the difference in pressure between the reactants and steam which is about 200 psi in the case of F-T but may be up to 1000 psi for methanol. The design of these tubesheets imposes a considerable mechanical problem.

Bechtel's slurry reactor design uses bayonet tubes with a double tubesheet arrangement to support the tubes and segregate the flowing coolant. Steam generation is within the tubes and the reacting mixture is contained within the shell outside the tubes. The vessel walls must withstand reacting pressure, which is on the order of 300 psi for the baseline case. If Shell can contemplate a diameter of 10 meters for their fixed-bed F-T reactors, there would appear to be no reason (from a mechanical standpoint) why the slurry reactor could not also be 10 meters in diameter.

Shell's four reactors were shop fabricated in 26 months at two of Bellili's manufacturing plants. It seems unlikely that reactors of this size would be field fabricated. During the mechanical design phase of this study, it is recommended that manufacturers be contacted regarding the possibility of field fabrication and the size limitations that would be imposed.

Transportation Limitations. The coal hydrogenation reactors in the Direct Liquefaction Study (DE-AC22-90PC89857) had a metal ID of 15 feet and an 11.6-inch metal thickness, so that the external diameter was 16.93 feet. The height of each was 85.5 feet and total weight of each was 1282 short tons. A 6-inch refractory lining was installed in the field, but HRI deemed that field construction of the reactors themselves was impractical. A brief survey was made by HRI and Bechtel's Houston office to assure that vessels close to 17 feet in diameter could be transported to the plant site outside of DuQuoin, Illinois. It was found that this would be feasible by a combination of river transport to a Mississippi River port such as East St. Louis and highway transport roughly 75 miles to the plant site.

Transportation options to the western site in Wyoming are somewhat more limited and studies done for the other synfuel projects outside of Gillette, Wyoming, found a maximum diameter limitation of 15 feet.

Shop vs Field Fabrication. The issues in deciding between shop and field fabrication are complex but, as a general rule, it can be stated that field fabrication does not produce very large cost savings in the majority of cases. Whatever savings are to be obtained in cost of materials are, to a large extent, negated by the higher cost of field labor, particularly in a remote location. Of course, certain complicated vessels, such as FCC reactors, must be field fabricated to a large extent and refractory linings are commonly installed in the field.

In a study done for the Syncrude Project in 1973, three shop-fabricated gas oil hydrotreater reactors (12-inch diameter) were compared with a single field-fabricated reactor (20.5-inch diameter). The shop-fabricated reactor trains cost an estimated $12.2 million, and the field-fabricated train cost an estimated $13.7 million. The study was carried through the stages of process design, reactor mechanical design, P&IDs and conceptual layouts, piping takeoffs and instrument counts. In the multireactor case, the cost of separate preheaters and intercoolers was included, but a common hydrogen recirculation system was used. The study was carried out for a reactor pressure of 800 psi. The final design pressure was 1500 psi and shop-fabricated reactors were used.

When all was said and done, there was little savings in materials cost for the large single reactor system and the high cost of field labor swung the economics towards shop fabrication. Admittedly, northern Alberta was then and still is a high-cost labor area but, even allowing for this, it is difficult to see how field fabrication could have been favored.

Conclusions. Based on this brief survey, it is concluded that a 15-foot OD should be the general limit on vessel size for the indirect liquefaction study, provided that, in special cases, diameters of 17 feet be considered feasible for the Illinois site. Such special cases would include the F-T reactors which have a number of significant pieces of auxiliary equipment that also have to be duplicated along with the reactors.

While some investigation into the limits of field fabrication should be carried out with vessel manufacturers, this would be primarily for the purpose of aiding future design work. Shop fabrication should be the basis for the present study and the chances of missing a significant cost savings by doing so are considered nil. Although Shell used 10-meter-diameter reactors in its Malaysian plant, the choice was based on shop fabrication and ocean shipping. This option is not feasible for a mine mouth location in the United States.

Future Work. Using this limitation on vessel size and other equipment size limitations, an examination will be made of the number of trains required for each process step in the baseline case. Shell has already set the capacity of the gasifiers as 2000 stpd of Illinois No. 6 coal, washed and dried to 5% moisture. The baseline design will employ 10 operating gasifiers, which equates to roughly 40,000 bpsd of liquid product. Work is also proceeding to establish a reasonable overall operating factor and determine whether spare gasifiers are necessary to achieve this factor.

Site-Related Criteria. Based on information from the direct liquefaction study, site related design factors are as shown in Table 3-17.

3.2.2 F-T Reactor Yield Correlation

Final F-T Reactor Yield Model

Background. The F-T reactor yield model is based on correlations of the Mobil first-stage pilot plant data according to triple α Schulz-Flory theory as described later in this section. The reactor yield model, there presented, requires the user to estimate values of α_2 and the methane factor (MF) corresponding to graphical correlations of α_2 vs wax yield and methane yield vs wax yield. The proper value of α_3 is then determined by trial and error calculation until the estimated wax yield is exactly predicted. This is obviously not a suitable correlation for a computerized process flow simulation program and the prediction has been automated. The prediction of oxygenates has also been automated so that it is not necessary to use the charts presented later.

Basically, the user starts with a trial wax yield and the program estimates the entire product distribution, including a new wax yield which may differ by up to ±1.0 wt% units from the trial value. If desired, a new trial value can be assumed until the desired wax yield is exactly matched and graphical guidance is provided as to the proper trial yield to assume. The entire product distribution including the olefin paraffin split and the oxygenates is then estimated. Table 3-18 is a spreadsheet documenting the results of the calculation at 50% wax yield and showing how the results can be integrated into a simulation of the entire F-T recycle loop. All results are well within experimental deviations but the method is limited to the range from 9.6 to 76% wax yield.

Derivation of Equations. The trial and error estimating procedure described above was used to estimate values of α_2, methane factor, and α_3 at wax yields of 9.6, 25, 50, 60, and 76 wt%. The results are given below (α_1 is calculated from α_2 and the methane factor):

Wax Yield	α_1	α_2	α_3	MF
9.6	.485	.79	.87	6.0
25	.520	.806	.932615	6.165
50	.498	.829	.95963	8.5
60	.471	.837	.966464	10.7
76	.419	.85	.9765	15

These values of α_2, α_3, and methane factor (MF) were then regressed against wax yield to obtain polynomial curve fits up to third order. The correlation coefficient for α_3 was not satisfactory and it was decided to reverse the procedure and correlate wax yield against a third order polynomial in α_3. This fit was quite good. Similarly, it was judged that wax yield correlated against a second order polynomial in α_2 was a better representation of the data, within the desired limits of wax yield, than the reverse correlation. This complicates the issue somewhat by requiring the solution of a cubic and a quadratic equation, respectively, but this has been automated and does not pose a problem.

Polynomial expressions have also been developed to predict water soluble and hydrocarbon soluble oxygenates yields based on methane yield (which was the only available parameter in most cases). Since the methane yield is predicted from the wax yield, there is some loss in accuracy, but, all in all, the limited available data are duplicated quite well. In view of the lack of data for other than a few final Mobil runs, oxygenates present in the vapor phase have been estimated to remain constant at an average measured value of 0.39 wt%.

Average values were obtained for the C, H, and O numbers of these same three oxygenate fractions based on averaging the results of all the analyses provided by Mobil in their reports. With two exceptions these numbers were assumed to remain constant as wax yield varies. The exceptions were the C and H numbers of the hydrocarbon soluble oxygenates. Since product breakdowns were available only for the low wax case and since the C number of the oxygenates should parallel the C number of the corresponding C_2-C_{19} hydrocarbon fraction, the latter was used to prorate the former for wax yields other than 9.6 wt%. (The carbon number of the C_2-C_{19} fraction is calculated from the value of α_2.) The H number of the hydrocarbon soluble oxygenates is calculated from the C number, assuming that the ratio of H_{2n}/C_n to H_{2n+2}/C_n constituents remains constant at all wax yields. The O Number for the wax is assumed to remain constant at 0.231 and is based on 22 wt% oxygenates, a number published by Mobil after their final report was written.

The calculation also provides olefin/paraffin ratios for each carbon number and these stay constant regardless of wax yield.

Procedure. The results of the correlations have been incorporated into an Excel spreadsheet which simulates the F-T reactor loop, including CO_2 removal, hydrocarbon recovery, hydrogen recovery, autothermal reforming and recycle to the F-T reactor. Table 3-18 documents the results of the calculation at 50% wax yield. The α values, correlation constants and the final yield distribution are shown on pages 4 and 5 of the spreadsheet in Table 3-18. The F-T reactor calculation uses the overall stoichiometric coefficients thus determined to run an elemental balance on the reactor assuming a given approach to water gas shift equilibrium. This determines the total hydrocarbon yield and individual components are then prorated from the yield distribution shown.

Values of the correlation constants are truncated in the printout, the extended value of the constants is given below.

Dep Var	Ind Var	A	B	C	D
%Wax	α_2	1400.862011	-4427.319882	3374.924039	
%Wax	α_3	-37006.47812	126869.57423	1.450249E-06	55290.3754
MF	%Wax	6.41280781	-0.0579554	0.001645086	7.986126E-06
OxW	%Wax	1.1282877	0.055580513		
OXHC	%Wax	1.35096875	0.133087676	0.110532834	

If the dependent variable is y and the independent variable is x, the form of these equations is:

$$y = A + B \cdot x + C \cdot x^2 + D \cdot x^3$$

For α_2, the familiar quadratic formula is used:

$$\alpha_2 = \{- B + [B^2 - 4 \cdot C \cdot (A - \%Wax)]^{0.5}\} / (2 \cdot C)$$

Only the positive root is used. Remember that A, B, and C are switched from their usual roles in the quadratic formula.

For α_3, Cardan's method as outlined in Perry's *Chemical Engineer's Handbook 3rd Edition*, page 67, is used. The calculation is simplified by defining some new terms as shown on the spreadsheet. The terminology parallels that in Perry's *Handbook*.

$$a = C/D$$
$$b = B/D$$
$$c = (A - \%Wax)/D$$
$$a' = - a^2/3 + b$$
$$b' = - a^3/27 + a^3/9 - a \cdot b/3 + \%Wax$$

$$y = [- b'/2 + (b'^2/4 + a'^3/27)^{0.5}]^{1/3} - [+ b'/2 + (b'^2/4 + a'^3/27)^{0.5}]^{1/3}$$
$$\alpha_3 = y - a/3$$

As described above, when a trial value of wax yield is entered into the program, a slightly different wax yield results. To aid in the use of the program, Figure 3-10 provides a correlation of the actual resulting wax yield against the delta which must be subtracted to get the trial wax yield.

Recommendations. It is recommended that this spreadsheet procedure be adapted by Amoco for yield prediction in the ASPEN SP process flow sheet simulator. It is also recommended that it be used now for the baseline case so that results will later conform to those predicted by the process flow sheet simulator. Actually all that is required now is that the C, H and O numbers for the overall product conform exactly to those predicted for a wax yield of 50% and that the hydrocarbon breakdown follow spreadsheet procedures already being used in the ASPEN SP modeling of the F-T loop. The oxygenates then need to be accounted for in the various product phases.

Future Work. The above procedures predict the molecular weight distribution and the olefin to paraffin ratio of the hydrocarbon product but do not identify iso to normal ratios or the fraction naphthenes (aromatics are absent). For most purposes, simulations can be carried out assuming all normal paraffin and all 1-olefin but, for downstream upgrading, further breakdown of the C_4, C_5, and possibly C_6 fractions will be useful.

A review of Mobil's ZSM-5 second step yield data has been commenced for the alternative case. The primary reactions occurring are olefin and oxygenate conversion into aromatics, naphthenes, paraffins, and water, along with isomerization. Appropriate component deltas must be developed.

Schulz-Flory Theory and Graphical Method. The basic Schulz-Flory relationship is given by:

$$C_n = (1 - \alpha) \cdot \alpha^{n-1}$$

where C_n is the mol fraction of C_nH_{2n} on total product. Note that:

$$\sum C_n = (1 - \alpha) \cdot \sum \alpha^{n-1} = 1, \text{ since}$$

$$\sum \alpha^{n-1} = 1/(1 - \alpha)$$

Let W_n be the weight of C_nH_{2n} per total mol of product. The molecular weight of C_nH_{2n} is $14.016 \cdot n$. Thus

$$W_n = 14.016 \cdot n \cdot (1 - \alpha) \cdot \alpha^{n-1}$$

$$\sum W_n = 14.016 \cdot (1 - \alpha) \cdot \sum n \cdot \alpha^{n-1} = 14.016/(1 - \alpha)$$

since

$$\sum n \cdot \alpha^{n-1} = 1/(1 - \alpha)^2$$

$$\text{Thus weight fraction, } wf = W_n/\sum W_n = n \cdot (1 - \alpha)^2 \cdot \alpha^{n-1}$$

$$wf/n = (1 - \alpha)^2 \cdot \alpha^{n-1}$$

This is the form usually plotted, giving a straight line on semilog paper when wf/n is plotted against n, with a slope of log α:

$$\log (wf/n) = 2 \log (1 - \alpha) + (n - 1) \log \alpha$$

This relationship holds strictly for olefins; it is less accurate, but still reasonable, for paraffins.

Double α. It can be shown that the above summations can be generalized:

$$\sum_{n=2}^{n=\infty} \alpha^{n-1} = 1/(1 - \alpha) - 1 = \alpha/(1 - \alpha)$$

$$\sum_{n=3}^{n=\infty} \alpha^{n-1} = 1/(1 - \alpha) - (1 + \alpha) = \alpha^2/(1 - \alpha)$$

$$\sum_{n=i}^{n=\infty} \alpha^{n-1} = \alpha^{i-1}/(1-\alpha)$$

and

$$\sum_{n=2}^{n=\infty} n \cdot \alpha^{n-1} = 1/(1-\alpha)^2 - 1 = \{2 \cdot \alpha - \alpha^2\}/(1-\alpha)^2$$

$$\sum_{n=3}^{n=\infty} n \cdot \alpha^{n-1} = 1/(1-\alpha)^2 - (1 + 2 \cdot \alpha) = \{3 \cdot \alpha^2 - 2 \cdot \alpha^3\}/(1-\alpha)^2$$

$$\sum_{n=i}^{n=\infty} n \cdot \alpha^{n-1} = \{i \cdot \alpha^{i-1} - (i-1) \cdot \alpha^{i}\}/(1-\alpha)^2$$

Therefore,

$$\sum_{n=i}^{n=\infty} C_n = \alpha^{i-1}$$

and

$$\sum_{n=i}^{n=\infty} wf = i \cdot \alpha^{i-1} - (i-1) \cdot \alpha^{i}$$

If α changes at $n = i$ from α_1 to α_2, then in order to make $wf_1 = wf_2$ at $n = i$, calculated wf_1 and wf_2 values must be multiplied by constants x and y, respectively, so that both expressions give the same value of wf_i and $\Sigma wf = 1$

$$wf/i = x \cdot (1-\alpha_1)^2 \cdot \alpha_1^{\,i-1} = y \cdot (1-\alpha_2)^2 \cdot \alpha_2^{\,i-1}$$

thus

$$y/x = [(1-\alpha_1)^2 \cdot \alpha_1^{\,i-1}]/[(1-\alpha_2)^2 \cdot \alpha_2^{\,i-1}]$$

$$\sum_{n=i}^{n=\infty} wf_2 = \{ i \cdot \alpha_2^{\,i-1} - (i-1) \cdot \alpha_2^{\,i} \} \cdot y$$

$$\sum_{n=1}^{n=i-1} wf_1 = \{1 - [i \cdot \alpha_1^{\,i-1} - (i-1) \cdot \alpha_1^{\,i}]\} \cdot x$$

In order to make the total $\Sigma\ wf_1 + \Sigma\ wf_2$ become equal to 1

$$x = 1 / \{1 - i \cdot \alpha_1^{\,i-1} + (i-1) \cdot \alpha_1^{\,i} + y/x \cdot [i \cdot \alpha_2^{\,i-1} - (i-1) \cdot \alpha_2^{\,i}]\}$$

It is then possible to solve for x and y for any given values of α_1, α_2 and i, and the wt% wax can be calculated from

$$\sum_{n=i}^{n=\infty} wf_2 = \{ i \cdot \alpha_2^{\,i-1} - (i-1) \cdot \alpha_2^{\,i} \} \cdot y$$

One interpretation of the double alpha phenomenon in the slurry reactor is that α_1 represents the chain growth parameter in the vapor phase and α_2 represents that in the liquid phase. If so, the relationship is complicated by vapor-liquid equilibrium considerations. The Mobil data indicate that, above C_{20}, most of the product is in the liquid phase and constitutes the so-called "wax" product. Between C_{15} and C_{25}, there is a transition from vapor to liquid and one would expect the molecular weight distribution to be smeared, which the Mobil data appear to corroborate.

Stoichiometry. In the Appendix to their article on slurry reactor modeling, Stern, Bell, and Heinemann show how the stoichiometric coefficients for the single α case can be written in closed form as a function of α, the chain growth probability factor, and γ, the fraction of the C2+ product which is olefinic. The double α case can be developed in similar fashion.

Assuming 100% olefinicity, the average carbon number of the total product from $n = i$ to $n = \infty$ is given by the relationship:

$$x = \sum_{n=i}^{n=\infty} n \cdot \alpha^{n-1} / \sum_{n=i}^{n=\infty} \alpha^{n-1}$$

where x is the average chain length in the formula C_xH_y. A similar relationship can be developed for a carbon number range from n = i to n = j:

$$x = [\sum_{n=i}^{n=\infty} n \cdot \alpha^{n-1}] - [\sum_{n=j}^{n=\infty} n \cdot \alpha^{n-1}] / [\sum_{n=i}^{n=\infty} \alpha^{n-1}] - [\sum_{n=j}^{n=\infty} \alpha^{n-1}]$$

Using the equations for these summations given above and remembering that:

$$\alpha^{i-1} = \alpha^{i} / \alpha$$

the resulting expression for x from i to infinity reduces to:

$$x = i + \alpha / (1 - \alpha)$$

If i = 1, this in turn reduces to

$$x = 1 / (1 - \alpha)$$

which is the result given by Stern et al.

Figure 3-11 shows the carbon number of the C_i+ as a function of α for i = 20 and is representative of the Mobil waxes which are predominantly C_{20}+.

The value of y can readily be calculated from the value of γ, the mol fraction of olefins, once x is known. Since the formula for olefins is C_nH_{2n} and the formula for paraffins is C_nH_{2n+2}, the value of y is given by

$$y = 2 \cdot x + (1 - \gamma) \cdot 2.$$

This, of course, assumes that γ is constant over the entire range. It also assumes that no other components than paraffins and olefins are present. Except for the oxygenates, this is a good assumption. The evidence indicates that the α for oxygenates is significantly lower than for hydrocarbons, so that the concentration in the wax should be quite low, even if an allowance is made for a double α there too.

It is also of value to have a way of estimating the average carbon number between n = i and n = j. The value of x is given by:

$$x = [(i + \alpha / (1 - \alpha)) \cdot \alpha^{i} - [(j + \alpha / (1 - \alpha)) \cdot \alpha^{j})] / (\alpha^{i} - \alpha^{j})$$

High Methane Yield – Triple α. It is commonly observed that methane yield is somewhat higher than expected by Schulz-Flory theory. With cobalt catalysts, this difference is quite pronounced and the ethane yield is, at the same time, lower than theory. Huff has shown how this can be accounted for by considering polymerization of not just C_1 but also of C_2 and C_3, each at its own chain growth factor. For iron catalysts, only the methane yield is high and the following discussion shows how this can be accounted for by using a lower chain growth probability factor for methane. In other words, there can now be a triple α situation, where α_1 is for methane, α_2 is for C_2 to C_i, and α_3 is for C_i plus. For these three carbon number ranges, normalizing factors x, y, and z, respectively, are also defined.

In single α theory, methane yield is given by $(1 - \alpha)^2$. For the triple α case, assume that the methane yield is higher than would be predicted from α_2 by a factor C. Thus, α_1 can be defined such that

$$(1 - \alpha_1)^2 = C \cdot (1 - \alpha_2)^2$$

Since the expressions in α_1 and α_2 must give the same value for weight fraction ethane:

$$y \cdot (\alpha_2 \cdot (1 - \alpha_2)^2) = x \cdot (\alpha_1 \cdot (1 - \alpha_1)^2) = C \cdot x \cdot (\alpha_1 \cdot (1 - \alpha_2)^2)$$

and

$$x / y = \alpha_2 / (C \cdot \alpha_1) \; .$$

As in the double α case, the ratio z / y is given by

$$z / y = [(1 - \alpha_2)^2 \cdot \alpha_2^{\,i-1}] / [(1 - \alpha_3)^2 \cdot \alpha_3^{\,i-1}]$$

and the weight fractions summed over the three carbon number ranges are

$$\sum_{n=1}^{n=1} wf_1 = wf_1 = (1 - \alpha_1)^2 \cdot x = C \cdot (1 - \alpha_2)^2 \cdot x$$

$$\sum_{n=2}^{n=i-1} wf_2 = \{1 - [\, i \cdot \alpha_2^{\,i-1} - (i - 1) \cdot \alpha_2^{\,i} \,] - (1 - \alpha_2)^2\} \cdot y$$

$$\sum_{n=i}^{n=\infty} wf_3 = \{ i \cdot \alpha_3{}^{i-1} - (i-1) \cdot \alpha_3{}^{i} \} \cdot z$$

And y is given by

$$y = 1 / (\sum wf_2 + \sum wf_3 \cdot z / y + wf_1 \cdot x / y).$$

Figure 3-12 shows how the weight percent wax varies with α_2 and α_3 for $i = 20$ (the carbon number marking the initiation of wax formation) and an MF of 4. The correlation of α_2 with wax yield developed from the Mobil pilot plant data is shown by the heavy circles and is nearly a straight line between 10 and 75% wax. It is apparent that once α_2 is fixed, along with the MF, there is only one value of α_3 which will match the observed wax yield.

Figure 3-13 shows a correlation of observed wax yields and methane yields taken from selected Mobil data. This is a good match to Figure IV-23 in Mobil's second report. Figure 3-14 shows the values of the MF required to match the correlation line in Figure 3-13. Both MF and α_3 depend on wax yield, but the relation with α_3 is much more sensitive. A trial and error procedure can be used to determine the best fit. These results lead to the three triple alpha plots given in Figure 3-15 for 76, 46, and 9.5% wax, respectively.

Oxygenates Production. Mobil measured oxygenates production in only a few runs, mostly at low to medium wax yield conditions, but the wax yields are often not given. A correlation against methane yield was obtained and is shown in Figure 3-16. Methane yield was used instead of wax yield to obtain a more consistent plot, but the two are related as shown in Figure 3-13. There appears to be a definite decrease in the oxygenates found in the overhead liquid hydrocarbon phase as methane yield decreases, but this may simply represent a decrease in the C_2/C_{19} fraction. The concentration does not drop and may even increase. This probably explains why the oxygenates soluble in the water phase remain almost constant as methane yield varies.

Figure 3-17 shows how α_1, α_2, and α_3 vary over the experimental range of the data to match observed yields of wax and methane. These yields are then worked up into an overall product distribution and stoichiometric constants using observed average olefin contents and oxygenate yields for the various carbon number ranges.

3.2.3 Environmental Strategy

With some minor modifications, the environmental compliance strategy developed for the Direct Coal Liquefaction Baseline Design Study and System Analysis (DOE Contract No. DE-AC22-91PC90027) can also be used for the Indirect Liquefaction Study. All of the major federal and Illinois environmental considerations to be addressed and the timing for same apply equally to

Illinois environmental considerations to be addressed and the timing for same apply equally to both facilities. Specific pollutants/hazards and their sources identified for direct liquefaction are listed in Table 3-19. This list will require modification for an indirect liquefaction facility, and the indirect liquefaction facility should be more environmentally benign. Some specific comments are as follows:

- No coal-fired boiler is planned in the indirect facility so certain pollutants, such as beryllium, lead, mercury, and halogens should not be present in the stack gases.
- The facility will be fueled by byproduct gas from the F-T recycle gas loop, supplemented by clean syngas, if necessary. Both of these are free of sulfur compounds and the stack gas from boilers and heaters will have no problem meeting SO_2 and particulate matter limitations. NO_x limitations will be the primary restriction.
- Coal receiving and handling differ only in degree and the same restrictions will apply.
- Both plants have coal gasifiers. The Shell gasifiers, in the indirect design, are dry feed gasifiers operating at higher temperature and produce a somewhat different slag. The Texaco gasifiers, used for hydrogen production in the direct design, feed a coal-water slurry. Both slags tie up the hazardous constituents of coal and are considered non-hazardous solid byproducts.
- Essentially all of the sulfur is removed from syngas in the indirect case by a combination of hydrolysis and acid gas removal (Selexol or Rectisol) and sulfur polishing with beds of zinc oxide. The zinc sulfide thus produced is an additional non-hazardous solid byproduct.
- The products of indirect liquefaction are sulfur and nitrogen free and have essentially no aromatics content prior to catalytic reforming. In contrast the products of direct liquefaction contain some sulfur and nitrogen compounds, depending on the depth of hydrotreating, and are high in aromatics. Depending on the upgrading route, oxygenated byproducts may be produced in quantity as an F-T byproduct. Recovery of alcohols and inclusion in gasoline is a possibility. These differences may affect TSCA requirements.
- Removal of oxygenates from F-T wastewater will be required unless the water is recycled. VOC control will certainly be required.
- Where Table 3-19 refers to the hydrotreaters (HTUs) for direct liquefaction, substitute the words *product upgrading units* for indirect liquefaction. The main difference is that different catalysts are used which may require different methods of handling and disposal. Upgrading units being considered include oligomerization (ZSM-5), wax hydrocracking, hydrotreating, cat poly, isomerization, alkylation, and cat reforming.

There is no FCC unit and no coker in the present indirect liquefaction cases, although consideration of FCC is a possible future option.

3.3 TASK 7 – PROJECT MANAGEMENT AND ADMINISTRATION

During the reporting period, the major activities in Task 7 were issue the final project management plan, hold the first technical progress meeting, prepare the subsequent conference note, and complete the Bechtel and Amoco subcontract agreement.

The first technical progress meeting was held on February 26, 1992 in Bechtel's San Francisco offices and attended by representations of PETC, Amoco, Bechtel, Mitre Corporation and Burns and Roe (consultants to PETC). The preliminary results of the tradeoff studies and the design criteria were reviewed. The overall project schedule status at the end of the reporting period is shown in Figure 3-18.

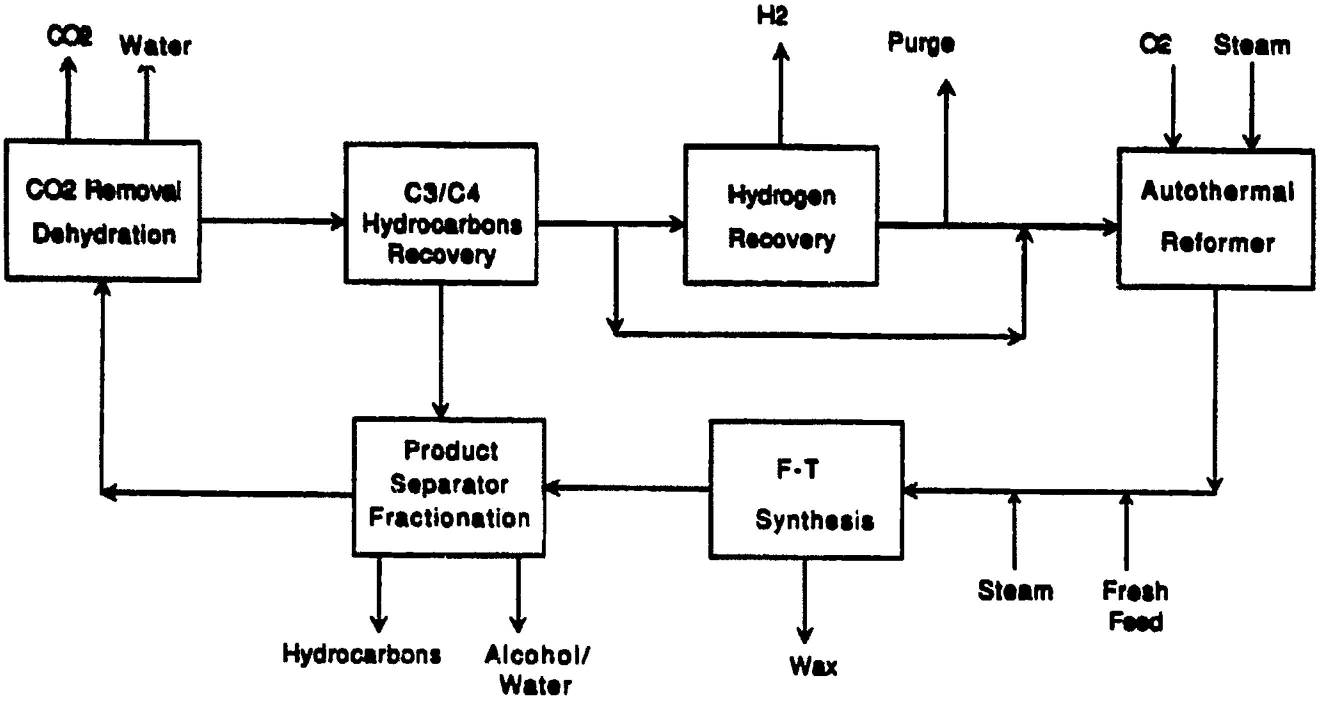


Figure 3-1 Block Flow Diagram for the F-T Recycle Loop

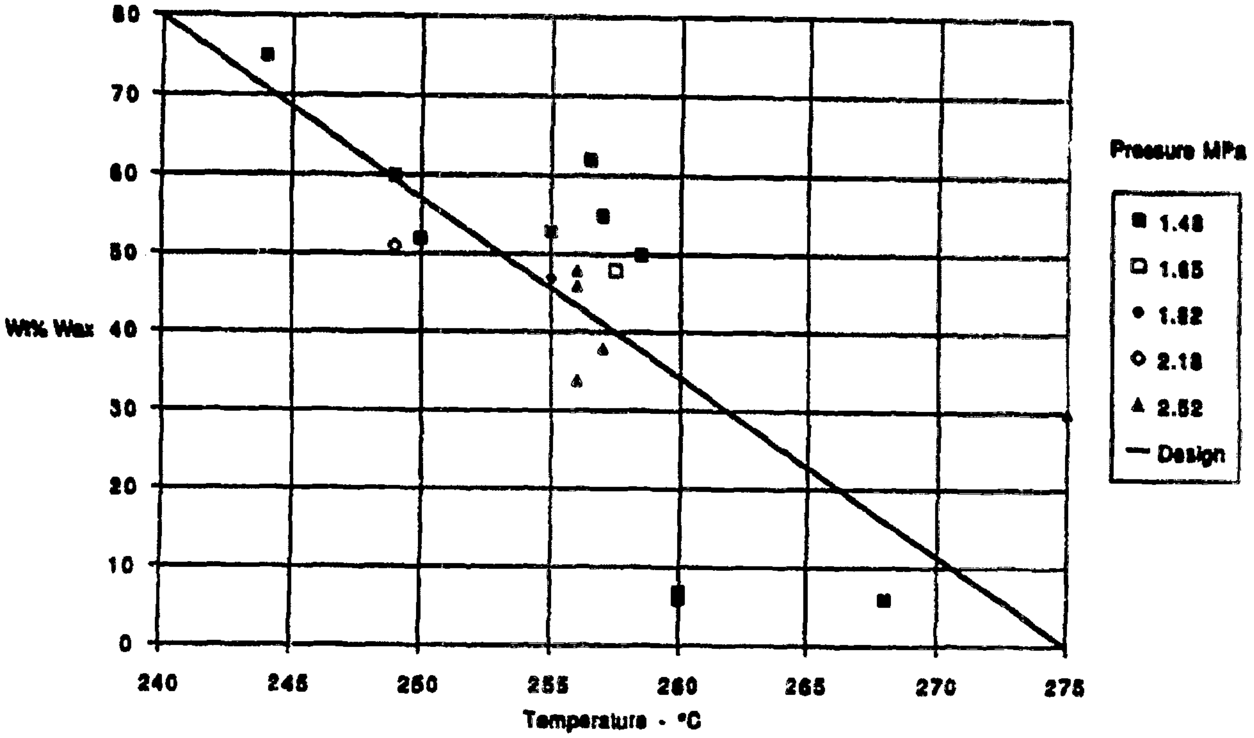


Figure 3-2 Wax Yield Versus Temperature and Pressure

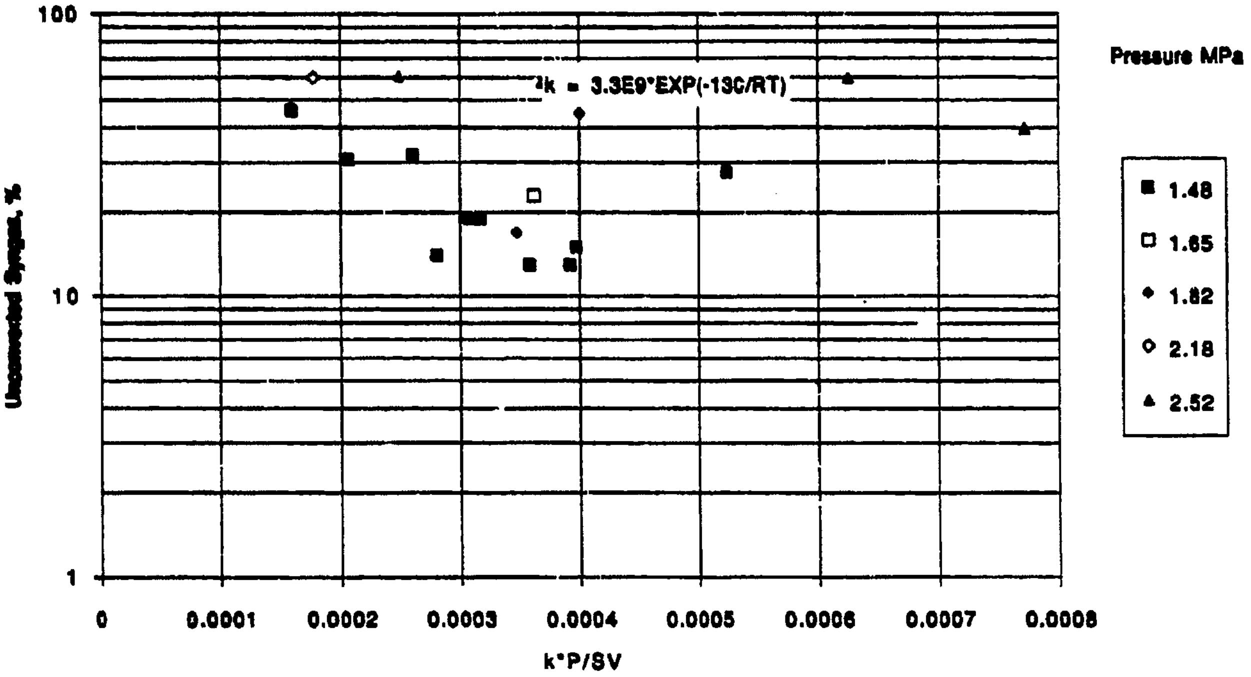


Figure 3-3 **F-T Kinetic Data Correlation**
Percent Unconverted Syngas Versus Correlation Parameter (K*P/SV)
K* = 3.3E09*EXP(-130/RT)

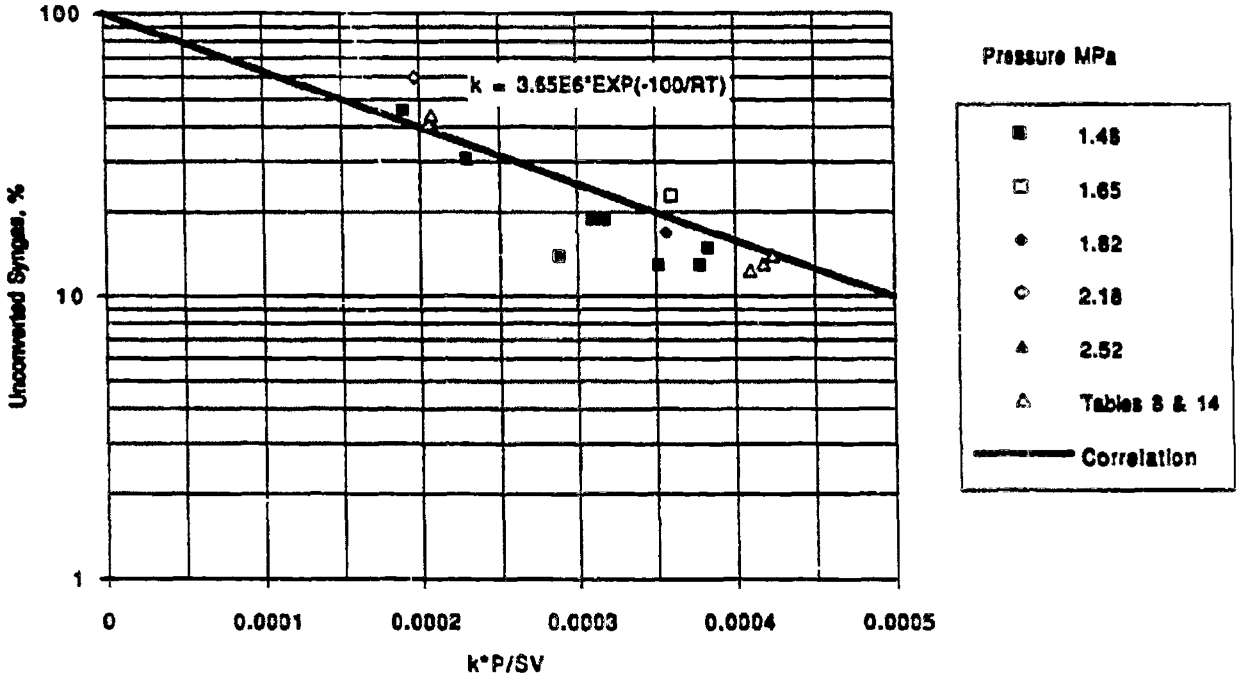


Figure 3-4 **F-T Kinetic Data Correlation**
Percent Unconverted Syngas Versus Correlation Parameter (K*P/SV)
K* = 3.65E06*EXP(-100/RT)

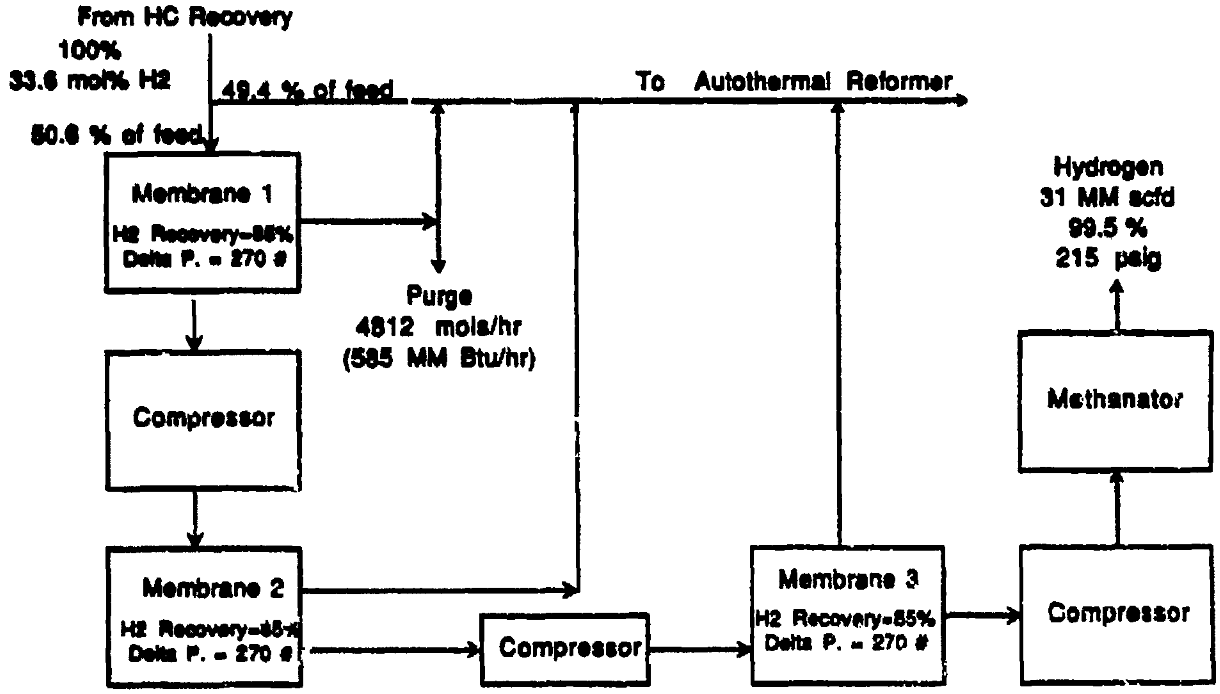


Figure 3-5 Hydrogen Recovery Tradeoff – Membrane/Methanator Case

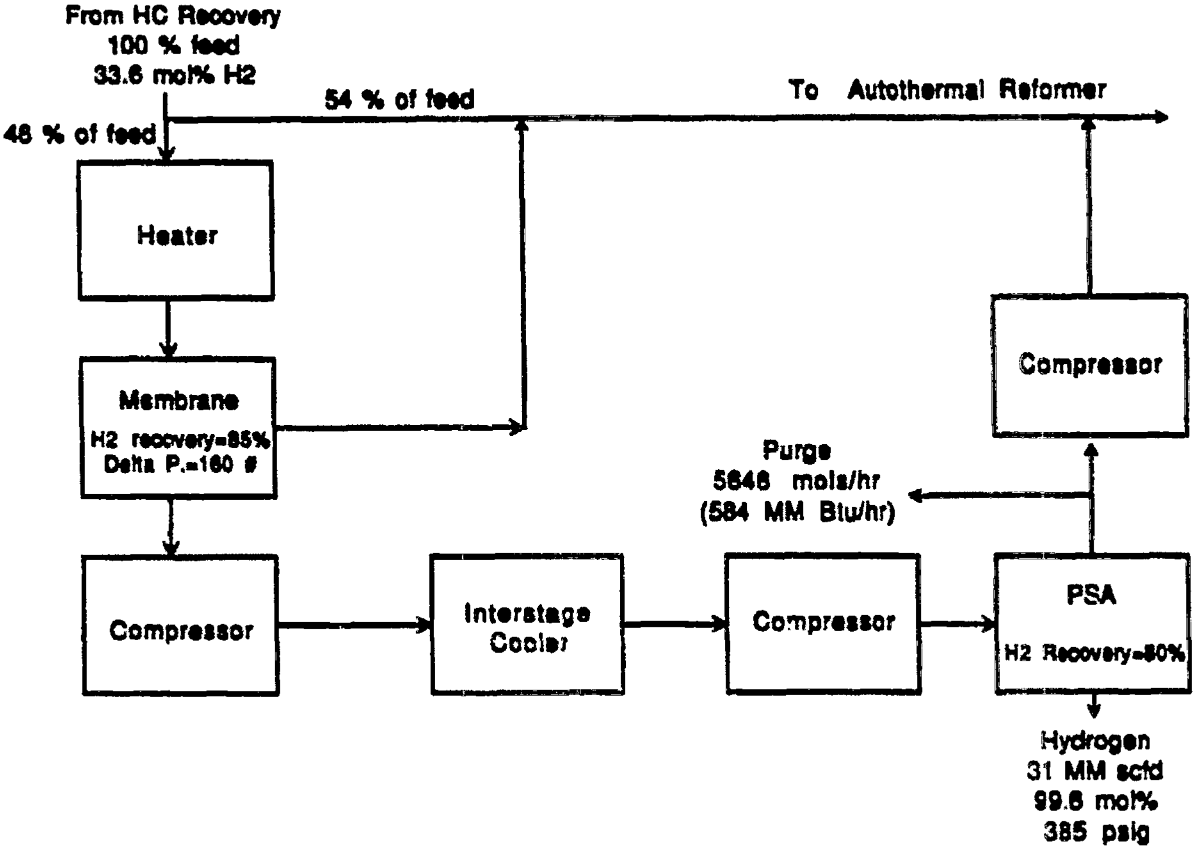


Figure 3-6 Hydrogen Recovery Tradeoff – Membrane/PSA Case

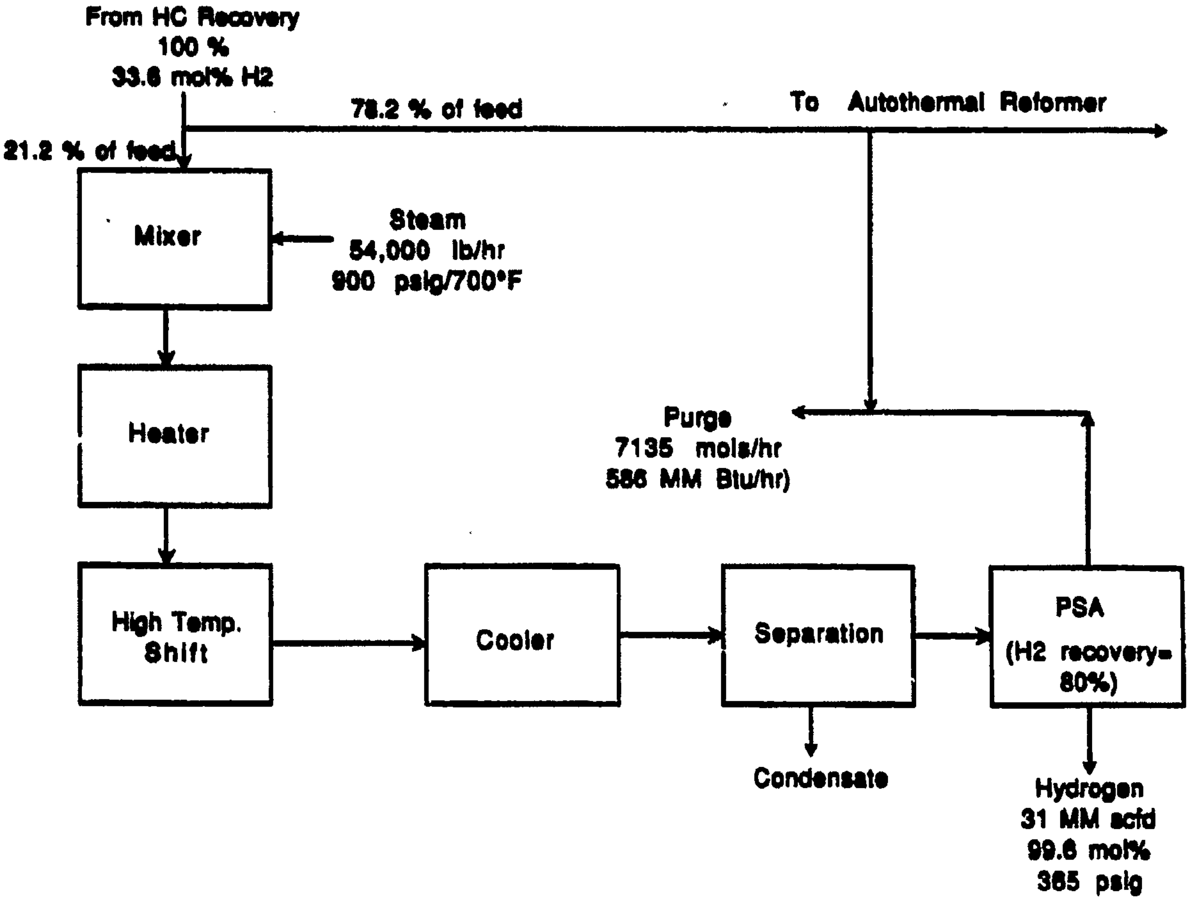


Figure 3-7 Hydrogen Recovery Tradeoff – Shift/PSA Case

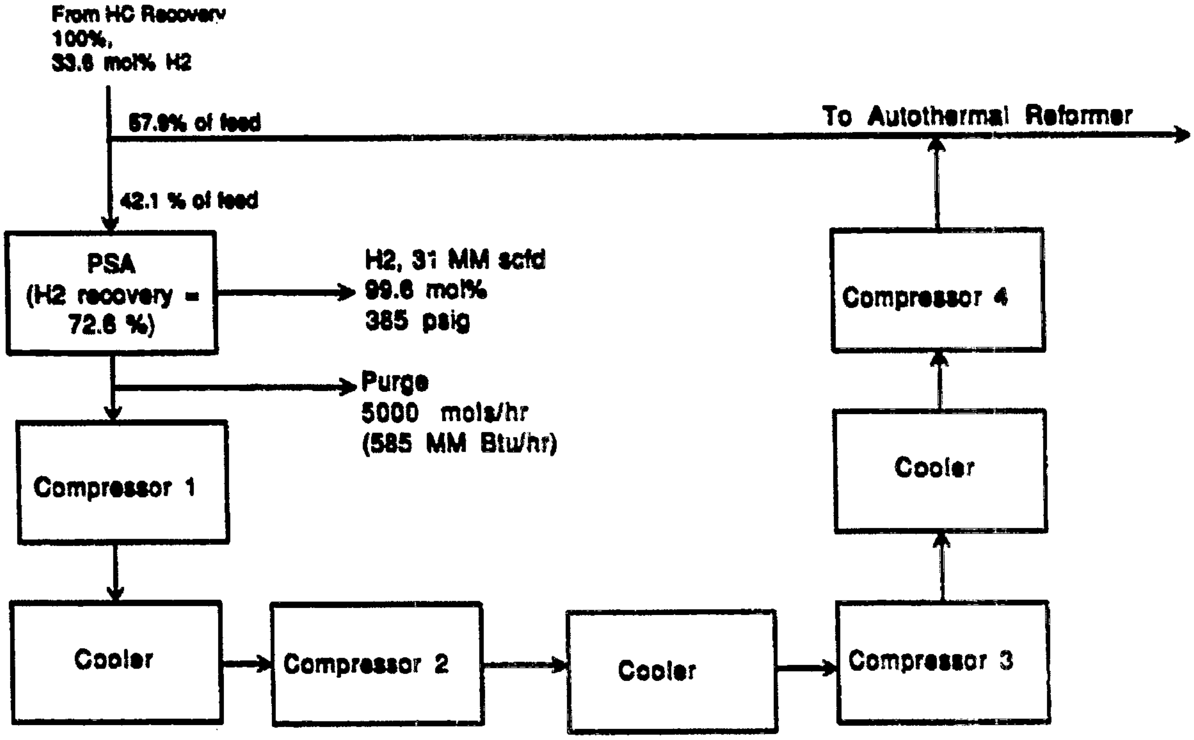


Figure 3-8 Hydrogen Recovery Tradeoff – PSA-Only Case (Water Injection, 4000 mols/hr)

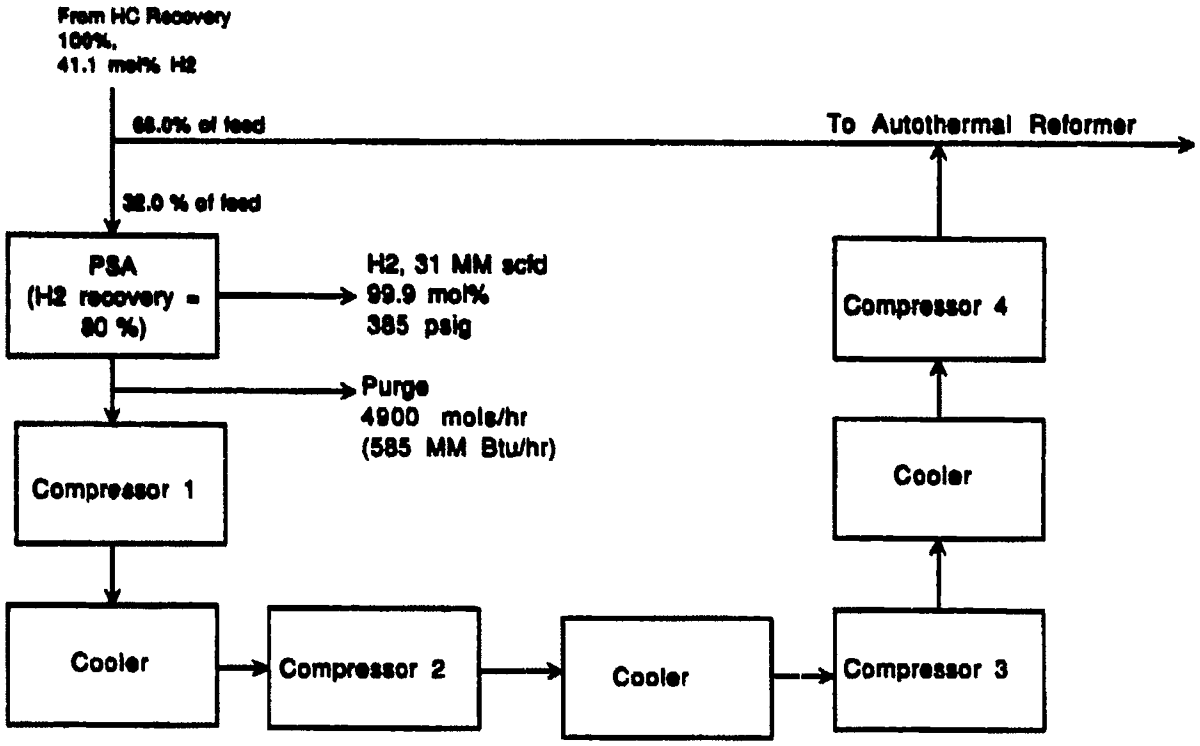


Figure 3-9 Hydrogen Recovery Tradeoff – PSA-Only Case (Water Injection, 6000 mols/hr)

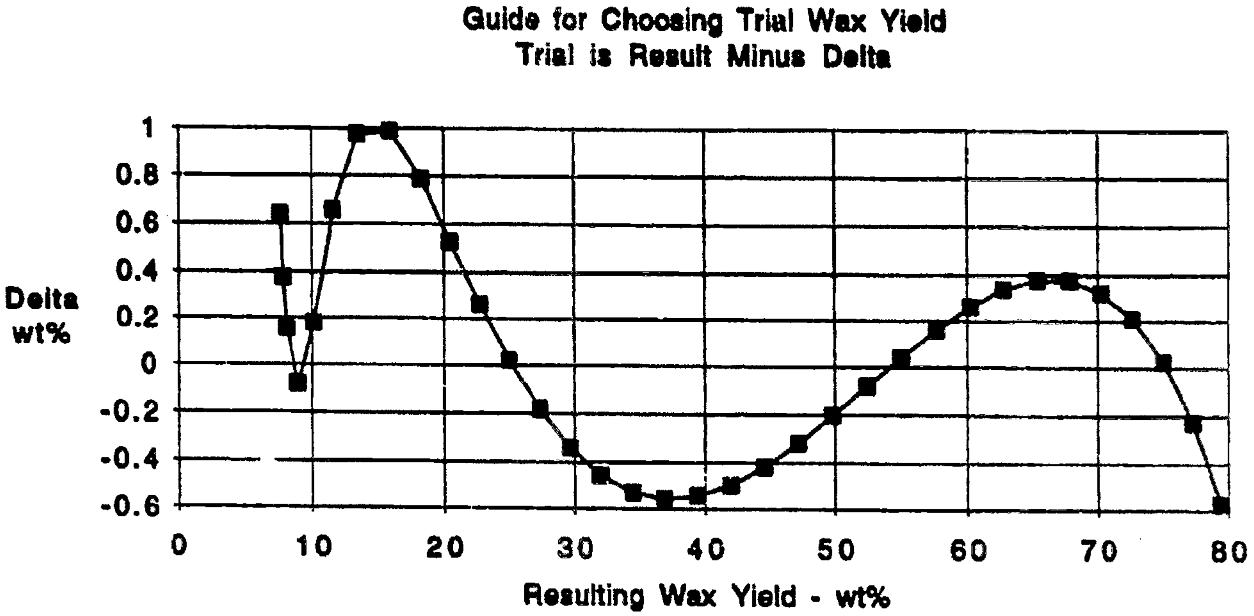


Figure 3-10 Guide for Choosing Trial Wax Yield

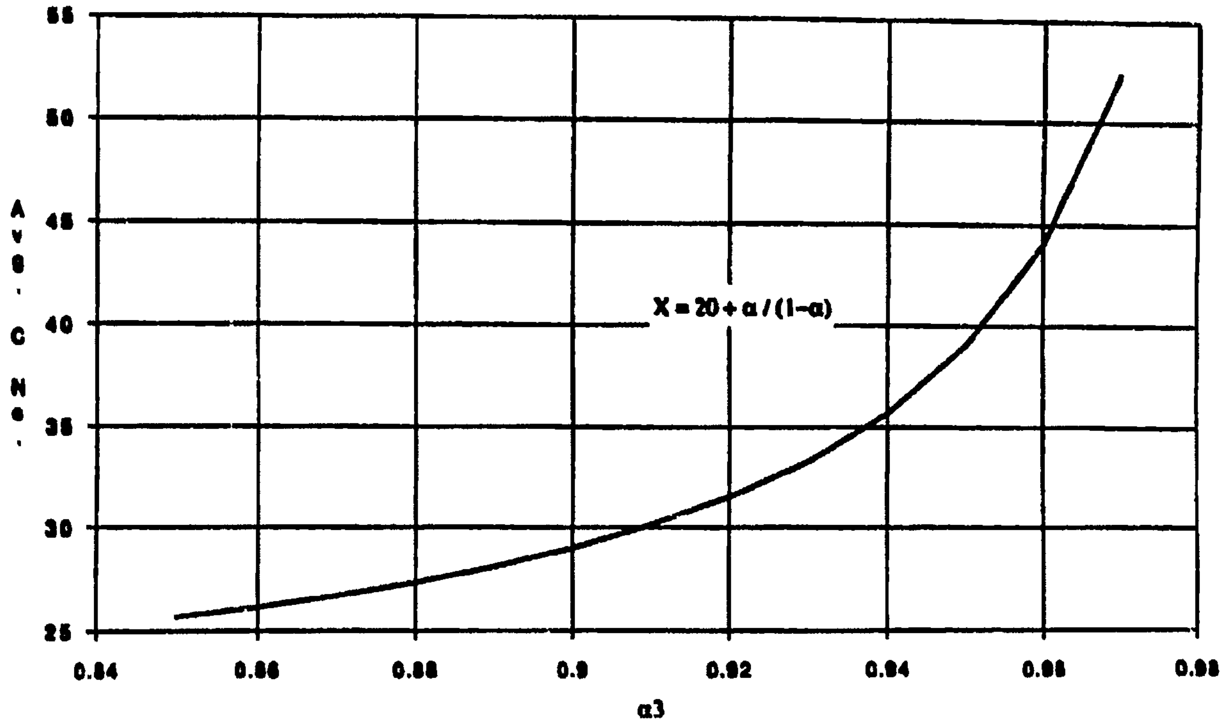


Figure 3-11 Average Carbon Number of C_{20+} Wax

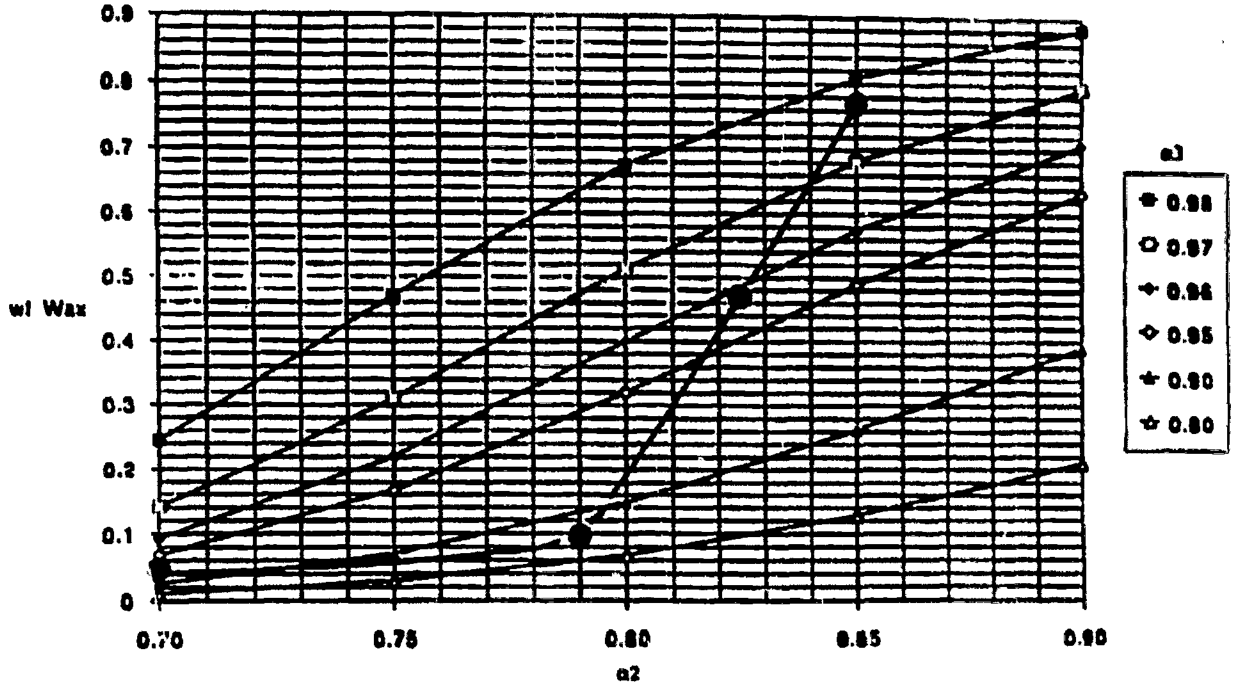


Figure 3-12 Weight Percent Wax Versus Double Alpha (I=20, MF=4)

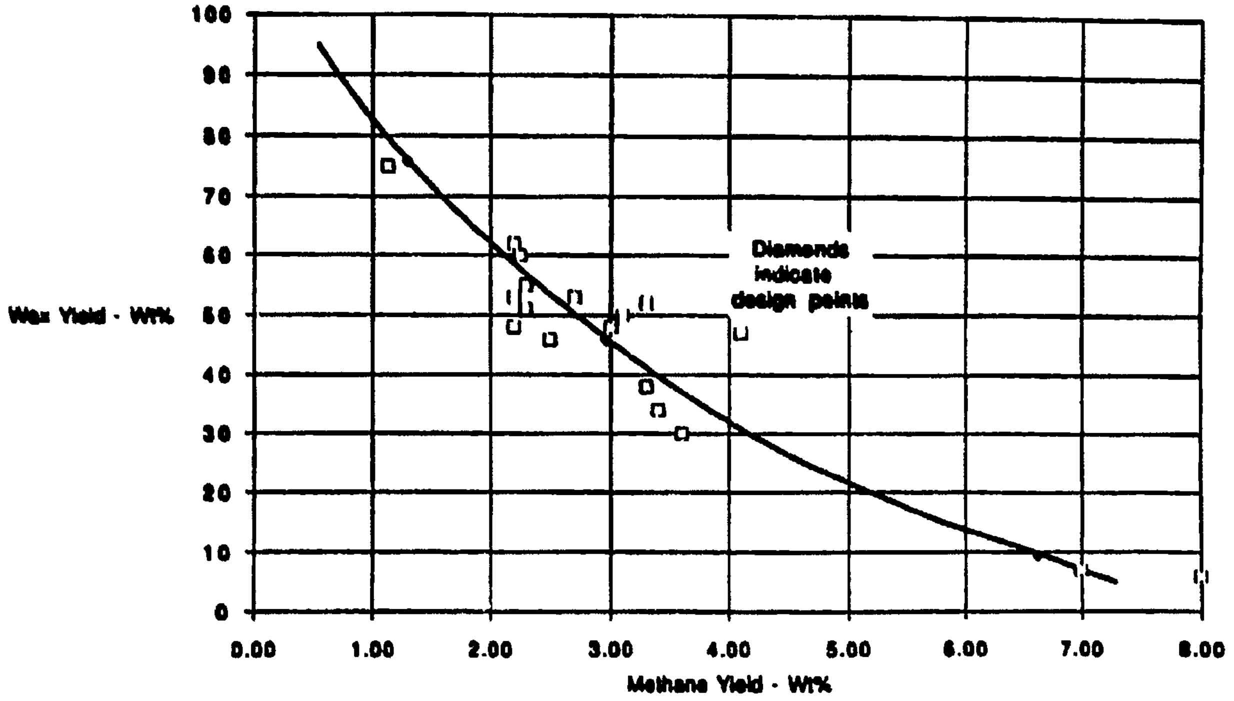


Figure 3-13 Correlation of Observed Wax and Methane Yield

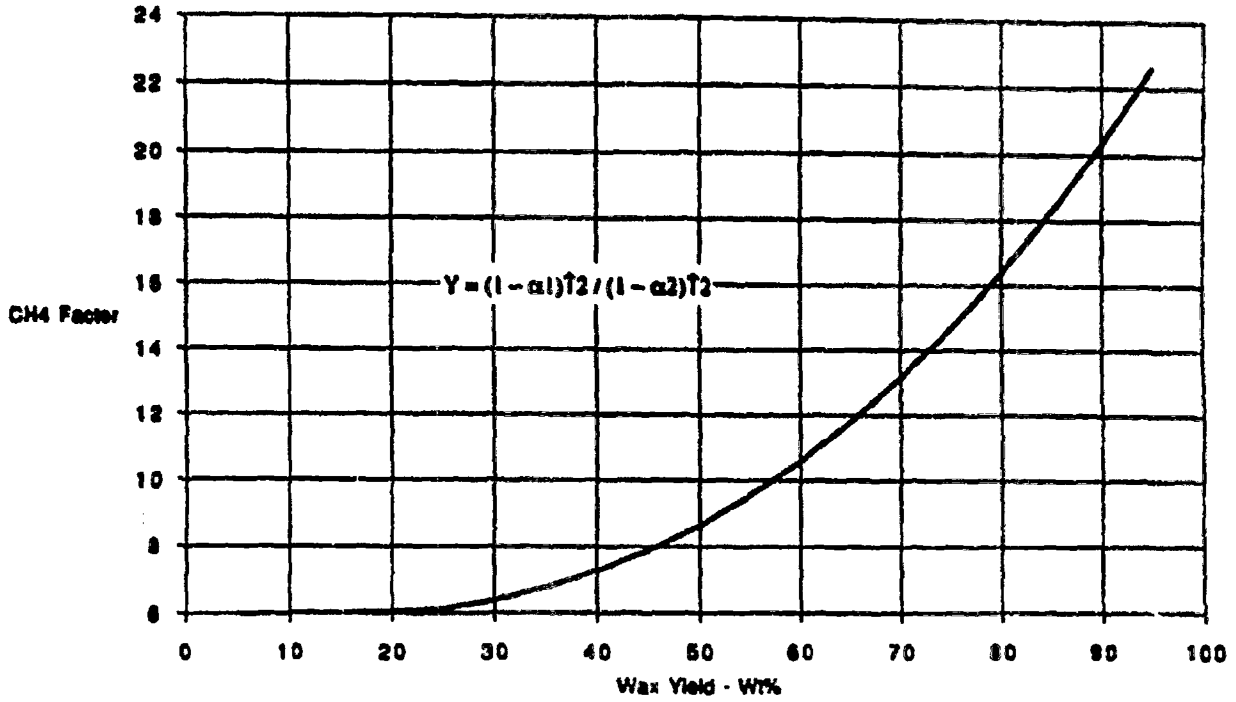


Figure 3-14 Methane Factor Required to Match Correlation in Figure 3-13

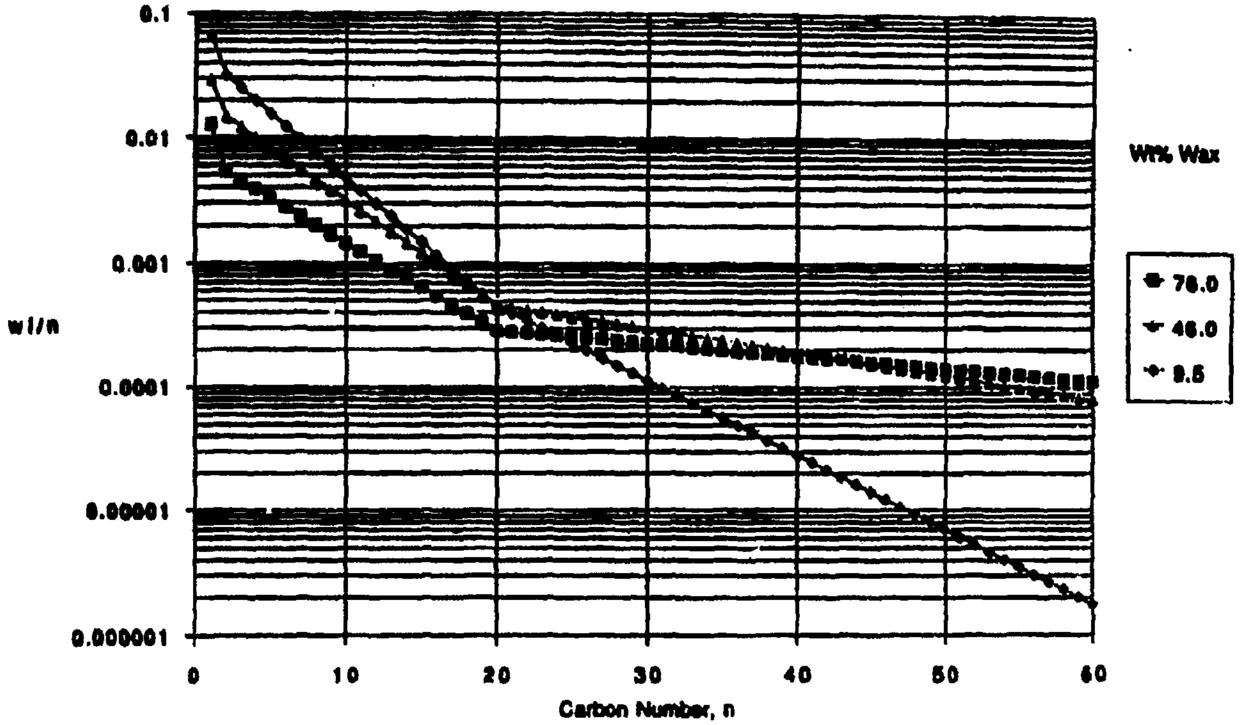


Figure 3-15 Design Schulz-Flory Plots

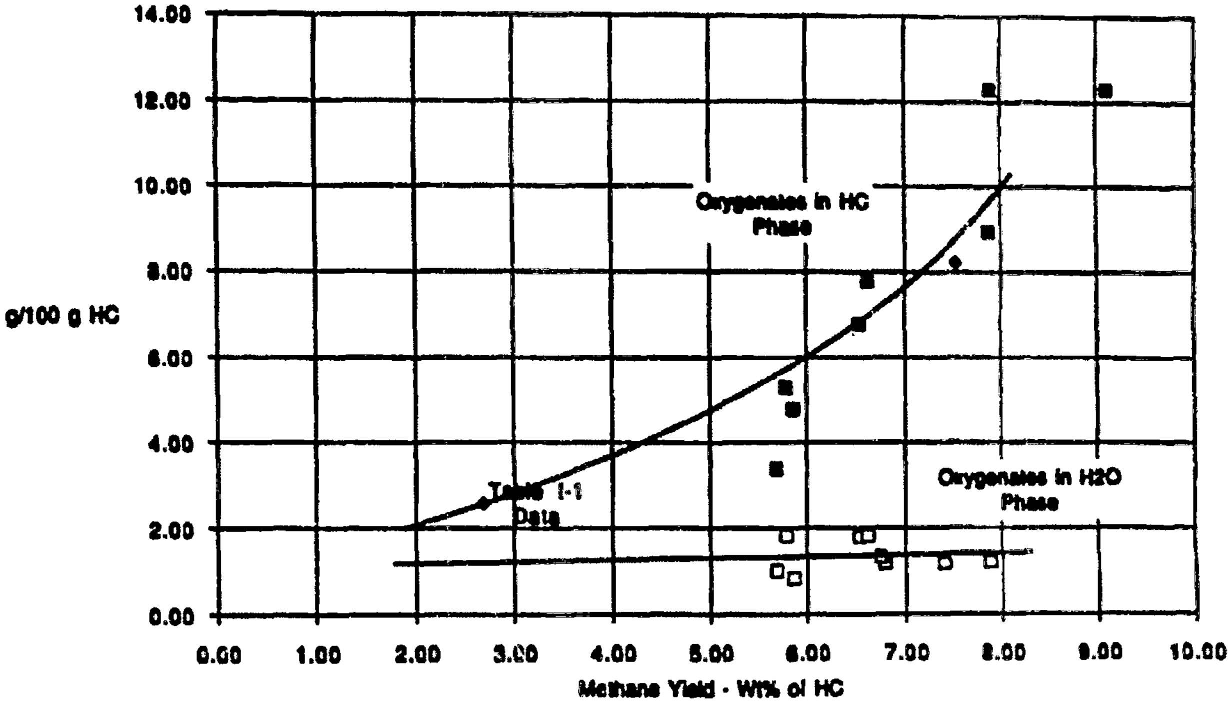


Figure 3-16 Oxygenates Versus Methane Yield (Mobile First-Stage Data)

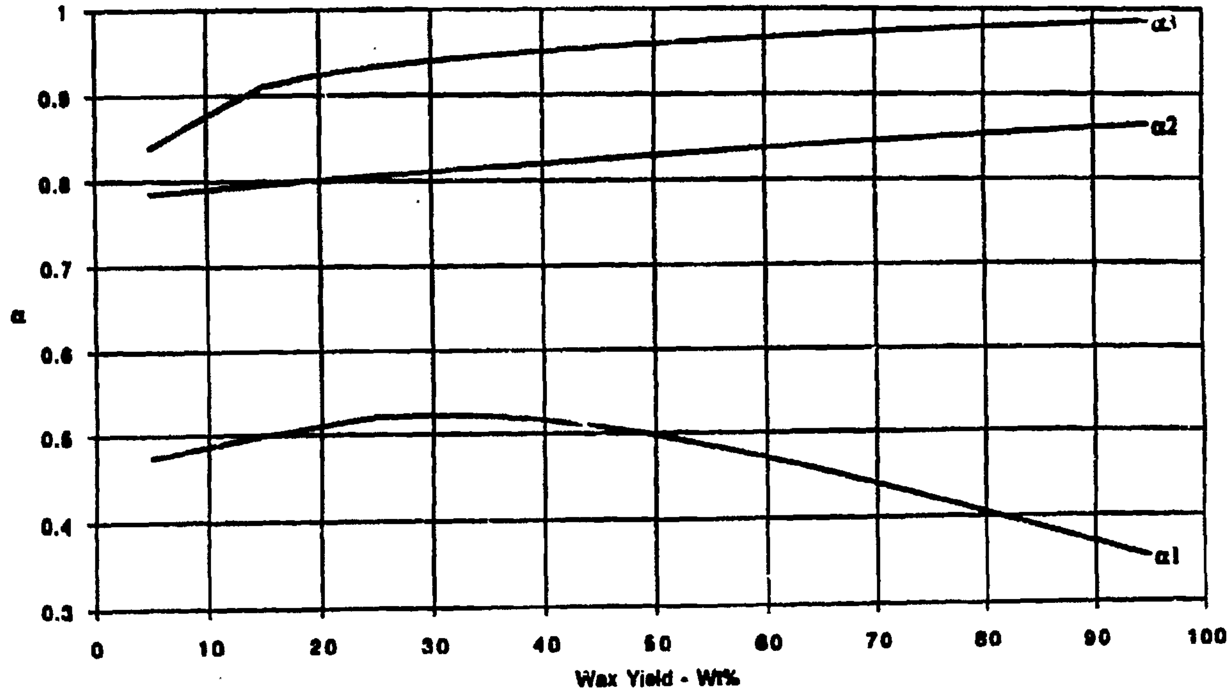


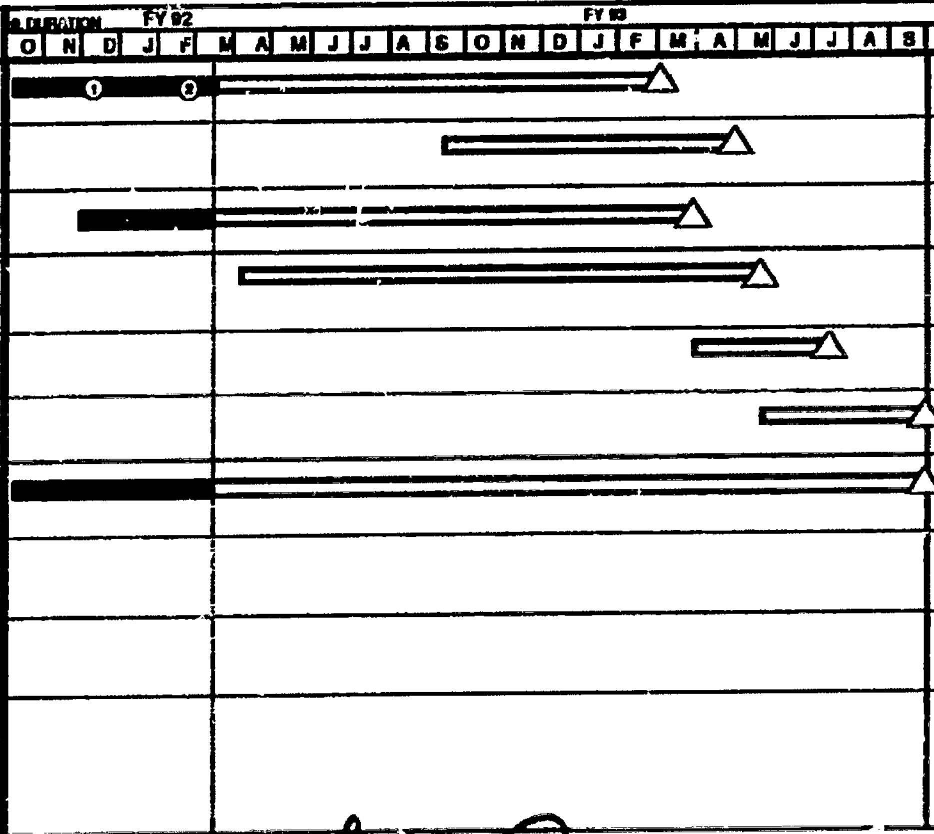
Figure 3-17 Triple Alpha Schultz-Flory Correlation

DOE F1332.3
(11.84)

☑ PLAN ■ STATUS REPORT

FORM APPROVED
OMB NO 1901.1400

1. TITLE Baseline Design/Economics for Advanced Fischer-Tropsch Technology	2. REPORTING PERIOD 2/17/92 to 3/15/92	3. IDENTIFICATION NUMBER DE-AC22-91PC90027
4. PARTICIPANT NAME AND ADDRESS	Bechtel Corporation 50 Beale Street San Francisco, CA 94105	5. START DATE 9/26/91 6. COMPLETION DATE 9/25/93



7. ELEMENT CODE	8. REPORTING ELEMENT	10. PERCENT COMPLETE a. Plan	b. Actual
Task 1	Baseline Design	26	21
Task 2	Economic Evaluation		
Task 3	Engineering Design Criteria	30	13
Task 4	Process Flowsheet Simulation Model		
Task 5	Sensitivity Studies		
Task 6	Documentation and Training		
Task 7	Project Management & Administration	28	28

△ Completion
① ASPEN/SP software delivered
② First progress meeting

11. SIGNATURE OF PARTICIPANT'S PROJECT MANAGER AND DATE Samuel S. Tam 5-10-92

Figure 3-18 Overall Milestone Schedule (as of March 15, 1992)

Table 3-1
Tradeoff Study Basis - Operating Cost and Product Values

Item	Value
Operating Costs	
Electric Power	5.1¢/kWh
50 psig Steam	$5.00/1,000 lb
Product Values	
Fuel Gas	$1.80/MM Btu
C_3 LPG	$0.43/gal
C_4 LPG	$0.47/gal
C_3/C_4 LPG	$0.10/lb
Gasoline	$23/bbl
Diesel	$26/bbl
Alcohol	$1.80/MM Btu
Four-Year Simple Payout	
Plant Cost Estimate (for comparison purpose only)	
Purchased Power	

Table 3-2
Oxygen Purity Tradeoff Case
Summary of Key Process Conditions

Basis:
50% Wax Yield
Overall Syngas Conversion - 82%
H_2 Recovery - Membrane/PSA
Purge Stream - 585 MM Btu/hr

Item	Oxygen Purity Mol%	
	99.5	95
F-T Reactor Overhead Flow, MMscfd	297	641
Feed to F-T, MMscfd	1,508	1,848
No. of F-T Reactors	26	32
Hydrocarbons Recovery Feed, MMscfd	334	678
Recycle Gas Flow Rate, MMscfd	315	578
Feed to Reformer, MMscfd	220	485
O_2 to Reformer, tpd	560	852
Steam to Reformer, mph	7,566	7,130
Purge to Fuel, mph	5,000	13,680

Table 3-3
Oxygen Purity Tradeoff Case
Comparison of Capital and Operating Cost

Item	Oxygen Purity Mol%	
	99.5	95
Capital Costs, $MM		
O_2 Plant	360	330
F-T Reactors	68	78
HC Recovery	23	37
Recycle Gas Compressor	7	10
Autothermal Reformer	17	29
H_2 Recovery (Membrane/PSA)	19	26
Total	494	510
Annual Operating Costs, $MM/yr		
O_2 Plant	122.4	113.9
HC Recovery Compressor	0.5	1.0
HC Recovery Plant HP Steam	9.5	19.2
HC Recovery Plant MP Steam	2.8	5.7
HC Recovery CW/Chemicals	0.4	0.8
Recycle Gas Compressor	4.5	8.3
Autothermal Reformer Steam	8.0	7.5
H_2 Recovery	3.6	7.7
Total	151.7	164.1

Table 3-4 Analysis of Mob

Run No.	Periods	Wt% CH4	Wt% Wax	H2+CO Conv.	Sup Vel. cm/s	T - °C	P - MP
256-1 (a)	34 - 43	8.0	6	68	1.7	268	
256-2	7 - 15	8.0	6	85	3.5	260	
256-3	32 - 39	7.0	7	87	3.45	260	
256-5	3 - 5	2.3	60	69	3.5	249	
256-5	8 - 12	1.1	75	54	3.2	244	
256-8 (a,b)	26 - 35	3.3	62	72	2.2	250	
256-11	2 - 6	3.1	50	87	5.3	258.5	
256-12	2 - 9	2.7	53	86	4.3	255	
256-13	3 - 10	2.2	62	81	4.2	256.5	
256-13	11 - 22	2.3	55	81	4.1	257	
256-13	25 - 29	3.0	48	77	3.6	257.5	
256-8 (b)	11 - 19	2.2	53	55	3.6	266	
256-9	4 - 9	4.1	47	83	4.8	255	
256-6	4 - 14	2.3	51	40	3	249	
256-4 (a)	21 - 28	2.5	46	40	2.2	256	
256-4 (a)	29 - 32	2.2	48	40	2.2	256	
256-7	36 - 44	3.4	34	39	4	256	
256-7 (b)	45 - 52	3.3	38	42	4	257	
256-7 (b)	59 - 66	3.6	30	60	4.2	275	

(a) Low superficial gas velocity

(b) Apparent catalyst activity loss

(1) Kuo, J.C. W. et al., " Slurry Fischer-Tropsch/ Mobil Two-Stage Process of Converting Syngas to High Octane Gasoline," under DOE Contract No. DE-AC22-80PC 30022, Final Report, June 1983, prepared by Mobil R&D Corp., Paulsboro, N. J.

(2) Kuo, J.C. W. et al., " Two-Stage Processes for Conversion of Synthesis Gas to High Quality Transportation Fuels," under DOE Contract No. DE-AC22-83PC 60019, Final Report, October 1985, prepared by Mobil R&D Corp., Paulsboro, N. J.

First-Stage Data (1, 2)

SV	1/SV	k	k*P/SV	100-H2+CO Conv.	Catalyst	Catalyst - gms
5.30	0.19	0.00093278	0.00028047	32	1 - A	252
2.25	0.44	0.00060462	0.00039771	15	1 - B	1241
2.28	0.44	0.00060462	0.00039247	13	1 - B	1207
2.35	0.43	0.00032595	0.00020667	31	1 - C	1221
2.25	0.44	0.00024401	0.00015942	46	1 - C	1162
0.98	1.02	0.00034516	0.00052478	28	1 - C	1838
2.30	0.43	0.0005566	0.00035816	13	1 - B'	1844
2.40	0.42	0.00045804	0.00028055	14	1 - B"	1433
2.40	0.42	0.0004981	0.00030716	19	1 - B"	1405
2.39	0.42	0.00051216	0.00031715	19	1 - B"	1376
2.40	0.42	0.00052659	0.00036203	23	1 - B"	1340
2.08	0.48	0.00045804	0.00040078	45	1 - C	1714
2.40	0.42	0.00045804	0.00034734	17	1 - B'	1981
4.00	0.25	0.00032595	0.00017764	60	1 - D	900
2.90	0.34	0.00048439	0.00042092	60	1 - B	1038
1.95	0.51	0.00048439	0.00062599	60	1 - B	1544
4.90	0.20	0.00048439	0.00024912	61	1 - B	1117
3.50	0.29	0.00051216	0.00036876	58	1 - B	1561
4.40	0.23	0.00134905	0.00077264	40	1 - B	1261

Table 3-5 Mobil Pre

						Mobil Table 8 &	
Run No.	Periods	Wt% CH4	Wt% Wax	H2+CO Conv.	Sup Vel. cm/s	T - °C	P
256-1	56.6	9		59	1.8	268	
256-1	56.8	9		58	1.8	268	
256-1	56.9	11		59	1.8	268	
256-1	57.6	10		56	1.8	268	
256-2	12.1	9.6		87.6	3.5	263	
256-2	14.2	8.3		86.9	3.5	263	
256-2	15.5	7.5		85.9	3.5	263	

(1) Kuo, J.C. W. et al., " Slurry Fischer-Tropsch/ Mobil Two-Stage Process of Converting Syngas to High Octane Gasoline," under DOE Contract No. DE-AC22-80PC 30022, Final Report, June 1983, prepared by Mobil R&D Corp., Paulsboro, N.

(2) Kuo, J.C. W. et al., " Two-Stage Processes for Conversion of Synthesis Gas to High Quality Transportation Fuels," under DOE Contract No. DE-AC22-83PC 60019, Final Report, October 1985, prepared by Mobil R&D Corp., Paulsboro,

ure Effect Data (1, 2)

ata (80PC30022)

a	SV	1/SV	k	k*P/SV	100-H2-CO Conv.	Catalyst	Catalyst - gms
1.48	5.8	0.17	0.00093278	0.00023802	41	1-A	244
1.83	7.2	0.14	0.00093278	0.00023708	42	1-A	243
1.14	4.5	0.22	0.00093278	0.0002363	41	1-A	242
1.48	5.8	0.17	0.00093278	0.00023802	44	1-A	244
1.14	1.84	0.54	0.00071245	0.00044141	12.4	1-B	1162
1.48	2.34	0.43	0.00071245	0.00045061	13.1	1-B	1187
1.82	2.84	0.35	0.00071245	0.00045657	14.1	1-B	1202

J.

Table 3-6
Wax Yield Tradeoff Case
Key Process Conditions

Item	76 wt% Wax	50 wt% Wax	9.6 wt% Wax
F-T Reactor Feed, MMscfd	1,506.5	1,543.3	1,635.9
Recycle, MMscfd	350.7	387.5	480.0
PSA Feed, MMscfd	167.6	170.4	173.6
CO_2 Produced, MMscfd	478.5	483.3	493.9
Autothermal Reformer Feed, MMscfd	349.6	374.6	434.4
O_2 Required, tpd	444.3	621.0	1115.4
Lt. Ends Make, lb/hr	7,313	8,440	10,593
C_3/C_4s, lb/hr	42,800	42,123	40,261
Gasoline, bpsd	13,785	18,523	25,770
Diesel, bpsd	26,331	19,168	10,440
Alcohols in Aq. Phase, lb/hr	8,103	9,543	12,947

Table 3-7

Wax Yield Tradeoff Case
Comparison of Capital Costs
($ MM)

Item	Capital Cost		
	76 wt% Wax	50 wt% Wax	9.6 wt% Wax
F-T Reaction Section	116.4	99.9	94.0
Hydrocarbon Recovery	16.7	17.8	19.9
PSA	22.4	22.7	23.0
Autothermal Reformer	19.9	20.9	23.0
Oxygen Plant	-	2.0	7.7
Subtotal	**175.4**	**163.3**	**167.0**
Upgrading			
Wax Hydrocracking	42.0	32.4	11.9
F-T Hydrocracking	20.1	30.4	40.7
Cat Reforming	29.2	31.9	34.8
Alkylation	31.5	41.0	50.8
Cat Polymerization	10.3	19.8	34.4
Subtotal	**133.1**	**155.5**	**172.6**
Total	**308.5**	**318.8**	**340.2**

Table 3-8
Wax Yield Tradeoff Case
Comparison of Operating Cost and Revenues
($MM/yr)

Item	Unit Price	76 wt% Wax	50 wt% Wax	9.6 wt% Wax
			Revenues	
Lt. Ends	$1.8/MM Btu	2.3	2.3	3.4
C_3/C_4	$0.45/gal	33.8	33.3	31.8
Gasoline	$23/Btu	109.9	147.7	205.5
Diesel	$26/Btu	237.4	172.8	94.1
Alcohols	$1.8/MM Btu	1.8	2.1	2.9
Total		385.2	358.6	337.7
			Operating Costs	
Power		3.48	4.41	6.61
Steam		-	1.20	4.00
Total		3.48	5.61	10.61
Net Revenue		381.7	352.99	327.1

Table 3-9
Autothermal Reformer Tradeoff Case
Comparison of Key Process Unit Conditions

Basis and Assumptions:
Oxygen Purity - 99.5 mol%
Wax Yield - 50 wt%
Overall Syngas Conversion - 80 mol%
Import Electricity

Item	With Autothermal Reforming	Without Autothermal Reforming
Feed to F-T Reactors, MMscfd	1,534	1,682
Number of Reactors	26	29
Feed to H_2 Recovery, MMscfd	165	293.2
Mol% H_2 in Feed	23.6	13.3
PSA Reject Gas Compressor, bhp	31,730	62,134
Gas Recycle Rate, MMscfd	378.2	413.0
Recycle Compressor, bhp	15,810	18,550
Autothermal Reformer Feed, MMscfd	364.7	-
O_2 Feed to Autothermal Reformer, tpd	612.5	-
C3 + Hydrocarbon Products, Mlb/hr	490.0	484.5

Table 3-10
Autothermal Reformer Tradeoff Case
Comparison of Capital and Operating Cost

Item	50 wt% with Autothermal Reforming	50 wt% w/o Autothermal Reforming
Capital Costs, $MM		
F-T Reactor Section	67.6	70.0
PSA Unit	25.4	38.0
Hydrocarbon Recovery	17.2	21.1
Autothermal Reformer	20.52	-
Oxygen Plant	7.0	-
Upgrading Plants	1.2	-
Total Capital Costs	138.9	129.1
Net Revenue, $MM/yr		
Product Revenue, $M/yr	353.4	349.4
Operating Cost, $MM/yr	7.5	26.0
Net Revenue	345.9	323.4

Table 3-11
Hydrocarbons Recovery Tradeoff Case
Key Process Unit Conditions and Yields

Basis and Assumptions:
- Oxygen Purity - 99.5 mol%
- Wax Yield - 50 wt%
- Overall Syngas Conversion - 82 mol%
- Import Electricity
- Purge to Fuel - 5,000 mols/hr

Item	Deep Refrig -130°F Cooling	Medium Refrig -30°F Cooling
F-T Feed, MMscfd	1538.2	1574.0
No. of F-T Reactors	26	26
F-T Reactor Effluent, MMscfd	382.4	418.3
HC's Recovery Feed, MMscfd	347.3	359.9
Recycle Compressor, bhp	14,915	14546
Propane Compressor, bhp	5,873	2,127
Ethylene Compressor, bhp	2,900	0
Propane Condenser Duty, kW	271	98
PSA Feed, MMscfd	167.3	167.8
PSA Offgas Compressor, bhp	32,268	32,390
Autothermal Reformer		
Reformer Feed, MMscfd	368.7	386.5
Reformer O_2 Usage, tpd	619.2	830.3
O_2 Plant, kW	8,607	11,542
Reformer Steam Usage, Mlb/hr	179.9	188.6
Saleable Products		
Lt. End Make, lb/hr	9,349	9,611
C_3/C_4s, lb/hr	45,252	45,408
Gasoline, bpsd	17,536	15,994
Diesel, bpsd	22,694	23,342

Table 3-12
Hydrocarbons Recovery Tradeoff Case
Comparison of Installed Costs ($MM)[a]

Item	Deep Refrig. -130°F Cooling	Medium Refrig. -30°F Cooling
Reaction Section		
F-T Reaction/Recycle System	67.6	68.7
HC Recovery		
Exchanger	7.7	2.9
Compressors	13.4	5.8
Autothermal Reformer	20.7	21.3
Dehydration	4.5	3.3
Oxygen Plant	0.0	2.4
Subtotal	**113.9**	**104.4**
F-T Product Upgrading Section		
Wax Hydrocracker	34.6	35.2
F-T Hydrotreater	29.1	29.4
Catalytic Reformer	32.9	33.5
Alkylation	42.1	39.5
Catalytic Polymerization	18.8	9.8
Subtotal	**157.5**	**147.4**
Total	**271.4**	**251.8**

(a) Installed costs of the process units shown are for comparison purpose only.

Table 3-13
Hydrocarbons Recovery Tradeoff Case
Comparison of Net Revenues ($MM/year)

Item	Deep Refrig. -130°F Cooling	Medium Refrig. -30°F Cooling
Product Revenues		
Lt. Ends	3.0	3.0
C3/C4	35.8	35.9
Gasoline	139.9	127.6
Diesel	204.6	210.4
Total	**383.3**	**376.9**
Operating Cost (a)		
Power	22.4	21.6
Net Revenue	**360.9**	**355.3**

(a) Only the annual operating costs of the process units that are affected by the selected options are shown in this table for comparison purpose.

Table 3-14
Hydrogen Recovery Tradeoff Case
Effects of Water Injection Rates on F-T Reactor Performance

Basis and Assumptions:
- Oxygen Purity - 99.5 mol%
- Wax Yield - 50 wt%
- HC Recovery - "-130°F " Refrigeration
- Overall Syngas Conversion - as indicated below
- H_2 Content in Clean Syngas from Gasifier - 25.6 mol%

Water Injection Rate, mols/hr	0	4,000	5,000	6,000
H_2 Conversion, %	80	75	72.5	70.5
CO Conversion, %	81.1	85.0	86.1	87.1
Overall Syngas Conv., %	80.8	82.0	81.9	81.9
Recycle Gas Rate, x 10^3 mols/hr	42	35	34	33
H_2 Content in Feed to H_2 recovery unit, mol%	23.6	33.6	37.5	41.1

Table 3-15
Hydrogen Recovery Tradeoff Case
Summary of Key Process Conditions and Flow Rates

Basis and Assumptions:
Hydrogen Product Purity - 99.6 mol%
Hydrogen Product Rate - 31 MM scfd
Hydrogen Product Pressure - 400 psia
F-T Recycle Loop Purge - 585 MM Btu/hr

Case Number **Case Description**	**1** **Membrane/ Methanation**	**2** **Membrane/ PSA**	**3** **Shift/ PSA**	**4A** **PSA-Only**	**4B** **PSA-Only**
Water Injection to F-T Reactor, mol/hr	4000	4000	4000	4000	6000
H_2 Recovery Feed, mol% H_2	33.6	33.6	33.6	33.6	41.1
PSA Feed, MM scfd		91.4	80.7	124.9	94.4
PSA Feed, mol% H_2		42.6	48.0	33.6	41.1
H_2 Recovery%		80.0	80.0	72.6 (a)	80.0

(a) This is the hydrogen recovery achievable via PSA due to low hydrogen content in the feed stream.

Table 3-16
Hydrogen Recovery Tradeoff Case
Comparison of Capital and Operating Cost

Case Number **Case Description**	**1** **Membrane/ Methanation**	**2** **Membrane/ PSA**	**3** **Shift/ PSA**	**4A** **PSA-Only**	**4B** **PSA-Only**
Installed Plant Cost, $MM					
Membrane Separation	9.4 (3-stage)	5.1 (1-stage)			
Compression	6.6	4.6		5.0	1.1
Methanation	0.2				
PSA		8.4	7.5	15.4	8.4
Shift			2.7		
	16.2	18.1	10.2	20.4	9.5
Annual Operating Cost (a), $MM/yr					
Steam	0.61	0.51	3.61		
Power	3.58	2.47		3.65	0.83
Others	0.09	0.06	0.25		
	4.28	3.04	3.86	3.65	0.83

(a) Only the annual operating costs of the process units that are affected by the selected options are shown in this table for comparison purpose.

Table 3-17

Site-Related Design Factors

Site Location	Inland, Southern Illinois
Site Elevation	650 ft above sea level
Seismic Zone	2
Design Amb. Temp. (Dry Bulb)	
- Summer/winter	95°F/-6°F
Max/Min Amb. Temp.	104°F/-18°F
Nominal Design RH	
- Summer/winter	75%/45%
Design Rainfall	
- Max 1 hr/max 24 hr	2.6 in./5.6 in.
- annual	40 in.
Snowfall	
- Max 24 hr/max 1 mo	10 in./20 in.
- annual	14 in.
Wind Velocity	
- Design/max	15 mph/90 mph

Table 3-18
Unified Loop Design Spreadsheet
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	A	B	C	D	E	F	G	H	I
1	6/15/92				F-T Reactor	Heat and Mass Balance		U	a
2	Design Case with Autothermal Reform	Wt% Wax =		60.00	Try Wax =	60.195		0.373	-0.5802
3	Using Hysim -130°F Balance		C	H	O	H2 Conv %	CO Conv %	SynGas Conv - %	
4	Yields based on % Wax Correlation		6.6743	18.2490	0.1073	70.48	86.80	81.66	
5	Stream No	1	2	3	4	5		5	
6	Stream Name	Feed Gas	Recycle	Steam	Comb Feed	E(I)		E(I)	
7	Composition								
8	CH4 - MPH	22.4	323.0201	0	345.4201	345.4201		1296.10	
9	C2H4	0	0	0	0	0		388.67	
10	C2H6	0	0	0	0	0		97.17	
11	C3H6	0	0	0	0	0		344.89	
12	C3H8	0	0	0	0	0		60.88	
13	C4H8	0	0	0	0	0		289.12	
14	C4H10	0	0	0	0	0		87.28	
15	C5H10	0	0	0	0			209.20	
16	C5H12	0	0	0	0			69.73	
17	C6H12	0	0	0	0			173.87	
18	C6H14	0	0	0	0			57.89	
19	C7OP	0	0	0	0			191.87	
20	C8OP	0	0	0	0			159.30	
21	C9OP	0	0	0	0			132.18	
22	C10OP	0	0	0	0			109.84	
23	C11OP	0	0	0	0			90.84	
24	C12OP	0	0	0	0			75.43	
25	C13OP	0	0	0	0			62.68	
26	C14OP	0	0	0	0			51.89	
27	C15OP	0	0	0	0			43.73	
28	C16OP	0	0	0	0			35.69	
29	C17OP	0	0	0	0			29.59	
30	C18OP	0	0	0	0			24.54	
31	C19OP	0	0	0	0			20.35	
32	Wax	0	0	0	0			455.91	
33	OX Vap	0	0	0	0			43.15	
34	OXHC	0	0	0	0			158.66	
35	OXH2O	0	0	0	0			158.13	4532.27
36	F-T Product	0	0	0	0	4532.274	4532.27		
37	CO2	3143.9	2224.378	0	5368.278	53073.69		53073.69	
38	N2	949.7	3397.661	0	4347.361	4347.361		4347.36	
39	O2	0	0	0	0	0		0.00	
40	CO	90343.4	9907.442	0	100250.8	13231.16		13231.16	
41	H2	32435	13645.6	0	46080.6	13602.99		13602.99	
42	H2O	0	5040.106	6000	11040.11	2162.882	2162.882	2162.88	
43	Total - MPH	126894.4	34538.2	6000	167432.6	91295.78	2162.88	91295.78	
44	C atoms	93509.7	12454.84	0	105964.5	105964.5	6.01E-09	105964.5	
45	H atoms	64959.6	38663.49	12000	115623.1	115623.1		115623.1	
46	O atoms	96631.2	19396.3	6000	122027.5	122027.5		122027.5	
47	N atoms	1899.4	6795.322	0	8694.722	8694.722		8694.722	
48	Total - #/hr	2761263	594073.3	108091.2	3463428	3463428		3463428	
49	C atoms in inert HC	22.4	323.0201	0	345.4201	345.4201			
50	H atoms in inert HC	89.6	1292.08	0	1381.68	1381.68			
51	Conditions								
52	Temp - Deg F	222	500	100	210.0	497.6			
53	Press - Atm	16.32653			16.07	14.61			
54	MM Btu/hr	-4355.37	-1149.63	-702.182	-6174.92	-9309.28	-3134.34		
55	Ratios				-6207.18				
56	recycle/feed				0.272181				
57	steam/carbon				0.056623				
58	H2/CO	0.359019	1.377309		0.459653	1.028102			
59	Boudouard Ratio					1.894443			
60	Delta T Approach - Deg F					-140			
61	Eq Temp - Deg K					604.0694			
62	Equilibrium Constants								
63	K - WGS					25.229			
64	K - SM					6.11E-07			
65	K - Boudouard					3.01E+08			
66									
67									
68									
69									

Table 3-18
Unified Loop Design Spreadsheet
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	J	K	L	M	N	O	P	Q	R	S
1	6/15/92									
2	Design Case with Autothermal Reformer						Product Separation Mass Balance			
3	Using Hysim -130°F Balance						%H2 Rec. =	90.00	% Purge =	69.76
4	Yields based on % Wax Correlation									
5	Stream No	5	6	7	8	9	9A	11	12	13
6	Stream Name	Effl	Water	HC Prod	CO2	Vapor	To PSA	H2	Purge	Ref Feed
7	Composition									
8	CH4 - MPH	1296.10	0	0	0	1296.095	407.9181	0	284.5744	1011.521
9	C2H4	388.67	0	0.413727	0	388.2569	122.1955	0	85.24881	303.0101
10	C2H6	97.17	0	3.045671	0	94.12188	29.62287	0	20.6657	73.45629
11	C3H6	344.86	0	292.1892	0	52.66946	16.57627	0	11.56404	41.10442
12	C3H8	60.86	0	53.82379	0	7.033448	2.213627	0	1.544284	5.489184
13	C4H8	289.12	0	284.7567	0	4.367622	1.374615	0	0.958969	3.408655
14	C4H10	67.28	0	66.43513	0	0.845941	0.266242	0	0.185737	0.660203
15	C5H10	209.20	0	208.9736	0	0.228673	0.07197	0	0.050208	0.178465
16	C5H12	69.73	0	69.65782	0	0.076224	0.02399	0	0.016736	0.059488
17	C6H12	173.67	0	173.6399	0	0.03003	0.009451	0	0.006594	0.023437
18	C6H14	57.89	0	57.88413	0	0.005865	0.001846	0	0.001288	0.004577
19	C7OP	191.87	0	191.8669	0	0.002326	0.000732	0	0.000511	0.001815
20	C8OP	159.30	0	159.2955	0	0.00091	0.000287	0	0.0002	0.00071
21	C9OP	132.16	0	132.1612	0	0.000809	0.000255	0	0.000178	0.000632
22	C10OP	109.64	0	109.6359	0	0.000708	0.000223	0	0.000156	0.000553
23	C11OP	90.94	0	90.94252	0	0	0	0	0	0
24	C12OP	75.43	0	75.43106	0	0	0	0	0	0
25	C13OP	62.56	0	62.56216	0	0	0	0	0	0
26	C14OP	51.89	0	51.88672	0	0	0	0	0	0
27	C15OP	43.03	0	43.03156	0	0	0	0	0	0
28	C16OP	35.69	0	35.68673	0	0	0	0	0	0
29	C17OP	29.59	0	29.59483	0	0	0	0	0	0
30	C18OP	24.54	0	24.54258	0	0	0	0	0	0
31	C19OP	20.35	0	20.35246	0	0	0	0	0	0
32	Wax	455.91	0	455.9147	0	0	0	0	0	0
33	OX Vap	43.15	0	43.14601	0	0	0	0	0	0
34	OXHC	158.86	0	158.8597	0	0	0	0	0	0
35	OXH2O	158.13	158.1285	0	0	0	0	0	0	0
36	F-T Product	0.00	0	0	0	0	0	0	0	0
37	CO2	53073.68	0.014944	0.054715	52808.32	265.2988	83.49709	0	58.24976	207.049
38	N2	4347.36	0	0	0	4347.361	1368.238	0	954.5192	3392.842
39	O2	0.00	0	0	0	0	0	0	0	0
40	CO	13231.16	0	0	0	13231.16	4164.225	0	2905 073	10326.09
41	H2	13602.98	0	0	0	13602.98	4281.25	3425	597.3425	9580.65
42	H2O	2162.88	2162.882	0	0	0	0	0	0	0
43	Total - MPH	91295.78	2321.026	2875.885	52808.32	33290.55	10477.49	3425	4920	24946.56
44	C atoms	105984.5	308.3675	38887.51	52808.3	15958.8	5022.7	0.0	3504.0	12464.8
45	H atoms	115623.1	5238.171	75454.77	0.0	34927.4	10992.6	6850 0	2890.0	25187.4
46	O atoms	122027.5	2324.204	324.906	105616.6	13761.8	4331.2	0 0	3021.6	10740.2
47	N atoms	8694.722	0	0	0.0	8694.7	2736.5	0.0	1908.0	6785.7
48	Total - #/hr	3463428	46169.22	624305	2324084.0	569073.2	179040.6	6904 8	120086.5	441691.9
49	C atoms in inert HC									
50	H atoms in inert HC						LHV(Btu/SCF)=		313.9951	
51	Conditions						LHV(MM Btu/hr)=		586.2729	
52	Temp - Deg F							%N2=	19.4008	800.0
53	Press - Atm					%H2=	43.86142			23.57
54	MM Btu/hr									-374.78
55	Ratios									
56	recycle/feed									
57	steam/carbon									
58	H2/CO									
59	Boudouard Ratio									
60	Delta T Approach - Deg F									
61	Eq. Temp - Deg K									
62	Equilibrium Constants									
63	K - WGS									
64	K - SM									
65	K - Boudouard									
66										
67										
68										
69										

Table 3-18
Unified Loop Design Spreadsheet
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	T	U	V	W	X	Y	Z	AA	AB	AC
1	6/15/92									
2	Design Case with Autothermal Reformer				Autothermal Reformer Heat and Mass Balance					
3	Using hysim -130°F Balance									
4	Yields based on % Wax Correlation									
5	Stream No.	14	15	14 +15	16	17	18		19	9
6	Stream Name	Steam	Oxygen	H_2O+O_2	Prehtd. Fd	Comb Feed	Effl		Cool Out	Recycle
7	Composition									
8	CH_4 - MPH	0.0	0.0	0.0	1011.5	1011.5	323.0	323.0	323.0	323.0
9	C_2H_4	0.0	0.0	0.0	303.0	303.0	0.0	323.0	0.0	0.0
10	C_2H_6	0.0	0.0	0.0	73.5	73.5	0.0	1.1E-08	0.0	0.0
11	C_3H_6	0.0	0.0	0.0	41.1	41.1	0.0		0.0	0.0
12	C_3H_8	0.0	0.0	0.0	5.5	5.5	0.0		0.0	0.0
13	C_4H_8	0.0	0.0	0 0	3.4	3.4	0.0		0.0	0.0
14	C_4H_{10}	0.0	0.0	0.0	0.7	0.7	0.0		0.0	0.0
15	C_5H_{10}	0.0	0.0	0.0	0.2	0.2	0.0		0.0	0.0
16	C_5H_{12}	0.0	0.0	0.0	0.1	0.1	0.0		0.0	0.0
17	C_6H_{12}	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0
18	C_6H_{14}	0	0.0	0.0	0.0	0.0	0		0.0	0.0
19	C7OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
20	C8OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
21	C9OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
22	C10OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
23	C11OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
24	C12OP	0	0.0	0 0	0.0	0.0	0		0.0	0.0
25	C13OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
26	C14OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
27	C15OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
28	C16OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
29	C17OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
30	C18OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
31	C19OP	0	0.0	0.0	0.0	0.0	0		0.0	0.0
32	Wax	0	0.0	0.0	0.0	0.0	0		0.0	0.0
33	OX Vap	0	0.0	0.0	0.0	0.0	0		0.0	0.0
34	OXHC	0	0.0	0.0	0.0	0.0	0		0.0	0.0
35	OXH2O	0	0.0	0.0	0.0	0.0	0		0.0	0.0
36	F-T Product	0	0.0	0.0	0.0	0.0	0		0.0	0.0
37	CO_2	0.0	0.0	0.0	207.0	207.0	2224.4		2224.4	2224.4
38	N_2	0.0	4.8	4.8	3392.9	3397.7	3397.7		3397.7	3397.7
39	O_2	0.0	959.0	959.0	0.0	959.0			0.0	0.0
40	CO	0.0	0.0	0.0	10328.1	10328.1	9907.4		9907.4	9907.4
41	H_2	0.0	0 0	0.0	9580.7	9580.7	13645.6		13645.6	13645.6
42	H_2O	6738 1	0.0	6738.1	0.0	6738.1	5040.1	5040.1	5040.1	5040.1
43	Total - MPH	6738.068	963.8438	7701.912	24945.65	32647.48	34538.2	5040.1	34538.2	34538.2
44	C atoms	0.0	0.0	0.0	12454.8	12454 8	12454.8	4.27E-08	12454.8	12454.8
45	H atoms	13476.1	0.0	13476.1	25187.4	38663.5	38663.5		38663.5	38663.5
46	O atoms	6738.1	1918.0	8656.1	10740.2	19396.3	19396.3		19396.3	19396.3
47	N atoms	0.0	9.6	9.6	6785.7	6795.3	6795.3		6795.3	6795.3
48	Total - #/hr	121393 0	30823.8	152216.8	441881.9	594098.7	594098.7		594098.7	594098.7
49	C atoms in inert HC									
50	H atoms in inert HC									
51	Conditions									
52	Temp - Deg F	650.0	500.0	630.9	1070.0	1400.0	1800.0		1500.0	490.0
53	Press - Atm	24.75	23.57	24.75	23.57	23.57	21.43		20.41	19.44
54	MM Btu/hr	-631.74	6.54	-625.42	-161.30	-786.14	-789.61		-678.02	-1150.67
55	Delta H			-625.19	213.48	-786.71		-1.48	-88.40	-274.68
56	oxygen/carbon					0.0770				
57	steam/carbon					0.5410				
58	H_2/CO						1.377		1.38	1.38
59	(H_2-CO_2)/(CO+CO_2)						0.94		0.94	0.94
60	Boudouard Ratio						0.036525		0.038351	0.040289
61	% Nitrogen		0.5		0					
62	Delta T SMR - Deg F						15.0			
63	Eq. Temp - Deg K						1247.1			
64	Delta T WGS - Deg F						0.0			
65	Eq. Temp - Deg K						1255 4			
66	Equilibrium Constants									
67	K - WGS						0.607855			
68	K - SM						5951 92			
69	K - Boudouard						0.008251			

Table 3-18
Unified Loop Design Spreadsheet
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	AD	AE	AF	AG	AH	AI	AJ	AK	AL
1									
2									
3									
4			Separation Factors						
5									
6		F-T Eff	HC Btms	HC/Eff	H2O Rec	CO2 Rec			
7									
8	CH4 - MPH	1085.68	0	0	0	0	Yield Prediction Summary		
9	C2H4	384 7	0.4085	0.001064	0	0	Wax Yield Est.	50.195	9.569397
10	C2H6	96.17	3.0144	0.031344	0	0	Methane Yield Est.	2.69	
11	C3H6	341.26	289.141	0.847275	0	0	Alpha1	0.49731532	
12	C3H8	60.22	53.2602	0.884427	0	0	Alpha2	0.82916683	0.79
13	C4H8	266.27	261.9487	0.983771	0	0	Alpha3	0.85957605	
14	C4H10	66.57	65.733	0.987427	0	0	CH4 Factor	8.65658441	
15	C5H10	0	0	0.998907	0	0	Oxygenates in Vapor	0.38	
16	C5H12	275.92	275.6184	0.998907	0	0	C No	2.43	
17	C6H12	171.76	171.7303	0.999827	0	0	H No	5.69	
18	C6H14	57.25	57.2442	0.999889	0	0	O No	1	
19	C7OP	189.82	189.8177	0.999988	0	0	Oxygenates in Water	1.27675971	
20	C8OP	157.48	157.4781	0.999994	0	0	C No	1.85	
21	C9OP	130.83	130.8282	0.999994	0	0	H No	5.77	
22	C10OP	108.34	108.3393	0.999994	0	0	O No	1.02	
23	C11OP	89.85	89.8494	1	0	0	Oxygenates in HC	2.52140989	
24	C12OP	74.51	74.5095	1	0	0	C No	4.89413033	4.42
25	C13OP	61.79	61.7899	1	0	0	H No	11.5782607	10.43
26	C14OP	51.23	51.2297	1	0	0	O No	1.11	1.11
27	C15OP	42.48	42.4797	1	0	0	Olefin in C2+ HC	0.75300305	
28	C16OP	35.22	35.2198	1	0	0	Fraction CH2	0.205	0.205
29	C17OP	29.2	29 1998	1	0	0	O No of Wax	0.231	0.231
30	C18OP	24 21	24.2098	1	0	0	Wax Yield - Wt%	50.00	
31	C19OP	20.08	20.0799	1	0	0	CH4 Yield	2.70728022	
32	Wax	8.75	8.75	1	0	0	C2 - C19 Yield	47.29255	
33	OX Vap		0	1	0	0	H/C Ratio	2.10380749	
34	OX HC		0	1	0	0	O/C Ratio	0.01238418	
35	OXH2O		0	0	1	0	C No of C2-C19	6.22507656	
36	F-T Product		0	0	0	0	C No of Wax	43.7380327	
37	CO2	53058.75	0.0547	1.03E-06	8.81E-06	0.995	C No of Ci-Cj	6.21383786	5.489577
38	N2	5942.36	0	0	0	0	i	2	2
39	O2	0	959.0227	0	0	0	j	20	20
40	CO	21424.88	0	0	0	0			
41	H2	8687.56	0	0	0	0			
42	H2O	286.32	0.0006	0	1	0			
43	Total - MPH								
44		Alpha2 Prediction							
45		1400.88201	-4427.32	3374.924					
46		Methane Factor							
47		6 41280781	-0 05798	0.001645	7.98E-06				
48		Oxygenates in H2O							
49		1 12828768	0.055581						
50		Oxygenates in HC							
51		1 35098875	0.133088	0 110533					
52									
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Table 3-18
Unified Loop Design Spreadsheet
page 5 of 5

	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW
1	i						20				
2	alpha1						0.497315				
3	alpha2						0.829167				
4	alpha3						0.959578				
5	CH4 Factor						6.655584				
6	x/y						0.192559				
7	z/y						1.113219				
8	x						0.107138				
9	y						0.556389				
10	z						0.619383				
11	(sum wf1)/x						0.252692				
12	1-(sum wf2)/y						0.15001				
13	(sum wf3)/z						0.807258				
14	sum wf1						0.027073				
15	sum wf2						0.472926				
16	sum wf3						0.500002				
17	Total						1.000000				
18	C No of fraction 2						6.213938				
19	C No of fraction 3						43.73803				
20	Wt % C No Dist	C No.	H No.	O No.	MF Olefins	MW	WT %	mols	atom C	atom H	atom O
21	1	1	4	0	0.00	16.0426	2.71	0.168754	0.168754	0.675023	
22	2	2	4.4	0	0.80	28.45876	2.69	0.094626	0.189252	0.416354	
23	3	3	6.3	0	0.85	42.38277	3.35	0.07902	0.237061	0.497828	
24	4	4	8.4	0	0.80	56.51036	3.70	0.065521	0.262084	0.550377	
25	5	5	10.5	0	0.75	70.63785	3.84	0.054328	0.271639	0.570443	
26	6	6	12.5	0	0.75	84.66475	3.82	0.0451	0.270603	0.563756	
27	7	7	14.6	0	0.70	98.78234	3.69	0.037389	0.261726	0.545886	
28	8	8	16.6	0	0.70	112.8191	3.50	0.031026	0.248207	0.515029	
29	9	9	18.6	0	0.70	126.8459	3.27	0.025741	0.231668	0.478782	
30	10	10	20.6	0	0.70	140.8727	3.01	0.021354	0.213537	0.439887	
31	11	11	22.6	0	0.70	154.8995	2.74	0.017713	0.19484	0.400307	
32	12	12	24.6	0	0.70	168.9263	2.48	0.014692	0.176299	0.361413	
33	13	13	26.6	0	0.70	182.9531	2.23	0.012185	0.158406	0.324124	
34	14	14	28.6	0	0.70	196.9799	1.99	0.010106	0.141482	0.289028	
35	15	15	30.6	0	0.70	211.0067	1.77	0.008381	0.125718	0.256464	
36	16	16	32.6	0	0.70	225.0335	1.56	0.006951	0.11121	0.226591	
37	17	17	34.6	0	0.70	239.0603	1.38	0.005764	0.097991	0.19944	
38	18	18	36.6	0	0.70	253.0871	1.21	0.00478	0.086042	0.174952	
39	19	19	38.6	0	0.70	267.1139	1.06	0.003964	0.075318	0.153011	
40	Wax	43.74	88.08	0.231	0.70	617.8193	50.00	0.08093	3.539804	7.128168	0.018695
41	Total	8.98	18.73	0	0.592	128.4716	100.00	0.78	7.06	14.77	0.02
42	C2/C19	6.23	12.83	0	0.761	87.78978	47.29	0.54	3.35	6.88	0.00
43	C2+HC	11.13	22.74	0	0.763	156.5486	97.29	0.62	6.89	14.09	
44	Oxygenates in Vapor	2.43	5.69	1		50.92108	0.39	0.007659	0.018611	0.043579	0.007659
45	Oxygenates in Water	1.95	5.77	1.02		45.55842	1.28	0.02807	0.054736	0.161963	0.028631
46	Oxygenates in HC	4.99	11.58	1.11		89.41358	2.52	0.028189	0.140832	0.3265	0.031301
47	C2/C19 - Oxygenates	6.23	12.83	0	0.761	87.78978	43.10	0.490917	3.055895	6.348682	0.00
48	Total	8.67	18.25	0.11		261.4413	100	0.804531	6.978734	14.68191	0.086288
49	C5/C19	8.90	18.36	0	0.717	125.3802	37.54809	0.299474	2.664685	5.498112	0
50	H/C Ratio	2.1038									
51	O/C Ratio	0.0124									
52		Alpha3 Prediction							Pred a3		
53	Wax	Alpha3	Alpha3^2	Alpha3^3	Pred	c	b'	y	x		
54	50 195	0.9594	0 9205	0 8831	49.99995	-0.67022	-0.00073	0.085255	0.959578		
55											
56											
57		Regression Output									
58	Constant			-37006							
59	Std Err of Y Est			0 4287							
60	R Squared			0.9999							
61	No. of Observations			5							
62	Degrees of Freedom			1							
63						a	a/3	b			
64	X Coefficient(s)		126870	-1E+05	55290.38	-2 62297	-0.87432	2.294605			
65	Std Err of Coef		30869	33137	11915.14						
66						a'					
67						0.001284					
68											
69											

Table 3-19
Environmental Compliance Strategy
Identification of Specific Pollutants/Hazards
(Direct Liquefaction Study DEAC22-90PC89857
Third Quarterly Report – April 1991)

Section	**Page**	**Pollutant & Rule**	**Plant**
3.2.3.2	69	Air Pollution - PSD (BACT)	Table 3-20
3.2.3.2	76,89	SO_2 (BACT) Bulk Sulfur	Claus
3.2.3.2	81,87	PM from Incinerators	Waste Sludge
3.2.3.2	82	PM Fugitive	Storage Piles
3.2.3.2	85,96	VOC from Misc. Equip.	Water Treat
3.2.3.2	85	CO from Incinerators	Waste Sludge
3.2.3.2	85	CO from Pet. Ref.	CO_2 Removal
3.2.3.2	89	PM, SO_2 & CO from Pet. Ref.	FCC Regen.
3.2.3.2	93-100	VOC Leakage	Upgrading HTUs
3.2.3.2	97	Vinyl Chloride	Boilers
3.2.3.3	102	Solid & Hazardous Waste	Table 3-21
3.2.3.3	104	Sanitary Landfill Requirements	San. Waste
3.2.3.3	105-116	Hazardous Waste	WWTreat.
3.2.3.4	117	Process and Storm Water	All Plants
3.2.3.4	118	Organic Wastewater	F-T & Upgrading
3.2.3.4	120	Pet. Refinery Wastewater	Upgrading HTUs
3.2.3.4	122	Iron & Steel Wastewater	Coking Unit
3.2.3.4	122	Power Gen. Wastewater	Steam & Power Gen.
3.2.3.4	123	Coal Mining Wastewater	Coal Prep.
3.2.3.5	127	Toxic Substances Control Act	HC Products
3.2.3.6	128	Exposure Limits OSHA Reqts.	Table 3-22
3.2.3.7	129	Noise	All Plants
3.2.3.8	137	Stack Heights – GEP	All Stacks
2.2.3.6	137	Stack Heights – FAA Reqts.	All Stacks
3.2.3.8	137	Safety Planning	All Plants

Tables 3-20, 3-21, and 3-22 follow this table.

Table 3-20
Air Pollution PSD (BACT)

Air Emission Point Identification	Pollutant	Control Technology	Control Efficiency/ Reference
Fluid Bed Combustion (FBC)	PM	Electrostatic Precipitators	99.80%
H_2 Heaters	PM	None	NA
Slurry Heaters			
Fractionator Heaters	PM	None	NA
Hydrotreating Heaters	PM	None	NA
Transfer Houses	PM	Enclosed, Spray and Baghouses	99.80%
Transfer Houses	PM	Enclosed, Spray and Baghouses	99.80%
Coal Pulverizing and Drying	PM	Baghouses	99.80%
Active Storage Pile	PM	Chemical Spray	80.00%
Inactive Storage Pile	PM	Surfactant	80.00%
Dried Coal Storage Vent	PM	Baghouses	99.8%
Stacker	PM	Chemical Spray	80.00%
Haul Road	PM	Covered Truck and Paved Roads	NA
Non-Hazardous Landfills	PM	NA	NA
Coal Conveyors	PM	Covered	90.00%
Boiler Stacks	SO_2	None	NA
H_2 Heaters	SO_2	None	NA
Slurry Heaters	SO_2	None	NA
Fractionator Heaters	SO_2	None	NA
Hydrotreating Heaters	SO_2	None	NA
CO_2 Stripper	CO	NA	NA
Boiler Stacks	CO	NA	NA
H_2 Heaters	CO	NA	NA
Slurry Heaters	CO	NA	NA
Fractionator Heaters	CO	NA	NA
Hydrotreating Heaters	H_2S	NA	NA

PM: Particulate Matter

Table 3-20 (Cont'd)

Air Emission Point Identification	Pollutant	Control Technology	Control Efficiency/ Reference
Boiler Stacks	NO_x	Proper Boiler Design	40.00%
H_2 Heaters	NO_x	NA	10.00%
Slurry Heaters	NO_x	NA	10.00%
Fractionator Heaters	NO_x	NA	10.00%
Hydrotreating Heaters	NO_x	NA	10.00%
Boiler Stacks	VOC	NA	NA
H_2 Heaters	VOC	NA	NA
Slurry Heaters	VOC	NA	NA
Fractionator Heaters	VOC	NA	NA
Hydrotreating Heaters	VOC	NA	NA
600# Steam	VOC	NA	NA
Intermediate Storage Tanks	VOC	Floating Roofs and Temperature Constant	NA
Final Products Storage Tanks	VOC VOC	Floating Roofs and Temperature Constant	NA
Tank Cars/Truck Loading	VOC	Vapor Recovery System	NA
Fugitives (drains, seals, valves)	VOC	Dual Seals and Good Maintenance	NA
Boiler Stacks	Fluorides	ESP and Wet Scrubber	99.80%
Boiler Stacks	Beryllium	ESP and Wet Scrubber	99.80%
Boiler Stacks	Lead	ESP and Wet Scrubber	99.80%
Boiler Stacks	Mercury	ESP and Wet Scrubber	99.80%

VOC: Volatile Organic Compound

Table 3-21
Solid and Hazardous Waste

Source	Waste Identification
Coal Crushing/Washing	Refuse
Gasifier	Ash, Slag, and Soot
Water Treatment	Sludge
Miscellaneous	Facility Refuse and Flotsam
Wastewater Treatment	Filter Cake and Salts(a)

(a) Considered a possibly hazardous waste due to the potential presence of heavy metals.

Table 3-22
Exposure Limits for Compounds Found in Coal Liquefaction Plants[a]

Compound	Where Found	TLV-TWA mg/m³ (ppm)	TLV-STEL mg/m³ (ppm)
Acetic Acid	Gas stream	25(10)	37(15)
Acetone	Laboratory	1780(750)	2380(1000)
Ammonia	Gas stream	17(25)	24(35)
Aniline (skin)	Gas stream	7.6(2)	(b)
Antimony	Trace element in coal	0.5(b)	(b)
Arsenic	Trace element in coal	0.2(b)	(b)
Benzene	Laboratory gas	32(10)	(b)
Beryllium	Trace element in coal	0.002(b)	(b)
1,3-Butadiene	Gas stream	22(b)	(b)
Cadmium Fume Dust	Trace element in coal	0.05 (b,c)	(b)
Carbon Dioxide	Gas stream	9,000(5,000)	54,000(30,000)
Carbon Disulfide	Gas stream	31(10)	(b)
Carbon Monoxide	Gas stream	57(50)	458(400)
Carbon Tetrachloride	Laboratory	31(5)	(b)
Chromium (Soluble & Metal)	Trace element in coal	0.5(b)	(b)
Coal Dust (> 5% SiO_2)	Coal preparation area	2.4(b)	(b)
Coal Dust (< 5% SiO_2)	Coal preparation area	10(b)	(b)
Coal Tar Pitch Volatiles	Gas stream	0.2(b)	(b)
Cresol (Skin)	Gas stream	0.2(b)	(b)
Ethyl Mercaptan	Gas stream	1.3(0.5)	(b)
Hydrogen Chloride	Gas stream	7.5(5) (d)	(b)
Hydrogen Sulfide	Gas stream	14(10)	21(15)
Lead and Lead Compounds	Trace element in coal	0.15(b)	(b)
Manganese	Trace element in coal	5(b)	(b)
Mercury	Trace element in coal	0.05(b)	(b)
Methyl Ethyl Ketone	Laboratory	590(200)	885(300)
Methyl Mercaptan	Gas stream	0.98(0.5)	(b)
Naphtha (Coal Tar)	Gas stream	(b,e)(100)	(b)
Naphthalene	Gash stream	52(10)	79(15)
Nickel (Soluble and Metal)	Trace element in coal	1(b,c)	(b)
Phenol (Skin)	Gas and effluent stream	19(5)	(b)
Propane	Gas stream	(b,e)(1,000)	(b)
Pyridine	Gas stream	16(5)	(b)
Selenium Compounds	Trace element in coal	0.2(b)	(b)
Silica Dust (Total)	Trace element in coal	10(b)	(b)
Silica Dust (Respirable)	Trace element in coal	0.05(b)	(b)
Styrene (Skin)	Gas stream	215(50)	426(100)
Sulfur Dioxide	Thermal oxidizer	5.2(2)	13(5)
Vanadium	Trace element in soil	0.05(b)	(b)
Xylene (V_2O_5 Dust and Fume)	Gas stream	434(100)	651(150)

(a) From American Conference of Government and Industrial Hygienists, *Threshold Limit Values and Biological Exposure Indices for 1989-1990*.

(b) Value not available or adopted.

(c) Value recommended for change.

(d) Ceiling or not-to-be-exceeded value.

(e) From Sax, N. Irving and Lewis, Sr., Richard J., *Dangerous Properties of Industrial Material*.

Key Personnel Staffing Report

Section 4

Key Personnel Staffing Report

The key personnel staffing report for this reporting period (December 23, 1991 through March 15, 1992) as required by DOE/PETC is shown below.

Name	Function	% Time Spent[a]
Bechtel		
Bruce D. Degen	Process Manager	31
Charles R. Brown	Offsite Facilities	0[b]
G. Lucido	Cost Estimating	0[c]
Samuel S. Tam	Project Manager	38
Amoco		
J. J. Nicoholas	Subcontract Manager	8
S. S. Kramer	Process Model/Simulation	8

(a) Number of hours spent divided by the total available working hours in the period and expressed as a percentage.

(b) C. Brown of Bechtel did not spend any time in this reporting quarter because no offsite facilities work was required.

(c) G. Lucido of Bechtel did not spend any time in this reporting quarter because no cost estimating work was required.

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