3.0 FIXED-BED REACTOR DESIGN

3.1 Types of Fixed-Bed Reactors

A number of fixed-bed designs are in commercial use in methanol plants, but the two in most common use are the recycle-gas-quenched design of ICI and the tubular-fixed-bed reactor of Lurgi with steam generation. Topsoe. Mitsubishi and Kellogg have developed multi-bed designs with intercooling and Mitsubishi has also announced a fluidized-bed design. In each case, the objective is to remove heat efficiently and the tubular-fixed-bed and fluidized-bed designs do this most effectively at the expense of appreciably more expensive reactors. A sketch of the tubular fixed-bed ARGE reactors used at Sasol, South Africa, is shown in Figure 3.1[4].

The tubular-fixed-bed reactor has been chosen for comparison with the slurry reactor because it is the most comparable in terms of energy efficiency. In addition, this reactor is somewhat more flexible in terms of recycle to fresh feed ratio than other designs which remove the heat of reaction as sensible heat. The methanol reactor, being equilibrium limited, requires a recycle to fresh feed ratio in the range of 2 to 4. The Fischer-Tropsch reaction is not so limited and theoretically, at least, very high single pass conversions are feasible.

3.2 Fixed-Bed Reactor Design Principles

The design of a tubular-fixed-bed F-T reactor requires a careful balance between conversion, pressure drop and heat transfer. It is useful to review the design principles involved:

3.2.1 Heat Transfer

The heat transfer coefficient for an empty tube is obtained from the Nusselt type equation:

$$hD/k = 0.023\cdot(DG/\mu)^{0.8}\cdot(c\mu/k)^{1/3}$$

where h is the heat transfer coefficient, Btu/(h.ft^2·°F), D is the tube internal diameter, ft, k is the thermal conductivity, Btu/(h·ft^2·°F/ft), c is the heat capacity of the fluid, Btu/(lb·°F), μ is the viscosity, lb/(h·ft) and G is the superficial mass velocity, lb/(h·ft^2).

For packed tubes Colburn [IEC 23, 910 (1931)] related the heat transfer coefficient to that of the empty tube times a factor which depends on the ratio of packing diameter to tube diameter, d/D:

d/D	0.05	0.10	0.20	0.30
h/h(empty)	5.5	7.0	7.5	6.6

The range of interest is 0.05 to 0.10 where the heat transfer coefficient is increasing.

[4] From the Encyclopedia of Chemical Technology, 2nd Edition

3.2.2 Pressure Drop

The pressure drop in a packed-bed is given by the modified Ergun equation:

$$\Delta P/L = f \cdot C \cdot G^2/(\rho d)$$

where d is the effective particle diameter, ft, f is a friction factor dependent on the modified Reynolds Number, dG/μ, C is the pressure drop coefficient in $ft \cdot hr^2/in^2$, ρ is the fluid density, lb/ft^3 and $\Delta P/L$ is the pressure drop in psi/ft. Linde Bulletin F-2932 gives the value of C at a typical bed void fraction of 0.37 as $3.6 \cdot 10^{-10}$. At modified Reynold's Numbers above 500, which is typical, the friction factor, f, varies between 1.1 and 1.0.

3.2.3 Conversion

The conversion-space velocity relationship for a fixed-bed Fischer-Tropsch reactor is reviewed in Appendix C. Basically, the relationship is equivalent to that of a slurry reactor when space velocity is expressed per unit weight of catalyst, temperature is identical and mass transfer is not limiting the conversion.

3.2.4 Operating Variables

Operating variables at the disposal of the designer are tube diameter, particle diameter, pressure level, inerts level and conversion.These are, of course, interrelated. From a heat transfer standpoint, it is essential to maximize mass velocity within the limits imposed by pressure drop. Pressure drop can be minimized by increasing pressure level (increasing ρ) or by using larger diameter particles. Up to a limit, larger particles also improve heat transfer. There is a tradeoff on particle size, however, since intraparticle diffusion decreases the effectiveness of the catalyst.

Superficial velocity is a secondary variable in fixed-bed reactor design but is significant since pressure drop is proportional to mass velocity times superficial velocity. In general superficial velocities of 3 to 5 times those in a slurry reactor can be tolerated. This ratio increases as pressure is raised.

Tube diameter is important since smaller diameter tubes improve the ratio of heat transfer area to reaction volume without materially affecting the heat transfer coefficient unless the ratio of tube diameter to particle diameter gets too small. Also, for good gas distribution the ratio of tube diameter to particle diameter should be kept over 10. A typical choice might be 1/8" particles in a 1.25" tube.

The remaining variables are conversion per pass and the inerts level, which control the external recycle to fresh feed ratio and the ultimate conversion. Heat evolution in a given size reactor is proportional to the space time yield (STY) which is the product of volumetric space velocity and conversion. STY increases as conversion is lowered, but eventually lines out as recycle ratio becomes very large (see Appendix D). In low conversion per pass, high recycle ratio designs, high mass velocities are employed without a corresponding increase in heat evolution. The high mass velocity is conducive to improved heat transfer and if a temperature rise is allowed, sensible heat effects reduce the heat removal requirement. A low level of inerts is also very significant in this type of operation since it permits high ultimate conversion to be achieved without excessive buildup of inerts in the recycle gas.

3.3 Comparison with the Slurry Reactor

Some of the differences between a slurry reactor and a fixed-bed reactor have been pointed out elsewhere, but a review may be helpful at this point:

A primary difference is the preferred conversion level. The slurry reactor, because of its superficial velocity limitation, fits best into the high conversion end of the scale where the recycle to fresh feed ratio is low, the only limitation being that due to backmixing. The fixed-bed reactor of the quenched or intercooled variety requires a high recycle ratio to limit the temperature rise, but even the externally cooled, tubular design requires a high mass velocity to achieve good heat transfer characteristics. A recycle to fresh feed ratio of at least 2 is preferred with pressure drop being the limiting factor.

Cooling surface requirement in a slurry reactor is less than a quarter that in a tubular fixed-bed reactor. This is partially because the heat transfer film coefficient is improved but also because a higher ΔT is permissible between reactants and coolant. In the tubular fixed-bed reactor, hydrogen content of the gas improves the heat transfer coefficient significantly, another reason why that reactor may not be a good choice for very low H_2/CO ratio gases.

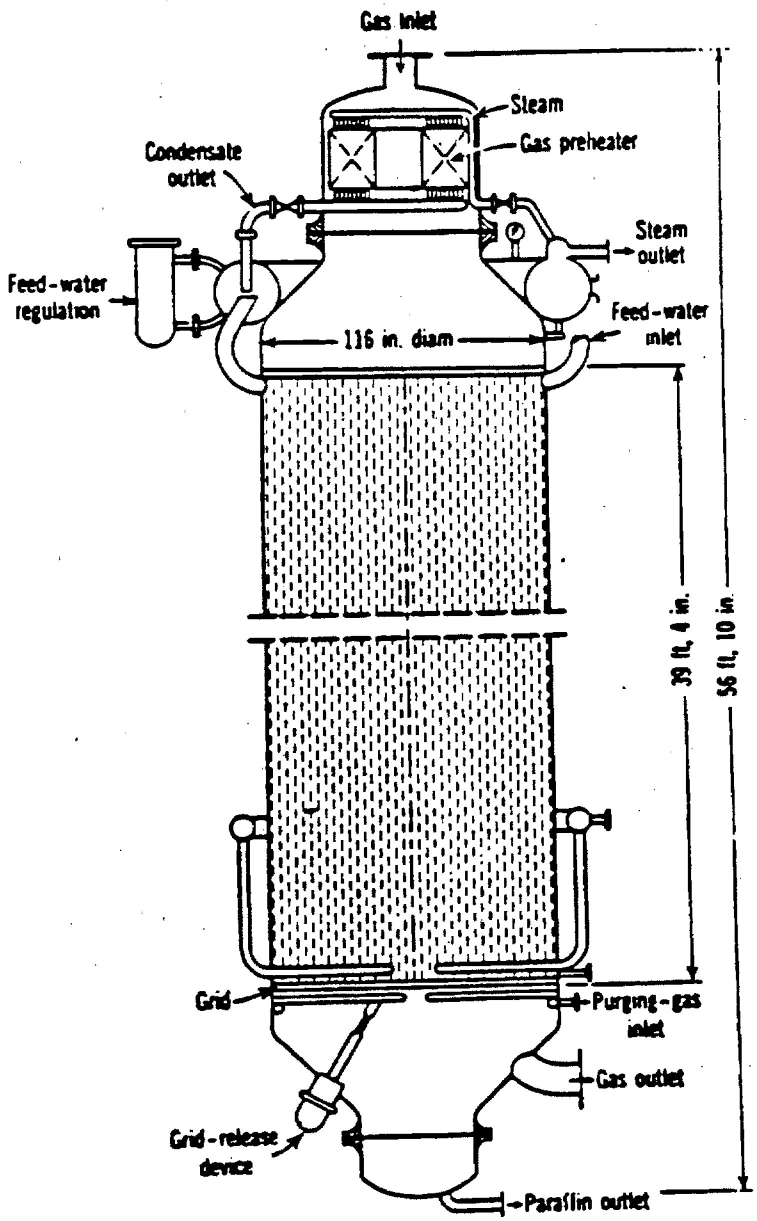
Increasing pressure level has significant advantages for either type of reactor, regardless of its effect on kinetics or equilibrium. At lower pressure, more slurry reactors are required because of the superficial velocity limitation. In the fixed-bed case, the limitation on superficial velocity is pressure drop. The higher the pressure level, the higher the permissible superficial velocity, so there is a double advantage. A high mass velocity is required for good heat transfer and this can more readily be achieved at high pressure. Higher pressure will permit a higher recycle ratio to be used without causing an increase in compressor horsepower. In either case, the vessel must be designed for the higher pressure but in the fixed-bed case the shell thickness is set by steam pressure rather than reaction pressure so there is less of an effect on cost.

Finally, in the fixed-bed reactor more catalyst can be loaded into a given volume. Since space velocity is normally expressed per unit weight of catalyst, this represents a significant potential advantage Since the fixed-bed reactor runs at lower conversion, space velocity would be expected to be higher as well. On the other hand, in F-T synthesis for distillate production, the slurry reactor is run at about 260 °C and, with catalyst addition, activity stays constant throughout the run. The fixed-bed reactor starts out at about 200 - 225 °C and temperature is gradually increased as activity declines. This temperature difference compensates for other effects and reaction volume requirements are actually somewhat less for the slurry reactor.

Some of these considerations are treated more fully in Appendix D.

Figure 3.1

FIXED-BED REACTOR DESIGN
ARGE REACTOR



4.0 PROCESS AND REACTOR DESIGN BASES[5]

This section discusses some of the key process design issues and provides overall block flow diagrams for the F-T and methanol cases. Reactor design bases are then defined. The fairest comparison is obtained when the maximum size reactor is used in each case. A 4.8 meter shell diameter was fixed as the maximum practical dimension.

Since the study is aimed at defining differences between the slurry reactor and the fixed-bed reactor, only those sections of the overall facility which are materially affected by the choice of reactor are included in the evaluation.

4.1 Methanol

There is much activity at the present time in the development of new methanol plant concepts. Low temperature designs have been proposed using soluble catalyst in a bubble column. Designs have been developed which use adsorbents or solvents to remove the product from the gas phase and increase conversion. A recent paper (J. B. Hansen, Haldor Topsoe, AIChE Spring National Meeting, Orlando, March 20, 1990) describes a high conversion, once-through, tubular, fixed-bed design in which operating conditions are such that the product condenses in the reactor. There have also been advances in feed gas preparation for conventional methanol plants. Both Davy McKee and Lurgi have designs which produce a stoichiometric or close-to-stoichiometric synthesis gas from natural gas. ICI is also working on this. For coal-based plants, synthesis gas may be produced from new, high efficiency coal gasifiers, but extensive shifting and CO_2 removal are required to produce a stoichiometric gas.

More to the point, Chem Systems have developed a slurry reactor design in which the catalyst is held in suspension in a heavy hydrocarbon oil. This has been proposed primarily for low conversion operation on as-produced, coal-derived synthesis gas, producing as much methanol as possible once-through and coproducing power from the tail gas. Air Products has piloted this design in a 2' diameter reactor at La Porte, Texas. While a similar type of operation may be possible in a fixed-bed reactor, the slurry reactor should give superior heat transfer characteristics with either internal cooling coils or with an external loop cooler. The use of a fixed-bed reactor for this application would be developmental and the necessary data are lacking for design. The comparison of once-through methanol/power coproduction, in a slurry reactor, with conventional high yield methanol production, in a fixed-bed reactor, has been the subject of other studies and introduces complications which are not pertinent to a one-for-one comparison of reactor designs.

It is possible to design a slurry reactor for high conversions to methanol using a stoichiometric synthesis gas. This may not be the optimum application for the slurry methanol reactor but this case does provide a one-for-one comparison of the slurry reactor with the fixed-bed reactor under normal synthesis conditions. This is the case selected for study.

4.1.1 Process Design.

The block flow diagram and overall material balance for the coal based methanol plant is shown in Figure 4.1. The Texaco gasifier has been selected for the methanol application since it permits synthesis gas to be generated at 5,600 kPa (55 atmospheres), sufficient to supply the fixed-bed reactor without further gas compression. An oxygen concentration of 99.5% is used since it gives

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[5] Changes to Topical Report Sections 4 and 5 are shown in italics.

a synthesis gas with very low inerts. This is beneficial in a recycle methanol operation. The gas is adjusted in composition by shift and CO_2 removal such that the ratio:

$$\frac{H_2 - CO_2}{CO + CO_2} = 2.05$$

and the CO_2 content is 3%. The steam content of the gas from the Texaco gasifier, after quenching, can be used effectively in the water gas shift reactor. The Rectisol Process is used for removal of CO_2, H_2S and other impurities. Processing closely follows that used in EPRI Report AP-1962. It turns out that, with the selected 4.8 m shell diameter, capacities are virtually identical for a fixed-bed reactor operating at 5600 kPa and *4.0* recycle to fresh-feed (R/FF) ratio and a slurry reactor operating at 10,000 kPa with a R/FF ratio of 2.2.

Only the methanol synthesis loop changes between cases. In addition to the differences in pressure and recycle ratio, there are differences resulting from slurry oil volatilization and recovery and catalyst makeup provisions in the slurry reactor case. The assumption is made that reactor configuration does not affect product distribution, so downstream product recovery facilities (after depressuring) are unchanged.

4.1.2 Reactor Design.

Design of the fixed bed methanol reactor is confidential to Lurgi who have requested that only overall dimensions and capacity be released publicly. The reactor has a shell diameter (ID) of 4.8 meters *(15.75 ft)* and a tangent-to-tangent length of *7.77 meters (25.5 ft)*. Total weight of catalyst provided is *78200* kg and the GHSV is 9.07 $Nm^3/(h \cdot kg\ Cat)$. Since a stoichiometric gas is used and the feed gas inerts are low, the reactor can be designed for a total pressure of 5600 kPa. Pressure drop is *25 psi (175 kPa) with a R/FF ratio of 4.0*[6]. Steam production is at 4100 kPa (40 atm).

The slurry reactor design is based on information developed by Air Products for the design of the internally-cooled La Porte pilot plant reactor (final report on DOE Contract DE-AC22-85PC80007), and on operating results from that reactor (Studer, et al, EPRI 14th Annual Conference on Fuel Science and Conversion, Palo Alto, May 18-19, 1989)). Cognizance has been taken of some stoichiometric-gas, high-conversion designs prepared by Chem Systems for an ongoing Bechtel study of IGCC power/methanol coproduction, but the design parameters have been independently established for this study, particularly the design heat flux. Reactor design variables are summarized in Table 4.1. Capacity at 0.15 m/s superficial velocity is *1685 short tons per day (STPD)* of methanol. At *0.146* m/s superficial velocity used for design, capacity is the same as a fixed-bed reactor of the same diameter *which is 1640 STPD.*

At the high design pressure (10,000 kPa), quite high conversions are theoretically possible and the R/FF ratio can be lowered, as indicated, to about 2.2. This combination of factors maximizes reactor throughput.

Air Products reports that the slurry methanol reactor can be designed to the same approach to equilibrium as a fixed bed reactor at the same space velocity *(30 °F and 9.07 $Nm^3/(h \cdot kgCat)$ in this study). Since the resulting CO conversion per pass is 88%, an allowance has been made for backmixing effects and the design approach is 45 °F giving a CO conversion of 83.6% at a GHSV of 8.7 $Nm^3/(h \cdot kgCat)$. Ultimate conversion is now virtually identical to the fixed-bed case. The*

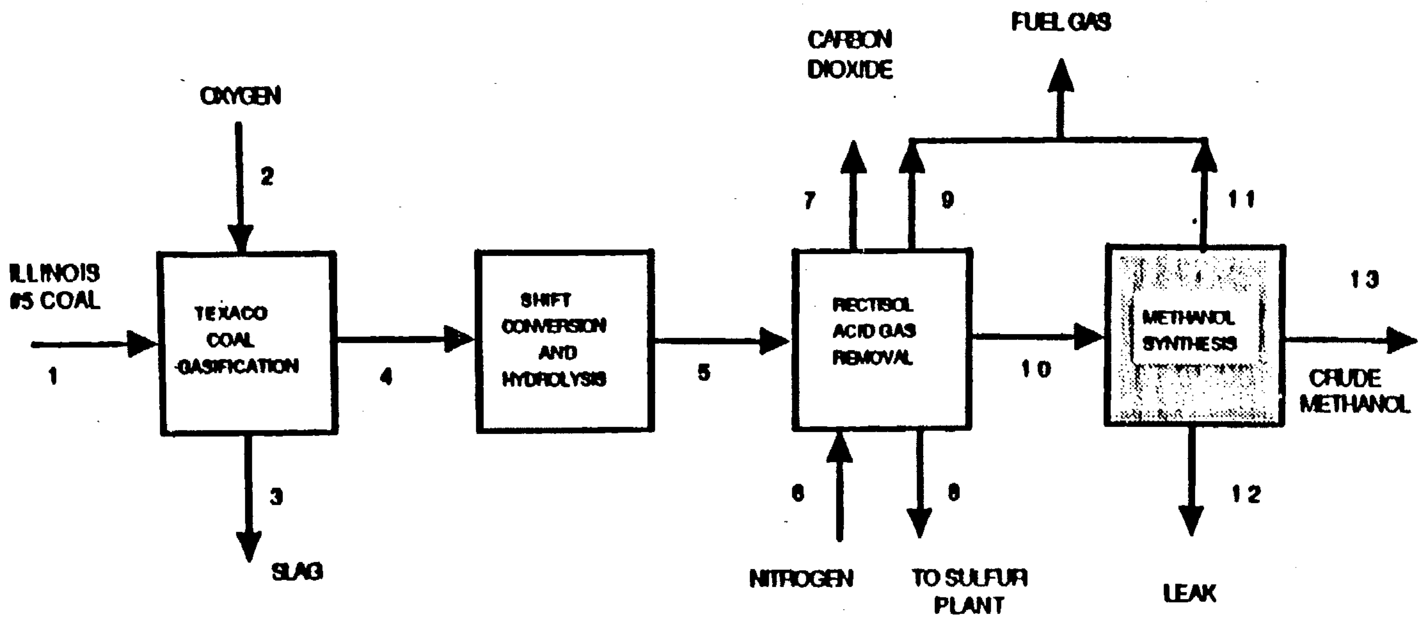
6 Information from Lurgi; Bechtel had originally used R/FF = 3.0.

resulting slurry bed height requirement of 12.6 meters is based on the bottom head volume being 15% effective for mass transfer and reaction. A total of 1245 cooling tubes are required. Methanol productivity (or STY), at 1.19 kg/(h·kg), is somewhat higher than in the fixed-bed reactor, at 0.794 kg/(h·kg), due to differences in conversion level. A more detailed analysis of backmixing might lead to a lower design GHSV than this. If so, the slurry eactor would be somewhat taller, productivity would be lower and fewer cooling tubes would be required.

Based on Air Products' recommendation, catalyst makeup requirement for the slurry reactor has been set equal to that for a fixed-bed reactor. The resulting makeup rate of 0.2% per day is roughly equivalent to total replacement every 18 months, which typically is the guaranteed life of a fixed-bed catalyst (replacement every 3 years is, however, not uncommon). At this low makeup rate, catalyst carryover will probably account for most of the required withdrawal but a separate catalyst withdrawal system is provided to allow for dumping a load of catalyst and recovering the liquid for reuse. Conventional materials of construction are used in both reactors since carbonyl poisoning of the catalyst should not occur with a stoichiometric feed gas. Overall yield in kg of methanol per kg of catalyst consumed is *9300* for the fixed-bed case and *13900* for the slurry reactor case.

Figure 4.1

SLURRY REACTOR STUDIES
METHANOL BLOCK FLOW DIAGRAM



MATERIAL BALANCE

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13
Description	Coal	Oxygen	Slag	Gasifier Outlet	Shifted Gas	Stripping Gas	CO2 Vent	Acid Gas	Fuel Gas	Methanol Syn Gas	Purge Gas	Leak Gas	Crude Methanol
Component - lb mph													
H_2				5890.0	8592.6		0.7	0.3	17.1	9584.7	443.9	60.5	25.3
CO				7815.0	4028.4		5.0	0.4	82.3	3870.0	33.9	7.1	4.9
CO_2				2109.2	5888.3		4727.3	320.0	488.1	452.1	21.9	2.0	20.0
H_2O				2878.2	0.0		0.0	0.0	0.0	0.0	0.1	0.3	388.5
O_2		4804.0		0.0	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0
N_2+Ar		36.0		118.6	118.8	550.0	542.7	0.2	2.4	113.0	91.0	0.8	10.3
CH_4				31.5	31.5		0.8	0.0	2.4	28.3	21.1	2.0	8.2
H_2S				149.9	150.3		0.0	158.2	0.0	0.0	0.0	0.0	0.0
COS				9.9	1.4		0.0	1.4	0.0	0.0	0.0	0.0	0.0
CH_3OH											3.7	0.3	4310.1
TOTAL - MPH		4840.0		18900.3	18817.2	550.0	5277.5	480.3	572.3	14128.0	615.3	71.4	4782.2
LBS/HR	177840	154925	27811	387352	405920	238869	223441	19463	23541	154204	6025	715	147420
Mol Wt		32.01		20.46	20.37	433.60	42.34	40.51	41.14	10.91	9.79	10.02	30.78

Table 4.1

SLURRY METHANOL REACTOR

DIMENSIONS	Design Case
Diameter, m	4.8
Straight Length of Bed, m	12.60
Xsect, m2	18.10
Head Vol, m3	28.95
Head Volume Effectiveness - %	15.00
Tube OD, mm	38.1
Tube ID, mm	34
Tube Length, m	12.10
No. of tubes	1245
Tube Area (OD), m2/tube	1.448
Tube Xsect (OD), m2/tube	0.001140
Tube Area (ID), m2/tube	0.000908
Net Xsect of Reactor, m2	16.68
Total Tube Area - m2 (OD)	1803.4
Reaction Volume, m3	214.44
CONDITIONS	
Feed Gas Temp., oC	150
Operating Temp, oC	250
Operating Pressure, atm	99
Slurry Concentration, wt%	35
Gas Holdup, %	25
Liquid Density, kg/m3	675
Particle Density, kg/m3	3000
Slurry Density, kg/m3	926.2
Catalyst Loading, kg/m3	243.1
Catalyst Weight, kg	52138.6
FF - kgmph	6324.3
TF - kgmph	20237.6
TF - m3/h	8777.7
TF - Nm3/h	453606
R/FF Ratio	2.20
MW of TF	9.72
MW of Effluent	11.99
CO2 in TF	2.808
CO2 Conversion per pass, %	30.02
CO in TF, %	10.434
CO Conversion per pass, %	83.64
Methanol Production, MTPD	1487.8
Heat Duty, MW	34.1
Inlet Superficial Velocity, m/s	0.146
GHSV, Nm3/h kgCat	8.70
Mass Velocity, kg/h m2	196649
Space Velocity, Nm3/h m3	2115
STY - kg Methanol/(h kgCat)	1.189
STY - kg Methanol/(h m3)	289
Heat Flux, kW/m2	18.912
Total Cooling Surface, m2	1803.4

4.2 Mixed Alcohols

The Lurgi Octamix process has been selected for the base case mixed alcohols process and Lurgi has provided the process design including a process flow diagram and equipment list. The data available to define the slurry reactor system for this application are very limited so only the reactors are sized. Relative costs may be compared by analogy with the methanol or Fischer-Tropsch systems. It is assumed that GHSV (in $Nm^3/(h \cdot kg\ Cat)$ and pressure level are identical regardless of which type of reactor is employed.

4.2.1 Process Design Basis

The overall block flow diagram is similar to that for methanol, the primary difference being that the synthesis gas has a 1.1 H_2/CO ratio and a CO_2 content of only 1.0%. Only a small amount of shifting is required and, while less CO_2 must be scrubbed out, a higher level of removal is achieved. The Rectisol unit employed for this purpose is integrated with that required for CO_2 removal from the gas recycled back to the synthesis reactor. Product recovery is somewhat more complicated than in a fuel grade methanol plant because of the higher alcohols in the product.

The synthesis loop is also more complicated since liquid methanol is recycled back to the reactor from the stabilizer reflux drum. Provisions may also be required for recovering heavier components of the product from the slurry oil. The assumption is made that syntheses gas preparation, the synthesis loop and product recovery are identical regardless of reactor selection.

4.2.2 Reactor Design.

Lurgi has given the capacity of the same tubular fixed-bed reactor used for 1640 STPD of methanol production as 460 STPD of mixed alcohols. The reactor is now designed for 10100 kPa rather than 5600 kPa operating pressure used for methanol. The primary effect is to increase the thickness of the heads and the tube sheets.

The slurry reactor design and sizing basis is summarized in Table 4.2. At the design GHSV of 2.7 $Nm^3/(h \cdot kg\ Cat)$, a slurry reactor designed for 0.15 m/s superficial velocity would have a slurry height of roughly 42.7 meters which is unrealistic. The superficial velocity is, therefore, reduced to 0.067 m/s, which should still be adequate to achieve the required agitation for heat and mass transfer. The slurry height is then reduced to 17.8 meters and the capacity is 460 STPD.

The heat release indicated by Lurgi in their fixed-bed design is about 50% higher per unit weight of product than in the methanol reactor. The same heat release has been used in the slurry reactor design. The design heat flux and gas holdup are reduced, at the lower superficial velocity, to 5,000 Btu/h x ft^2 x ^oF (15.76 kW/m^2) and 20%, respectively.

Since the reaction to mixed alcohols is controlled more by kinetics than equilibrium, the slurry reactor may benefit by a higher average temperature level, increasing the allowable space velocity. If the space velocity could be increased by 2.4 times, then it would be possible to double the capacity of the slurry reactor without increasing height, increasing the superficial velocity along with the space velocity. It is important, therefore, to obtain the kinetic data on which to base a valid design.

Table 4.2

SLURRY OCTAMIX REACTOR

DIMENSIONS	Design Case	Max. Sup. Vel.
Diameter, m	4.8	4.8
Straight Length of Bed, m	17.77	42.67
Xsect, m2	18.10	18.10
Head Vol, m3	28.95	28.95
Head Volume Effectiveness - %	15.00	15.00
Tube OD, mm	38.1	38.1
Tube ID, mm	34	34
Tube Length, m	17.27	42.17
No. of tubes	581	446
Tube Area (OD), m2/tube	2.067	5.048
Tube Xsect (OD), m2/tube	0.001140	0.001140
Tube Area (ID), m2/tube	0.000908	0.000908
Net Xsect of Reactor, m2	17.43	17.59
Total Tube Area - m2 (OD)	1199.8	2252.7
Reaction Volume, m3	314.07	754.80
CONDITIONS		
Feed Gas Temp., oC	200	200
Operating Temp, oC	245	245
Operating Pressure, atm	99	99
Slurry Concentration, wt%	35	35
Gas Holdup, %	20	25
Liquid Density, kg/m3	675	675
Particle Density, kg/m3	3000	3000
Slurry Density, kg/m3	926.2	926.2
Catalyst Loading, kg/m3	259.3	243.1
Catalyst Weight, kg	81453.0	183520.3
FF - kgmph	2322.3	5232.4
TF - kgmph	9811.9	22106.9
TF - m3/h	4215.1	9496.9
TF - Nm3/h	219923	495505
R/FF Ratio	3.225	3.225
MW of TF	22.90	22.90
MW of Effluent	26.57	26.57
CO2 in TF	0.96	0.96
CO in TF, %	62.49	62.49
CO Conversion per pass, %	16.2	16.2
Alcohols Production, MTPD	417.5	940.6
Heat Duty, MW	18.9	42.6
Inlet Superficial Velocity, m/s	0.0672	0.150
GHSV, Nm3/h kgCat	2.7	2.7
Mass Velocity, kg/h m2	224706	506282
Space Velocity, Nm3/h m3	700	656
STY - kg Alcohols/(h kgCat)	.214	.214
STY - kg Alcohols/(h m3)	55	52
Heat Flux, kW/m2	15.76	18.912
Total Cooling Surface, m2	1199.8	2252.7

4.3 Fischer-Tropsch

A modern coal gasifier of the Texaco or Dow design produces a synthesis gas with a H_2/CO ratio of about 0.75, the Shell gasifier produces something under 0.5 H_2/CO ratio. A 0.667 ratio is stoichiometric for the F-T reaction, without steam addition, where the catalyst has high water gas shift activity. Iron based catalysts have this activity. The reactions involved are:

$$2H_2 + CO \rightarrow -CH_2- + H_2O \quad (1)$$

$$H_2O + CO \leftrightarrow H_2 + CO_2 \quad (2)$$

giving the overall reaction:

$$H_2 + 2CO \rightarrow -CH_2- + CO_2 \quad (3)$$

Because equilibrium in reaction 2 heavily favors CO_2 production at F-T conditions, reaction 3 predominates over reaction 1.

Since the fixed-bed reactor is not applicable to low H_2/CO ratio operation, this study evaluates fixed-bed operation at a 2 to 1 ratio versus slurry bubble column operation at the low ratio out of a Shell gasifier. Because of the hydrogen deficiency in the as-produced gas, steam is added to conform with stoichiometry. The two processing schemes are quite different between the gasifier and the downstream processing units.

The Shell gasifier is believed to be the optimum choice in the case of the slurry reactor, which is capable of handling a very low H_2/CO ratio gas. The low oxygen requirement is a very definite advantage for this gasifier. It was considered appropriate to use the same gasifier for the fixed-bed case, leaving it to other studies to examine the difference between gasifiers. The Shell gas requires more shifting to achieve a 2.0 H_2/CO ratio but CO_2 removal requirements are virtually identical when compared to other gasifiers. The low inerts content resulting from the use of 99.5% oxygen and the CO_2 carrier gas favors the fixed-bed reactor because of the higher recycle ratio used in that design.

After consultation with catalyst experts, it was decided to go "generic" in terms of catalyst requirements and product distribution. In actual practice, fused or precipitated iron catalysts seem most appropriate for the slurry reactor, where high WGS activity is required, and cobalt type catalysts for fixed-bed synthesis where low WGS activity is needed. Some differences in product distribution can be expected when iron vs cobalt catalysts are compared, but it was decided that to identify such differences would confound the main purpose of the study. An attempt was made to rationalize space velocity requirements so that reactor sizing is not dependent on the particular catalyst chosen. This is described elsewhere in this report.

Basis for design is a plant which uses the gas produced from 7500 T/D of coal in three Shell gasifiers at 2500 TPD each. In either case, the plant produces roughly 20,000 BPSD of liquid distillates under conditions where the Schultz-Flory chain-growth probability factor is about 0.9. The detailed product distribution is given in Mobil's final report under DOE Contract DE-AC22-83PC60019 (October 1985). The only difference identified between cases was a higher degree of olefinicity at the lower H_2/CO ratio. There should also be much lower oxygenates production if a cobalt catalyst is used, but this has not been factored into the design. For the slurry reactor case, steam was added to the feed gas to compensate for the deficiency in product water and a close approach to WGS equilibrium was assumed. For the fixed bed reactor, an 8% yield of CO_2 on CO converted was assumed - a compromise between cobalt and iron based catalysts.

A catalyst makeup rate of 1.67% per day was used for the slurry reactor case, this being the level used by MITRE based on their review of the available design information. This corresponds to a catalyst life of 60 days without replacement. Sixty days is not a reasonable catalyst life for a fixed-bed system and it is believed that Shell expects to get over a year life in their Malaysian unit using a cobalt based catalyst. Catalyst life in a fixed-bed system is amenable to study by varying the operating cost and does not materially impact capital cost.

4.3.1 Process Design Basis.

The overall Block Flow Diagram for the slurry reactor Fischer-Tropsch case is given in Figure 4.2 The material balance is given in Table 4.3 which is keyed into Figure 4.2 by means of stream numbers. Plants for which process flow diagrams and equipment lists will be provided are shaded in the diagram.

While the design follows that developed by MITRE (Gray, et al, Sandia Report WP89W00144-1), there are some key differences. Both designs use Shell gasification of coal with CO_2 carrier gas to prepare synthesis gas. The Shell gasifier package includes a waste heat boiler and a scrubber for carbon removal. The gasifier product gas is subjected to COS/HCN hydrolysis, cooling and condensation of sour water. Bechtel's design eliminates the water-gas-shift step entirely. The gas is compressed such that the F-T synthesis pressure is 3050 kPa (440 psia). The Selexol process is used for selective H2S removal and, finally, zinc oxide beds are used for sulfur polishing. The gas is then sent to the Fischer-Tropsch reactor after combining with a small amount of recycle gas. Since the gas is below stoichiometric H_2/CO ratio, steam is added to the recycle gas to supplement the water produced by reaction 1, shifting additional CO to produce the required amount of hydrogen.

As described elsewhere in this report, conversion per pass is 80% in the F-T reactor, rather than the 90% conversion used by MITRE. This permits significant reduction in the number of F-T reactors at the expense of doubling the small amount of recycle gas. It was not found effective to carry out a partial oxidation of the recycle gas to convert hydrocarbon byproducts to synthesis gas The gas is recycled after product separation, CO_2 removal, cryogenic hydrocarbon recovery and recovery of enough hydrogen to treat the liquid product. A small purge is taken for inerts removal

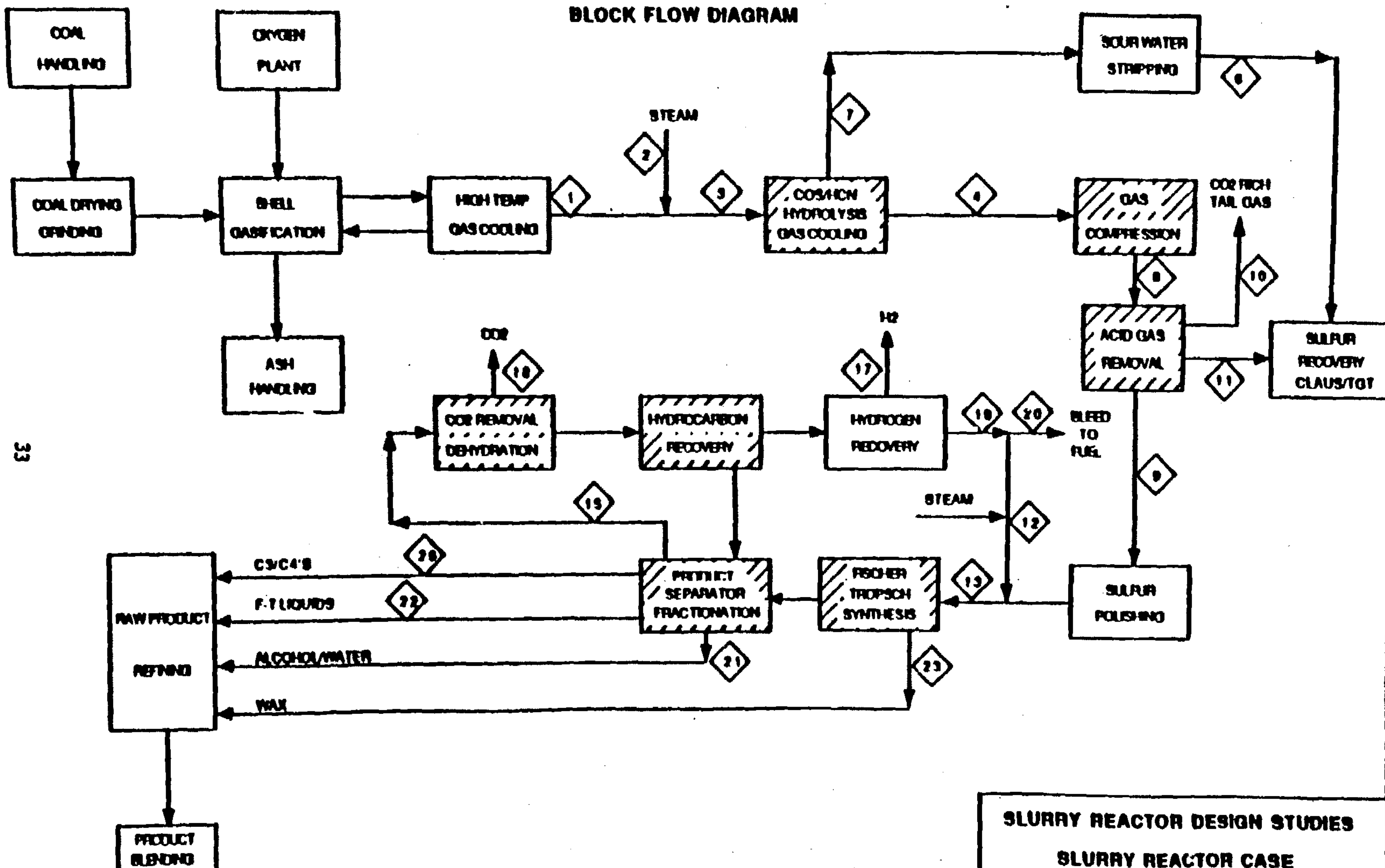
Product upgrading follows the sequence defined by MITRE and includes wax hydrocracking, distillate hydrotreating, catalytic polymerization of C3/C4's, heavy poly gasoline hydrotreating, isomerization of the C5/C6's and catalytic reforming of the naphtha from wax hydrocracking and middle distillate hydrotreating, and alkylation of cat poly olefins with isobutane from the cat reformer. MITRE shows "alcohols recovery" from the small amount of product water. Actually, there are other oxygenates present than just alcohols. This step has not been further defined but should be a minor part of the overall plant cost.

Figure 4.2

FISCHER TROPSCH SYNTHESIS

SLURRY REACTOR CASE

BLOCK FLOW DIAGRAM



SLURRY REACTOR DESIGN STUDIES

SLURRY REACTOR CASE

Table 4.3

MATERIAL BALANCE -BASIS 3 SHELL GASIFIERS 2500 T/D M/F COAL EACH - SLURRY REACTOR CASE

STREAM NO	1	2	3	4	7	9	11	12	13	14	15	16	17
DESCRIPTION	GASIFIER OUTLET	STEAM TO COS HYDR	COS HYD INLET	COS HYD OUTLET	SOUR WATER	SELEXOL OUTLET	SOUR GAS	RECYCLE GAS	REACTOR FEED	REACTOR PROD	OFF GAS	CO2 OFFGAS	H2 PROD
COMPONENT	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH
H2O	47.8	12879.0	12928.8	12880.9	12729.7	0.0	0.0	3193.8	3193.8	204.2	0.0	0.0	0.0
H2	14621.3	0.0	14621.3	14621.3	0.0	14620.2	1.1	3093.8	17714.0	4909.9	4909.9	0.0	943.8
CO	34280.4	0.0	34280.4	34280.4	0.0	34288.4	12.0	5264.6	39533.1	6749.7	6749.7	0.0	0.0
CO2	1920.9	0.0	1920.9	1966.7	15.5	1712.4	238.6	153.1	1865.6	19671.2	19671.2	19474.5	0.0
N2	190.5	0.0	190.5	190.5	0.0	190.0	0.5	672.9	862.9	862.9	862.9	0.0	0.0
H2S	433.9	0.0	433.9	479.7	1.7	0.4	477.5	0.0	0.0	0.0	0.0	0.0	0.0
NH3	17.2	0.0	17.2	17.2	17.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
COS	46.3	0.0	46.3	0.5	0.0	0.4	0.1					0.0	
C8H17O.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1830.3	0.0	0.0	0.0
C1	5.3	0.0	5.3	5.3	0.0	5.3	0.0	18.0	23.3	23.3	2052.2	0.0	0.0
C2=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	506.0	506.0	506.0	848.7	0.0	0.0
C2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	182.9	182.9	182.9	208.9	0.0	0.0
C3=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	301.0	301.0	301.0	454.4	0.0	0.0
C3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	33.2	33.2	33.2	59.1	0.0	0.0
C4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.8	3.6	3.6	25.1	0.0	0.0
C4=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	21.5	21.5	21.5	129.2	0.0	0.0
C5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	32.6	0.0	0.0
C5=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.3	6.3	6.3	136.4	0.0	0.0
C6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.2	0.2	22.6	0.0	0.0
C6=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.8	0.8	92.4	0.0	0.0
TOTAL	51563.5	12879.0	64442.4	64442.4	12764.1	50797.2	730.0	13432.8	64229.2	35287.9	36055.2	19474.5	943.8
LB/HR	1098389	232027	1330418	1330418	230372	1070180	27141.6	272356	1342499	1342498	1198365	857090	1902.3

Table 4.3 Cont.

MATERIAL BALANCE -BASIS 3 SHELL GASIFIERS 2500 T/D M/F COAL EACH-SLURRY REACTOR CASE

STREAM NO	18	19	20	CHECK		21	23	26	30	
DESCRIPTION	H/C REC	AFTER H2 REC	BLEED	RECYCLE GAS	F-T STEAM ADDITION	ALCOHOLS	WAX TO HYDRO-CRACKER	CAT POLY FEED	FT PROD HTU FEED	NET F-T YIELD
COMPONENT	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH	MPH
H2O	0.0	0.0	0.0	0.0	3193.8					
H2	0.0	3966.3	872.6	3093.7						
CO	0.0	6749.7	1484.9	5264.7						
CO2	0.0	196.7	43.3	153.4						
N2	0.0	862.9	189.8	673.1						
H2S	0.0	0.0	0.0	0.0						
NH3	0.0	0.0	0.0	0.0						
COS										
C8H170.1	0.0	0.0	0.0	0.0						
C1	0.0	2052.2	451.5	1600.7						446.4
C2=	0.0	648.7	142.7	506.0						142.7
C2	0.0	208.9	46.0	162.9						45.9
C3=	68.6	385.8	84.9	301.0				68.6		153.4
C3	16.5	42.5	9.4	33.2				16.5		25.9
C4	20.5	4.6	1.0	3.6				17.6		21.5
C4=	101.7	27.5	6.1	21.5				129.4		107.8
C5	31.3	1.3	0.3	1.0					31.3	31.6
C5=	128.3	8.1	1.8	6.3					128.3	130.1
C6	22.4	0.2	0.0	0.1					22.4	22.4
C6=	91.4	1.0	0.2	0.8					91.4	91.7
C7-C11									226.3	226.3
C12-C18									83.5	83.5
C19-C24							12.4			12.4
C25+							131.3			131.3
ALCOHOLS						157.6				157.6
TOTAL	480.7	15156.4	3334.4	11822.0	3193.8	157.6	143.8	232.0	583.2	1830.4
LB/HR	31389	307984	67756	240227	57539	10678	107474	10340	64938	210696

The BFD for the fixed-bed case is given in Figure 4.3 which differs from Figure 4.2 only in the location of some steam additions and the addition of a water gas shift step. The material balance is given in Table 4.4. In this case, extensive shifting and CO_2 removal are required ahead of the F-T converters. A selective Rectisol unit is used for CO_2 and H_2S removal in this case. This was chosen over Selexol since the latter would have required a double COS hydrolysis and CO_2 removal sequence to achieve adequate COS removal. A zinc guard bed is again employed for polishing.

The fixed-bed converters operate at 37% CO conversion per pass and 97% ultimate conversion with a 2.3 recycle to fresh feed feed ratio. This high level of conversions is only possible because of the very low inerts level (0.4%) in the syntheses gas.

The recycle loop and product recovery are similar to that provided for the slurry reactor case except that:

- Much less CO_2 is removed from the recycle gas,
- Less hydrogen recovery is required to supply the treating units, and
- Considerably more water must be handled.

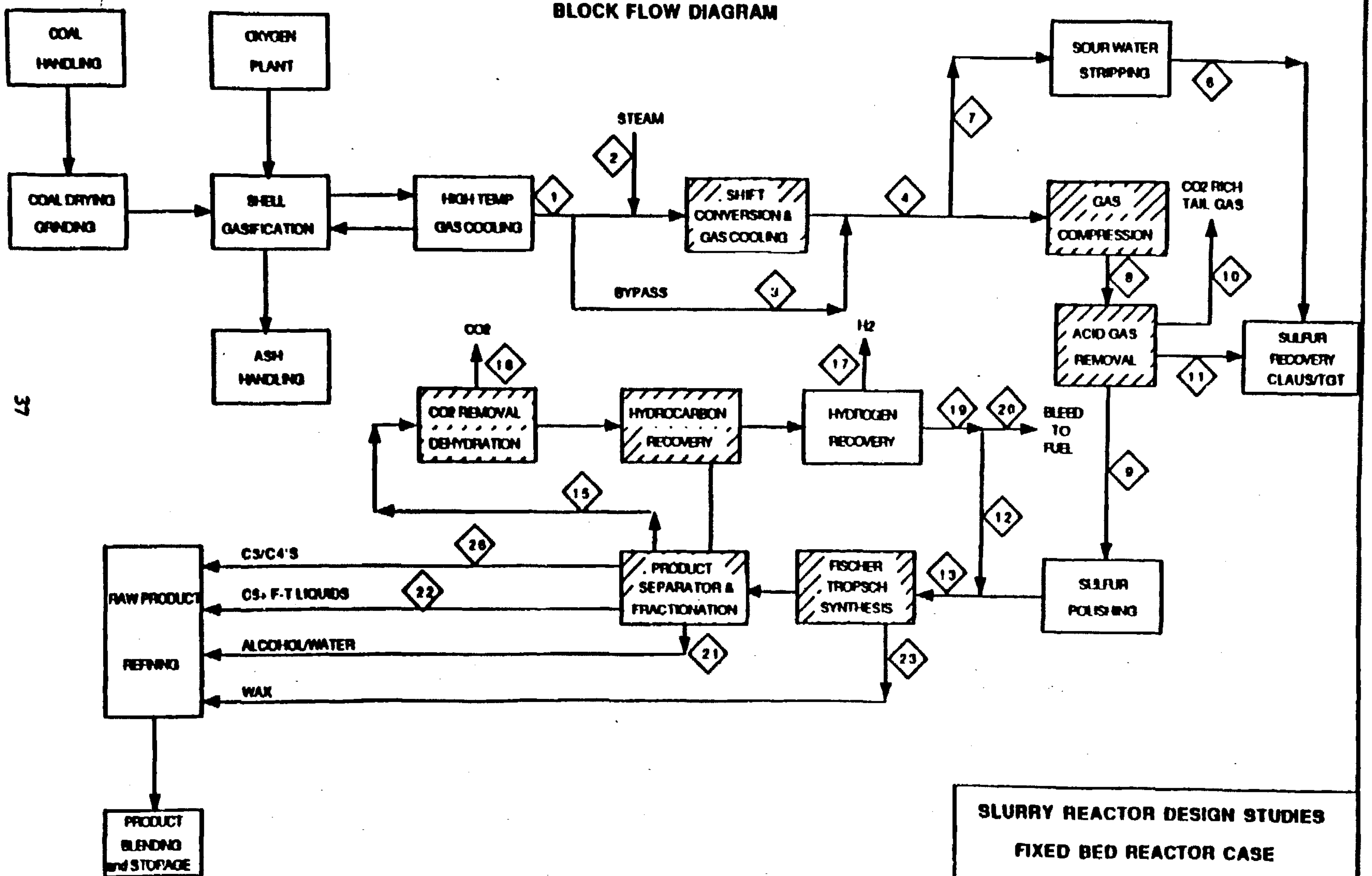
The question of oxygenates recovery from the product water is not addressed in this study. It could be more of a problem in the fixed-bed than in the slurry reactor case because of the larger quantity of water to be handled. On the other hand, if a cobalt based catalyst is used, oxygenates production could be so low that only a biotreatment step is required on the product water before its reuse as a utility.

Figure 4.3

FISCHER TROPSCH SYNTHESIS

FIXED BED REACTOR CASE

BLOCK FLOW DIAGRAM



SLURRY REACTOR DESIGN STUDIES

FIXED BED REACTOR CASE

BLOCK FLOW DIAGRAM

Table 4.4

MATERIAL BALANCE -BASIS 3 SHELL GASIFIERS 2500 T/D M/F COAL EACH - FIXED BED CASE

STREAM NO.	1	2	3	4	7	9	10	11	12	13	14	15	16	17
DESCRIPTION	GASIFIER OUTLET MPH	STEAM TO SHIFT MPH	SHIFT BYPASS MPH	SHIFT OUTLET MPH	SOUR WATER MPH	RECTISOL OUTLET MPH	CO2 OFF GAS MPH	SOUR GAS MPH	RECYCLE GAS MPH	REACTOR FEED MPH	REACTOR PROD MPH	OFF GAS MPH	CO2 OFFGAS MPH	H2 PROD MPH
H2O	47.6	46035.7	19.2	28904.7	28703.3	0.0	0.0	0.0	0.0	0.0	13535.6	0.0		0.0
H2	14621.3		5892.4	31799.9	0.0	31738.3	63.6	0.0	49908.3	51644.6	51645.9	51645.9		583.7
CO	34280.4		13815.0	17101.8	0.0	16930.8	171.0	0.0	26941.9	43872.7	27564.8	27564.8		0.0
CO2	1920.9		774.1	19099.5	15.3	977.1	17243.7	863.4	22.7	999.8	2304.5	2304.5	2281.4	0.0
N2	190.5		76.8	190.5	0.0	190.1	0.0	0.4	8224.4	8414.4	8414.4	8414.4		0.0
H2S	433.9		174.9	433.9	1.7	0.5	0.0	431.7	0.0	0.0	0.0	0.0		0.0
NH3	17.2		6.9	17.2	17.0	0.2	0.0	0.0	0.0	0.2	0.0	0.0		0.0
COS	46.3		18.6	46.3	0.0	0.0	0.0	46.3	0.0	0.0	0.0	0.0		0.0
C8H170.1	0.0		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1880.2	0.0		0.0
C1	5.3		2.1	5.3	0.0	5.2	0.1	0.0	21989.8	21994.9	21994.9	22498.5		0.0
C2=	0.0		0.0	0.0	0.0	0.0	0.0	0.0	1340.1	1340.1	1340.1	1371.1		0.0
C2	0.0		0.0	0.0	0.0	0.0	0.0	0.0	6557.3	6557.3	6557.3	6709.0		0.0
C3=	0.0		0.0	0.0	0.0	0.0	0.0	0.0	687.5	687.5	687.5	762.1		0.0
C3	0.0		0.0	0.0	0.0	0.0	0.0	0.0	634.5	634.5	634.5	736.9		0.0
C4	0.0		0.0	0.0	0.0	0.0	0.0	0.0	74.0	74.0	74.0	137.2		0.0
C4=	0.0		0.0	0.0	0.0	0.0	0.0	0.0	91.1	91.1	91.1	156.5		0.0
C5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.2	17.2	17.2	93.7	0.0	0.0
C5=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	29.3	29.3	29.3	114.6	0.0	0.0
C6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.4	2.4	2.4	55.4	0.0	0.0
C6=	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.7	3.7	3.7	64.9	0.0	0.0
TOTAL	51563.5	46035.7	20780.1	97599.1	28737.4	49840	17478.4	1341.8	116524	166364	136778	122629	2281.4	583.7
LB/HR	1098389	829379	442851	1927767	518141	586663	763831	55505	1744398	2331040	2331040	1920899	100408	1176.7

Table 4.4 Cont.

MATERIAL BALANCE -BASIS 3 SHELL GASIFIERS 2500 T/D M/F COAL EACH- FIXED BED CASE

STREAM NO.	18	19	20	CHECK	21	23	26	30	
DESCRIPTION	H/C REC MPH	AFTER H2 RECOV MPH	PURGE GAS MPH	RECYCLE GAS MPH	ALCOHOLS MPH	WAX TO HYDCRACK MPH	CAT POLY FEED MPH	FT PROD HTU FEED MPH	NET F-T YIELD MPH
H2O	0.0	0.0	0.0	0.0					
H2	0.0	51062.2	1154.0	49908.2					
CO	0.0	27564.8	623.0	26941.8					
CO2	0.0	23.0	0.5	22.5					
N2	0.0	8414.4	190.2	8224.3					
H2S	0.0	0.0	0.0	0.0					
NH3	0.0	0.0	0.0	0.0					
COS	0.0	0.0	0.0	0.0					
C8H170.1	0.0	0.0	0.0	0.0					
C1	0.0	22498.5	508.5	21990.0					503.6
C2=	0.0	1371.1	31.0	1340.1					31.0
C2	0.0	6709.0	151.6	6557.3					151.6
C3=	58.7	703.5	15.9	687.6			58.7		74.6
C3	87.8	649.1	14.7	634.5			87.7		102.4
C4	61.5	75.7	1.7	74.0			61.5		63.2
C4=	63.4	93.2	2.1	91.1			59.2		65.5
C5	76.1	17.6	0.4	17.2				76.0	76.4
C5=	84.5	30.0	0.7	29.3				84.5	85.2
C6	53.0	2.5	0.1	2.4				52.9	53.0
C6=	61.1	3.8	0.1	3.7				61.1	61.2
C7-C11								226.7	226.7
C12-C18								83.6	83.5
C19-C24						12.5			12.5
C25+						131.0			131.0
ALCOHOLS					158.8				158.8
TOTAL	271.3	119164.5	2693.1	116471.4	158.8	143.5	267.2	584.9	1880.2
LB/HR	34592	1784722	40335	1744388	10762	107458	13469	65518	212336

4.3.3 Reactor Design.

The design principles for both slurry and fixed-bed Fischer-Tropsch reactors are the subject of other sections of this report. In the following discussion, these principles (kinetics, heat, and mass transfer, hydraulics and batch-mixing effects) are translated into specific designs for the two F-T cases.

Table 4.5, for the slurry reactor, follows the same format as Tables 2.1 through 2.5 but uses operating variables specific to the proposed process design to establish the slurry bed height requirement for the three simplified reaction models. A bed height of 12.22 meters is required to provide the design 80% CO conversion using Model 2, the model proposed for the commercial reactor. In this calculation, the reactor is treated as cylindrical, the head volume and the volume occupied by the cooling tubes being neglected. As long as the cooling tubes occupy the entire slurry bed height, and the bottom head is assumed ineffective for reaction, the bed height calculation in Table 4.5 is still valid. The cooling tubes simply reduce the effective diameter of the vessel. Capacity is reduced but the bed height / space velocity relationship is unchanged.

Table 4.6, following the format of Tables 4.1 and 4.2 for methanol and mixed alcohols, *uses the design GHSV from Table 4.5 but assumes the bottom head volume is 15% effective and allows for the reactor volume occupied by the cooling tubes.The straight length of bed in Table 4.6 is the height of the slurry-gas interface above the bottom tangent line of the reactor. The tube length is that active for heat transfer and is equal to the bed length.* Design heat flux is 18.9 kW/m^2 [6,000 $Btu/(h \cdot ft^2)$]. The right hand column shows the maximum capacity at 0.15 m/s superficial velocity *and under these circumstances the required bed height is 13.16 meters. The middle column is at 1/6th the flow given in Table 4.3 for the design material balance. Superficial velocity is 0.136 m/s and the required bed height is 11.69 meters.* It is noted that *2481* tubes are required in a 4.8 m diameter reactor. These are 38.1 mm in diameter (1.5 ") and reduce the effective cross sectional area of the reactor to 84% of that for the empty vessel.

Because of the large number of cooling tubes required, an alternate design with an external pumparound cooling loop becomes worthy of consideration. The left hand column of Table 4.6 shows that in this case the number of reactors can be decreased to 5 and the required bed length is 11.91 meters.

Table 4.7 presents an analysis of fixed-bed F-T reactor design. *Table 4.8 repeats the same data in metric units for comparison with the slurry reactor.* Pressure drop and average heat transfer characteristics are shown *in Table 4.7* for two design cases requiring 8 reactors and 7 reactors, respectively, to handle the flow shown in Table 4.4. These designs are compared with similar calculations for the ARGE reactors (based on information given in the Encyclopedia of Chemical Technology, 2nd Edition, Vol. 4). Design space velocity is roughly the same at 1920 $Nm^3/(h \cdot m^3)$, though the per pass conversion has been increased from 26% to 37%. This increased is justified by the analysis given in Appendix C. Part of the effect is due to the higher pressure level and part is an assumed higher catalyst activity. The same catalyst bulk density of 850 kg/m^3 (53.1 lb/ft^3) has been used, even though there are indications that a cobalt-based catalyst would have a lower value. Gas properties used in Table 4.7 are derived using API Technical Data Book methods for gas mixtures and are averaged between inlet and outlet conditions.

It will be noted that somewhat longer tubes of significantly smaller diameter are used in the present design than were used in the ARGE reactors. The smaller diameter is to accommodate the higher heat release per unit reactor volume and the longer length is to accommodate the space velocity at the design throughput. While either the 7 reactor or the 8 reactor design might be satisfactory, the 8 reactor design has the shorter tubes and the lower pressure drop and was chosen as the design case. The longer reactor in the 7 reactor case might give fabrication problems.

Table 4.5

	A	B	C	D	E
1	CASE		COMMERCIAL DESIGN		6/12/90
2	uGo - cm/s		15		
3	alpha		-0.5658		
4	I		2.2317		
5	U		2.5604		
6	alpha'		-0.623348182		
7	T - oC		257		
8	Wt % Slurry		35		
9	Vol % Solids		10.43659272		
10	dR - cm		480		
11	L - cm		1222		
12	dp - micron		26		
13	rhoS - g/cm^3		3.1		
14	muL - poise		0.02474214		
15	rhoL - g/cm3		0.670865		
16	sigmaL - dyne/cm		16.5		
17	DA - cm2/s		0.00053911		
18	muSlurry - poise		0.046982128		
19	rhoSlurry - g/cm^3		0.924383927		
20	kLa Correction Factor		0.766055793		
21	REACTOR MODEL	MODEL 1	MODEL 2	MODEL 3	
22	epsilonG - Bukur's Model	0.233068105	0.241202372	0.242630391	
23	kLa - s^-1 (uncorr) for H	0.990384219	1.028471622	1.035171484	
24	kLa - s^-1 (corr) for H	0.758689567	0.787866644	0.792999112	
25	kH - (s*kgCat/m3)^-1		0.000507903	3.3e^9*exp(-130/RT)	
26	kH - s^-1		0.106883608	With pressure correction	
27	kH*epsilonL - s^-1	0.081972448	0.081103028	0.080950396	
28	He - (kPa cm^3)/mol		20064929.63		
29	RTL/(uGo*He) - s^-1		17.89073553		
30	kA - s^-1	0.073979364		0.07345229	
31	Stanton No. - target	1.323545234		1.314115489	
32	H2 Conversion	0.873587608		0.899774742	
33	Stanton No. - result	1.323542709		1.314115554	
34	Average uG - cm/s	10.91588064		11.72847515	
35	Stanton No. - reaction		1.45099283		
36	StantonM - target		14.09551375		
37	H2 Conversion		0.72608013		
38	n		0.500432287		
39	Y		0.726080164		
40	StantonM - result		14.09415988		
41	Average uG - cm/s		11.60549453		
42	Pressure - kPa		2600		
43	Reactor Xsect - m^2		18.09557368		
44	Reactor Vol. - m^3		221.1279104		
45	Feed Rate - m^3/h		9771.60979		
46	Feed Rate - Nm^3/h		129122.8672		
47	SV - Nm^3/(m^3 h)		583.9274967		
48	H2+CO Conversion	0.962441229	0.799930592	0.770949652	
49	CO Conversion	1.002255551	0.833022165	0.80284234	
50	STY - Nm^3/(h*m^3)	561.9958977	467.1014882	450.1787006	
51	STY - Nm^3/(kgCat h))	2.264935904	1.902875991	1.837200858	
52	GHSV - Nm^3/(kgCat h)	2.353323855	2.378551351	2.383036106	
53	Catalyst - kg	54868.20988	54286.26426	54184.10021	
54	Catalyst Loading kg/m^3	248.1288308	245.4971159	245.0351026	
55	Reaction Enthalpy - kJ/gmol -CH2-	214.6	214.6	214.6	
56	kgmol/h of H2+CO Conv (=3* -CH2-)	5544.435555	4608.243581	4441.290059	
57	Heat Release - kW	110169.988	91567.50671	88250.0784	
58	Heat Release - kW/m^3	498.218374	414.0929408	399.0906359	
59	Heat Release - Btu/(h ft^3)	48170.98637	40037.19342	38586.67321	
60	Mass Transfer Resistance - %	9.750939922	9.333240378	9.282594199	
61	DL - cm2/s	30932.8815	31545.0434	31651.62833	

Table 4.6

SLURRY FISCHER-TROPSCH BASE CASE DESIGN

DIMENSIONS	5 Reactors	6 Reactors	Max Capacity
Cooling Tube Design	External	Internal	Internal
Diameter, m	4.8	4.8	4.8
Straight Length of Bed, m	11.91	11.69	13.16
Xsect, m2	18.10	18.10	18.10
Head Vol, m3	28.95	28.95	28.95
Head Volume Effectiveness - %	15.00	15.00	15.00
Tube OD, mm	NA	38.1	38.1
Tube ID, mm	NA	34	34
Tube Length, m	NA	11.69	13.16
No. of tubes	NA	2481	2440
Tube Area (OD), m2/tube	NA	1.399	1.576
Tube Xsect (OD), m2/tube	NA	0.001140	0.001140
Tube Area (ID), m2/tube	NA	0.000908	0.000908
Net Xsect of Reactor, m2	18.10	15.27	15.31
Total Cooling Surface, m2 (OD)	NA	3471.3	3844.7
Reaction Volume, m3 (Effective)	219.92	182.80	205.93
Reaction Volume, m3 (Total)	244.53	207.41	230.54
CONDITIONS - PER REACTOR			
Feed Gas Temp., oC	149	149	149
Operating Temp, oC	257	257	257
Operating Pressure, atm	28.3	28.3	28.3
Slurry Concentration, wt%	35	35	35
Gas Holdup, %	23.0	22.8	24.1
Liquid Density, kg/m3	675	675	675
Particle Density, kg/m3	3000	3000	3000
Slurry Density, kg/m3	926.2	926.2	926.2
Catalyst Loading, kg/m3	249.6	250.3	246.1
Catalyst Weight, kg (Effective)	54898.1	45748.4	50670.0
Catalyst Weight, kg (Total)	61041.3	51907.5	56725.4
FF - kgmph	4608.4	3840.3	4253.4
TF - kgmph	5826.8	4855.7	5378.1
TF - m3/h	8959.4	7466.2	8269.4
TF - Nm3/h	130603	108835	120544
R/FF Ratio	0.2644	0.2644	0.2644
MW of TF	20.90	20.90	20.90
MW of Effluent	38.04	38.04	38.04
Syngas in TF - %	90.8	90.8	90.8
Syngas Conversion/Pass - %	80	80	80
'-CH2-Production, MTPD	474.9	395.8	438.4
Heat Duty, MW	78.8	65.6	72.7
Inlet Superficial Velocity, m/s	0.138	0.136	0.150
GHSV, Nm3/h kgCat	2.379	2.379	2.379
Mass Velocity, kg/h m2	121781	101484	112401
Space Velocity, Nm3/h m3	594	595	585
STY - kg -CH2-/(h kgCat)	.360	.360	.360
STY - kg -CH2-/(h m3)	90	90	89
Heat Flux, kW/m2	NA	18.912	18.912

Table 4.7

FISCHER TROPSCH TUBULAR REACTOR DESIGN 4/17/90

CASE	Prototype ARGE Design	Design 8 Reactors	Design 7 Reactors
Pressure - psia	368	425	425
Temperature - F at Inlet	392	392	392
Temperature - F at Outlet	437	437	437
CO Conversion/Pass - %	26.0	37.2	37.2
CO Ultimate Conversion - %	63.0	96.3	96.3
C5+ Selectivity - %	78.00	87.24	87.24
Shell ID - inches	116.00	188.98	188.98
Shell T-T - feet	45	50	56
Tube ID - inches	1.80	1.34	1.34
Tube OD - inches	1.96	1.50	1.50
Tube Length - feet	39.5	44.5	50.5
No of Tubes	2000	9602	9602
Tube xsection (ID) - sq ft	.0177	.0098	.0098
Tube Volume - cu ft	1396	4176	4739
Tube Area - sq ft	37228	149731	169920
Catalyst Bed Height - feet	36.5	41.5	47.5
Catalyst Volume - cu ft	1290	3894	4457
Catalyst Density - lb/cu ft	53.1	53.1	53.1
Catalyst Weight - pounds	68500	206776	236671
Catalyst Contact Area - sq ft	34400	156065	178629
Tube Xsect Area as % of Shell Area	57.099	60.176	60.176
Fresh Feed - lb mph per Reactor	2092.0	6230.0	7120.0
Total Feed - lb mph per Reactor	6903.6	20795.7	23766.6
Recycle/FF ratio	2.30	2.338	2.338
SV -FF Basis - Nm3/hxm3	582	574	574
SV -TF Basis - Nm3 /hxm3	1921	1917	1915
Prod - lb C5+/hrxlb cat	.062	.111	.111
C5+ HC - lb/hr	4281	22978	26260
Total HC - lb/hr	5544	26542	30334
MW of Inlet Gas	14.60	14.01	14.01
MW of Outlet Gas	16.38	17.04	17.04
Gas Viscosity - cp - Avg	0.0205	0.0201	0.0201
Gas Density - lb/cuft - Avg	.629	.705	.705
Gas Therm Cond - Btu/hrxftxF - Av	.060	.062	.062
Gas Sp. Ht. - Btu/lbxF - Avg	.556	.578	.578
Gas Prandtl No.	.458	.456	.456
Mass Velocity - lb/hrxsqft	2852	3105	3549
Reynold's Number - basis tube ID	8623	7958	9095
Catalyst Diam - feet	.0122	.0122	.0122
Reynold's Number - basis part diam	701	779	890
f	1.08	1.08	1.05
Press Drop - psi/ft	.41	.44	.55
Press. Drop - psi	15.0	18.1	26.3
Heat Release - MM Btu/hr	26.5	130.2	148.8
Heat Flux - Btu/hrxsqft	713	870	876
d/D	.081	.098	.098
Int Heat Trans Coef-Btu/hrxsqftxF	65	81	90
Film Temp Diff - F	11	11	10
Wall Resistance - k/t	938	953	953
Steam Side h - Btu/hrxsqftxF	250	250	250
Overall U	49.1	57.6	62.0
Overall Delta T - F	15	15	14
Gas Res. Time - sec	10.11	11.32	11.34
Tube area/tube volume	26.67	35.86	35.86
Heat Release/Unit Volume	19013	31188	31409

Table 4.8

FIXED-BED FISCHER TROPSCH BASE CASE DESIGN

DIMENSIONS	8 Reactors
Diameter, m	4.8
Straight Length of Bed, m	12.65
Xsect, m2	18.10
Tube OD, mm	38.1
Tube ID, mm	34.04
Tube Length, m	13.56
No. of tubes	9602
Tube Area (OD), m2/tube	1.623
Tube Xsect (OD), m2/tube	0.001140
Tube Area (ID), m2/tube	1.450
Tube Xsect (ID), m2/tube	0.000910
Net Xsect of Reactor, m2	8.74
Total Tube Area - m2 (ID)	13926
Total Tube Area - m2 (OD)	15589
Reaction Volume, m3	110.29
CONDITIONS - PER REACTOR	
Feed Gas Temp., oC	200
Operating Temp, oC	225
Operating Pressure, atm	28.3
Catalyst Loading, kg/m3	850
Catalyst Weight, kg	93747.4
FF - kgmph	2825.9
TF - kgmph	9432.9
TF - m3/h	13628.3
TF - Nm3/h	211428
R/FF Ratio	2.338
MW of TF	14.01
MW of Effluent	17.04
Syngas in TF - %	75.45
Syngas Conversion/Pass - %	36.89
'-CH2-Production, MTPD	294.6
Heat Duty, MW	38.2
Inlet Superficial Velocity, m/s	0.433
GHSV, Nm3/h kgCat	2.26
Mass Velocity, kg/h m2	15127
Space Velocity, Nm3/h m3	1917
STY - kg -CH2-/(h kgCat)	.131
STY - kg -CH2-/(h m3)	111
Heat Flux, kW/m2 (ID)	2.74

4.4 Key Design Parameters

An AIChE paper, reproduced as Appendix D, gives some criteria for comparing the fixed-bed and the slurry reactor. In this paper it is pointed out that the same GHSV [in $Nm^3/(h.kg\ Cat)$] should be required regardless of reactor type, to achieve the same conversion per pass. Owing to the lower catalyst loading, the slurry reactor will require a greater reaction volume. It was also noted that the fixed-bed reactor will generally run at a lower conversion/pass. The following discussion briefly summarizes the key design parameters in the final reactor selections of Section 4 and rationalizes these against Appendix D.

4.4.1 Methanol Design Parameters

Key methanol reactor design variables are summarized below:

	Slurry	Fixed-Bed
Temperature, °C	250	255 (outlet at end of run)
Pressure, atm	99	54
R/FF Ratio	2.2	4.0
CO in Total Feed, %	10.4	10.0
CO Conversion, %	83.6	55.9
Superficial Velocity, m/s (based on empty shell)	0.135	0.317
GHSV, $Nm^3/(h \cdot kgCat)$	8.7	9.1
SV, $Nm^3/(h \cdot m^3)$	2,115	11,333
STY, kg MeOH/(h·kgCat)	1.189	0.794
STY, kg MeOH/$(h \cdot m^3)$	289	992
(based on empty shell)	266	486
Effective XSect Area, %	92	49
Methanol Production, MTD	1488	1488

Both reactors have the same shell diameter, 4.8 meters. The slurry reactor has a tangent to tangent height of *15.1* meters, the fixed-bed reactor, *7.77* meters. The slurry reactor pressure has been raised in order to increase capacity to that of the fixed-bed. End of run temperature is shown since this limits the equilibrium conversion and hence the design. Lower start of run temperatures improve conversion.

Once the shell diameter is set, the capacity of a given reactor depends on the allowable superficial velocity (corrected for the effective cross sectional area) and the total volume of gas to be handled. The allowable superficial velocities based on an empty reactor are *0.135* and *0.317* m/s, respectively, a factor of *2.35* in favor of the fixed-bed. This is balanced by the difference in total gas handled (owing to differences in recycle ratio, conversion per pass and pressure level) so that the capacities are equal in terms of methanol production.

The required height of the reactor can be calculated from the STY in kg MeOH/$(h \cdot m^3)$, the capacity in kg methanol per hour and the available cross sectional area. The STY can, in turn, be calculated from the space velocity, the conversion per pass and the concentration of reactants in the reactor feed. As best as can be determined, the slurry reactor and the fixed-bed reactor are designed to the same GHSV in $Nm^3/(h \cdot kgCat)$ to achieve the same approach to equilibrium. As discussed in Appendix D, the catalyst loading in kg/m^3 of reactor volume is highly significant and gives the fixed-bed reactor a significantly lower height requirement. When all factors are combined, the slurry reactor is about twice the height of the fixed-bed reactor.

4.4.2 Fischer-Tropsch Design Parameters

In similar fashion to methanol, F-T design parameters are summarized below:

	Slurry	Fixed-Bed
Number of Reactors	6	8
Height of Bed, m	*11.69*	12.65
Reaction Volume, m3	*1097*	887
Temperature, °C	257	225 (outlet at start of run)
Pressure, atm	28.3	28.3
R/FF Ratio	0.264	2.34
Syngas in Total Feed, %	90.8	75.5
Syngas Conversion, %	80.0	36.9
Superficial Velocity, m/s	*0.136*	*0.433*
(based on empty shell)	*0.115*	*0.209*
GHSV, $Nm^3/(h \cdot kgCat)$	*2.38*	2.26
SV, $Nm^3/(h \cdot m^3)$	*595*	1917
STY, kg $-CH_2-/(h \cdot kgCat)$	*0.360*	0.131
STY, kg $-CH_2-/(h \cdot m^3)$	*90*	111
(based on empty shell)	*52.7*	*44.8*
Effective XSect Area, %	*84*	48
Hydrocarbon Production, MTD	2294	2312

A key difference is the higher design temperature in the slurry reactor case as compared to the fixed-bed reactor. Equilibrium is no longer a consideration so the improved activity at the higher temperature is significant. The result is that 80% conversion per pass is achieved in the slurry reactor as compared to 37% in the fixed-bed reactor, at the same pressure level and at roughly the same GHSV in each case. Comparisons given in Appendix D assume temperature is the same and the allowable space velocity rises as conversion level drops.

The allowable superficial velocity for the fixed-bed reactor, based on the empty shell, is *1.8 times* that for the slurry reactor. *Actual fixed-bed superficial velocity is set by pressure drop considerations and will vary depending on mass and space velocity, molecular weight of the gas, pressure level, reactor length and other variables.* Owing to differences in conversion per pass and recycle ratio, the fixed-bed reactors must handle *2.4* times the amount of gas as the slurry reactors for the same production. Consequently, six slurry reactors have roughly the same capacity as eigh fixed-bed reactors.

At roughly the same value of GHSV in $Nm^3/(h \cdot kgCat)$, the SV, in $Nm^3/(h \cdot m^3)$ is about 3 times greater in the fixed-bed case due to the higher catalyst loading. At the lower gas concentration and conversion level in the fixed-bed, the difference in STY is not nearly as great; 111 $kg/(h \cdot m^3)$ for the fixed-bed versus *90* for the slurry reactor. This ratio is only slightly *less* than the ratio in number of reactors and reaction bed heights are, therefore, roughly comparable.

4.5 Low Pressure Design

In order to ascertain the relative advantage for compressing the synthesis gas prior to acid gas removal and Fischer-Tropsch synthesis, designs have been prepared for both the slurry reactor and the fixed-bed reactor at half of the previous design pressure. The assumption is made that allowable GHSV increases as the square root of pressure in the fixed-bed case and that the reaction kinetic constant, k_H, decreases as the square root of pressure in the slurry reactor case. Thesae are almost equivalent assumptions, since the GHSV in the slurry reactor also increases by $P^{1/2}$ when mass transfer resistance is insignificant.

4.5.1 Slurry Reactor

Keeping the superficial velocity constant, capacity must vary in direct proportion to pressure if the cross sectional area is constant. Actually, the area occupied by the cooling tubes increases as capacity increases so the exponent on pressure is slightly less than 1. Since GHSV varies as $P^{1/2}$ and u is constant, reactor length must vary as $P^{1/2}$.

It turns out that if pressure is halved, the number of slurry reactors increases from 6 to 11. Table 4.9 shows that, as expected, the reactor length has been decreased from 12 meters to 8.5 meters and GHSV decreases from 2.42 to 1.71 to achieve 80% conversion per pass, Model 2. Table 4.10 shows how this fits into a slurry reactor design when the head volume and cooling tube volume corrections are made. Designs for 10, 11 and 12 reactors are shown. The 11 reactor design is under the limit of 0.15 m/s superficial velocity and results in a bed depth (to the tangent line) of 8.55 meters. In all cases the bottom head is assumed to be 15% effective.

4.5.2 Fixed-Bed Reactor

The assumption that allowable GHSV increases as $P^{1/2}$ turns out to be a good one from the standpoint of fixed-bed design since the reactor sizing does not change significantly but capacity increases in proportion to $P^{1/2}$. The reason is as follows:

- *To keep $\Delta P/L$ constant, uG is constant (superficial velocity times mass velocity).*
- *For the same reactor, capacity is proportional to GHSV.*
- *If reactor length is not varied, G varies as does GHSV (i.e. as $P^{1/2}$)*
- *Since gas density varies in direct proportion to P, u varies as $P^{1/2}/P = P^{-1/2}$, uG is constant, ΔP is constant.*
- *Heat flux varies as $P^{1/2}$.*
- *The internal film coefficient varies as $G^{0.8}$ or as $P^{0.4}$, film ΔT varies as $P^{0.1}$ but the effect on overall ΔT is quite small.*

The overall effect of halving the pressure is to increase the number of reactors from 8 to 11 (11/8 = 1.375). The resulting reactor design is given in Tables 4.11 and 4.12. Overall reactor dimensions remain unchanged.

Table 4.9

	A	B	C	D	E
1	CASE		COMMERCIAL DESIGN AT LOW PRESSURE		6/12/90
2	uGo - cm/s		15		
3	alpha		-0.5658		
4	l		2.2317		
5	U		2.5604		
6	alpha*		-0.623348182		
7	T - oC		257		
8	Wt.% Slurry		35		
9	Vol.% Solids		10.43659272		
10	dR - cm		480		
11	L - cm		864.5		
12	dp - micron		26		
13	rhoS - g/cm^3		3.1		
14	muL - poise		0.02474214		
15	rhoL - g/cm3		0.670865		
16	sigmaL - dyne/cm		16.5		
17	DA - cm2/s		0.00053911		
18	muSlurry - poise		0.046982128		
19	rhoSlurry - g/cm^3		0.824383927		
20	kLa Correction Factor		0.766055793		
21	REACTOR MODEL	MODEL 1	MODEL 2	MODEL 3	
22	epsilonG - Bukur's Model	0.233900696	0.241195733	0.243191644	
23	kLa - s^-1 (uncorr) for H	0.994276668	1.028440484	1.037805804	
24	kLa - s^-1 (corr) for H	0.761671401	0.78784279	0.795017148	
25	kH - (s*kgCat/m3)^-1		0.000507903	3.3e^9*exp(-130/RT)	
26	kH- s^-1		0.151156248	With pressure correction	
27	kH*epsilonL - s^-1	0.115800696	0.114698006	0.114396312	
28	He - (kPa cm^3)/mol		20064929.63		
29	RTL/(uGo*He) - s^-1		12.65674375		
30	kA - s^-1	0.100518386		0.10000625	
31	Stanton No. - target	1.272235449		1.265753475	
32	H2 Conversion	0.858672142		0.68940258	
33	Stanton No. - result	1.272238106		1.265754884	
34	Average uG - cm/s	10.98561211		11.77696616	
35	Stanton No. - reaction		1.451703272		
36	StantonM - target		9.97152431		
37	H2 Conversion		0.726202139		
38	n		0.500241442		
39	Y		0.726208105		
40	StantonM - result		9.970574259		
41	Average uG - cm/s		11.60492413		
42	Pressure - kPa		1300		
43	Reactor Xsect - m^2		18.09557368		
44	Reactor Vol. - m^3		156.4362345		
45	Feed Rate - m^3/h		9771.60979		
46	Feed Rate - Nm^3/h		64561.33359		
47	SV - Nm^3/(m^3 h)		412.7006367		
48	H2+CO Conversion	0.946008693	0.80006501	0.759522526	
49	CO Conversion	0.985143233	0.833162144	0.790942495	
50	STY - Nm^3/(h*m^3)	390.4183901	330.1873393	313.45543	
51	STY - Nm^3/(kgCat h))	1.575160343	1.344962645	1.280175317	
52	GHSV - Nm^3/(kgCat h)	1.665059057	1.681066698	1.685500131	
53	Catalyst - kg	38774.20043	38404.98041	38303.96236	
54	Catalyst Loading kg/m^3	247.8594589	245.4992638	244.853518	
55	Reaction Enthalpy - kJ/gmol -CH2-	214.6	214.6	214.6	
56	kgmol/h of H2+CO Conv (=3* -CH2-)	2724.885466	2304.508969	2187.73031	
57	Heat Release - kW	64144.48342	45791.44674	43471.01152	
58	Heat Release - kW/m^3	346.1121625	292.7163702	277.8832644	
59	Heat Release - Btu/(h ft^3)	33464.37052	28301.71872	26867.55777	
60	Mass Transfer Resistance - %	13.1970802	12.70834588	12.57913114	
61	DL - cm2/s	30995.77675	31544.54725	31693.44566	

Table 4.10

SLURRY FISCHER-TROPSCH - LOW PRESSURE DESIGN

DIMENSIONS	12 Reactors	11 Reactors	10 Reactors
Diameter, m	4.8	4.8	4.8
Straight Length of Bed, m	7.78	8.61	9.64
Xsect, m2	18.10	18.10	18.10
Head Vol, m3	28.95	28.95	28.95
Head Volume Effectiveness - %	15.00	15.00	15.00
Tube OD, mm	38.1	38.1	38.1
Tube ID, mm	34	34	34
Tube Length, m	7.78	8.61	9.64
No. of tubes	1865	1838	1805
Tube Area (OD), m2/tube	0.931	1.030	1.154
Tube Xsect (OD), m2/tube	0.001140	0.001140	0.001140
Tube Area (ID), m2/tube	0.000908	0.000908	0.000908
Net Xsect of Reactor, m2	15.97	16.00	16.04
Total Cooling Surface, m2 (OD)	1735.6	1893.5	2082.7
Reaction Volume, m3 (Effective)	128.51	142.03	158.92
Reaction Volume, m3 (Total)	153.12	166.64	183.53
CONDITIONS - PER REACTOR			
Feed Gas Temp., oC	149	149	149
Operating Temp, oC	257	257	257
Operating Pressure, atm	14.15	14.15	14.15
Slurry Concentration, wt%	35	35	35
Gas Holdup, %	22.3	23.3	24.6
Liquid Density, kg/m3	675	675	675
Particle Density, kg/m3	3000	3000	3000
Slurry Density, kg/m3	926.2	926.2	926.2
Catalyst Loading, kg/m3	251.9	248.7	244.4
Catalyst Weight, kg (Effective)	32371.6	35316.1	38846.1
Catalyst Weight, kg (Total)	38570.6	41435.4	44861.7
FF - kgmph	1920.1	2094.8	2304.2
TF - kgmph	2427.8	2648.6	2913.4
TF - m3/h	7466.0	8145.1	8959.3
TF - Nm3/h	54417	59366	65300
R/FF Ratio	0.2644	0.2644	0.2644
MW of TF	20.90	20.90	20.90
MW of Effluent	38.04	38.04	38.04
Syngas in TF - %	90.8	90.8	90.8
Syngas Conversion/Pass - %	80	80	80
-CH2-Production, MTPD	197.9	215.9	237.5
Heat Duty, MW	32.8	35.8	39.4
Inlet Superficial Velocity, m/s	0.130	0.141	0.155
GHSV, Nm3/h kgCat	1.681	1.681	1.681
Mass Velocity, kg/h m2	50741	55356	60889
Space Velocity, Nm3/h m3	423	418	411
STY - kg -CH2-/(h kgCat)	.255	.255	.255
STY - kg -CH2-/(h m3)	64	63	62
Heat Flux, kW/m2	18.912	18.912	18.912

Table 4.11

FISCHER-TROPSCH TUBULAR REACTOR DESIGN - LOW PRESSURE 6/12/90

CASE	Prototype ARGE Design	Design 11 Reactors	Design 10 Reactors
Pressure - psia	368	212	212
Temperature - F at Inlet	392	392	392
Temperature - F at Outlet	437	437	437
CO Conversion/Pass - %	26.0	37.2	37.2
CO Ultimate Conversion - %	63.0	96.3	96.3
C5+ Selectivity - %	78.00	87.24	87.24
Shell ID - inches	116.00	188.98	188.98
Shell T-T - feet	45	50	56
Tube ID - inches	1.80	1.34	1.34
Tube OD - inches	1.96	1.50	1.50
Tube Length - feet	39.5	44.5	50.5
No. of Tubes	2000	9602	9602
Tube xsection (ID) - sq ft	.0177	.0098	.0098
Tube Volume - cu ft	1396	4176	4739
Tube Area - sq ft	37228	149731	169920
Catalyst Bed Height - feet	36.5	41.5	47.5
Catalyst Volume - cu ft	1290	3894	4457
Catalyst Density - lb/cu ft	53.1	53.1	53.1
Catalyst Weight - pounds	68500	206776	236671
Catalyst Contact Area - sq ft	34400	156065	178629
Tube Xsect Area as % of Shell Area	57.099	60.176	60.176
Fresh Feed - lb mph per Reactor	2092.0	4530.9	4984.0
Total Feed - lb mph per Reactor	6903.6	15124.2	16636.6
Recycle/FF ratio	2.30	2.338	2.338
SV -FF Basis - Nm3/hxm3	582	418	401
SV -TF Basis - Nm3 /hxm3	1921	1394	1340
Prod - lb C5+/hrxlb cat	.062	.081	.078
C5+ HC - lb/hr	4281	16711	18382
Total HC - lb/hr	5544	19303	21234
MW of Inlet Gas	14.60	14.01	14.01
MW of Outlet Gas	16.38	17.04	17.04
Gas Viscosity - cp - Avg	0.0205	0.0201	0.0201
Gas Density - lb/cuft - Avg	.629	.401	.401
Gas Therm Cond - Btu/hrxftxF - Av	.060	.062	.062
Gas Sp. Ht. - Btu/lbxF - Avg	.556	578	.578
Gas Prandtl No.	.458	.456	.456
Mass Velocity - lb/hrxsqft	2852	2258	2484
Reynold's Number - basis tube ID	8623	5788	6367
Catalyst Diam - feet	.0122	.0122	.0122
Reynold's Number - basis part diam	701	566	623
f	1.08	1.11	1.10
Press Drop - psi/ft	.41	.42	.50
Press. Drop - psi	15.0	17.3	23.7
Heat Release - MM Btu/hr	26.5	94.7	104.2
Heat Flux - Btu/hrxsqft	713	633	613
d/D	.081	.098	.098
Int Heat Trans Coef-Btu/hrxsqftxF	65	63	68
Film Temp Diff - F	11	10	9
Wall Resistance - k/t	938	953	953
Steam Side h - Btu/hrxsqftxF	250	250	250
Overall U	49.1	47.7	50.6
Overall Delta T - F	15	13	12
Gas Res. Time - sec	10.11	8.85	9.21
Tube area/tube volume	26.67	35.86	35.86
Heat Release/Unit Volume	19013	22682	21986

Table 4.12

FIXED-BED FISCHER TROPSCH LOW PRESSURE DESIGN

DIMENSIONS	11 Reactors
Diameter, m	4.8
Straight Length of Bed, m	12.65
Xsect, m2	18.10
Tube OD, mm	38.1
Tube ID, mm	34.04
Tube Length, m	13.56
No. of tubes	9602
Tube Area (OD), m2/tube	1.623
Tube Xsect (OD), m2/tube	0.001140
Tube Area (ID), m2/tube	1.450
Tube Xsect (ID), m2/tube	0.000910
Net Xsect of Reactor, m2	8.74
Total Tube Area - m2 (ID)	13926
Total Tube Area - m2 (OD)	15589
Reaction Volume, m3	113.40
CONDITIONS - PER REACTOR	
Feed Gas Temp., oC	200
Operating Temp, oC	225
Operating Pressure, atm	14.15
Catalyst Loading, kg/m3	850
Catalyst Weight, kg	96387.5
FF - kgmph	2055.2
TF - kgmph	6860.3
TF - m3/h	19823.1
TF - Nm3/h	153766
R/FF Ratio	2.338
MW of TF	14.01
MW of Effluent	17.04
Syngas in TF - %	75.45
Syngas Conversion/Pass - %	36.89
'-CH2-Production, MTPD	214.3
Heat Duty, MW	27.8
Inlet Superficial Velocity, m/s	0.630
GHSV, Nm3/h kgCat	1.60
Mass Velocity, kg/h m2	11001
Space Velocity, Nm3/h m3	1356
STY - kg -CH2-/(h kgCat)	.093
STY - kg -CH2-/(h m3)	79
Heat Flux, kW/m2 (ID)	2.00

4.6 Baffled Slurry Reactors

The backmixing effects in a slurry reactor cause a decrease in the conversion level achievable with a given GHSV. One way of cutting down on backmixing would be to install baffles or trays. This has been done in gas/solid fluidized beds such as the fluid-bed MTG reactor, piloted by Mobil and UDHE in 1986. Extensive cold-model tests were run to check out the principle (Krambeck, F. J., Avidan, A. A., Lee, C. K. and Lo, M. N., "Predicting Fluid-Bed Reactor Efficiency using Adsorbing Gas Tracers", AIChE Journal, 33 , No.10, 1727-1734, 1987). Horizontal baffles were found to be particularly effective in improving fluid-bed reactor performance. The extension to slurry reactors would require piloting on a substantial scale plus similar cold-flow model testing. There are questions as to the extent of erosion of the baffles and whether salting out of the solids in inactive zones can be tolerated.

Preliminary reactor designs have been prepared to study the effect of backmixing using the simplified models described elsewhere in this report (Model 1 - plug flow vs Model 2, liquid phase fully backmixed, gas phase plug flow). These results give an indication of the maximum benefits to be achieved by baffling. These benefits should be balanced against the cost of reactor development and the cost of baffle installation and maintenance. It should also be understood that these are the maximum benefits to be expected and may be reduced somewhat when tested against more sophisticated reactor models.

Two cases are considered: (1) where conversion is kept constant and the size of the reactor is reduced and (2) where reactor size is kept roughly constant and conversion per pass is increased.

4.6.1 80% Conversion per Pass

Table 4.13 shows that in a plug flow reactor, 80% conversion should be achievable with an 8.7 meter bed height and a GHSV of 3.34, (Model 1). This compares with 12 meters and a GHSV of 2.42 for a liquid backmixed reactor, Table 4.5 - Model 2. Table 4.14 shows how this translates into a slurry reactor design. Because of the shorter bed length, more tubes are required and these take up more of the volume and more of the cross sectional area. The right hand column shows the maximum capacity case. The middle column, the design case, shows a 6 reactor design at a superficial velocity of 0.146 m/s, meeting the design GHSV requirement with a bed length of 9.01 meters. The number of cooling tubes increases to 3407.

The left hand column of Table 4.14 shows an alternate design with an external cooling loop. In this case the number of reactors can be decreased to 5 and the required height decreases to 8.54 meters.

4.6.2 95.5% Conversion Once-Through

Table 4.5 shows that the design slurry reactor should be capable of 95.5% conversion per pass if it were baffled to achieve 100% plug flow, (Model 1). The way to take advantage of higher conversion per pass is to relax on the inerts level in the synthesis gas. If 95% oxygen were used instead of 99.5% oxygen to the gasifier, the main effect would be a 10 fold increase in nitrogen content of the synthesis gas from 0.37% up to 3.7%. (Gasifier oxygen requirement would be increased, but negligibly). With once-through operation, total inerts in the F-T reactor feed gas are approximately the same and total feed gas is actually down from 64229 mph to 52510 mph.

Table 4.15 shows that the bed height must be increased to 11.99 meters, but that a 5 reactor design is feasible. The number of cooling tubes increases to 2955 (versus 2481 in the base design). Superficial velocity in the 5 reactor design is 0.138 m/s. Again, an external circulation loop decreases the number of reactors, this time from 5 to 4. Superficial velocity is 0.141 m/s with 4 reactors and the required bed height is 12.26 meters.

Table 4.13

	A	B	C	D	E
1	CASE		DEVELOPMENTAL DESIGN - BAFFLED REACTOR		6/12/90
2	uGo - cm/s		15		
3	alpha		-0.5658		
4	l		2.2317		
5	U		2.5604		
6	alpha*		-0.623348182		
7	T - oC		257		
8	Wt % Slurry		35		
9	Vol % Solids		10.43659272		
10	dR - cm		480		
11	L - cm		873.6		
12	dp - micron		26		
13	rhoS - g/cm^3		3.1		
14	muL - poise		0.02474214		
15	rhoL - g/cm3		0.670865		
16	sigmaL - dyne/cm		16.5		
17	DA - cm2/s		0.00053911		
18	muSlurry - poise		0.046982128		
19	rhoSlurry - g/cm^3		0.924383927		
20	kLa Correction Factor		0.766055793		
21	REACTOR MODEL	MODEL 1	MODEL 2	MODEL 3	
22	epsilonG - Bukur's Model	0.241197971	0.246449548	0.24805185	
23	kLa - s^-1 (uncorr) for H	1.028450982	1.053109211	1.060643168	
24	kLa - s^-1 (corr) for H	0.787850832	0.806740411	0.812511843	
25	kH - (s*kgCat/m3)^-1		0.000507903	3.3e^9*exp(-130/RT)	
26	kH- s^-1		0.106883608	With pressure correction	
27	kH*epsilonL - s^-1	0.081103499	0.080542191	0.080370931	
28	He - (kPa cm^3)/mol		20064929.63		
29	RTL/(uGo*He) - s^-1		12.78997263		
30	kA - s^-1	0.073533737		0.073136514	
31	Stanton No. - target	0.940494479		0.935414013	
32	H2 Conversion	0.726161003		0.598797798	
33	Stanton No. - result	0.940496206		0.935415654	
34	Avarage uG - cm/s	11.60511644		12.20055361	
35	Stanton No. - reaction		1.03013242		
36	StantonM - target		10.31818778		
37	H2 Conversion		0.628823785		
38	n		0.61043005		
39	Y		0.628856383		
40	StantonM - result		10.31720848		
41	Average uG - cm/s		12.06017678		
42	Pressure - kPa		2600		
43	Reactor Xsect - m^2		18.09557368		
44	Reactor Vol. - m^3		158.0829317		
45	Feed Rate - m^3/h		9771.60979		
46	Feed Rate - Nm^3/h		129122.6672		
47	SV - Nm^3/(m^3 h)		816.8033435		
48	H2+CO Conversion	0.800019691	0.69278219	0.659702225	
49	CO Conversion	0.833114949	0.721441242	0.686992823	
50	STY - Nm^3/(h*m^3)	653.4587585	565.8668093	538.8469831	
51	STY - Nm^3/(kgCat h))	2.661762304	2.321033759	2.214915339	
52	GHSV - Nm^3/(kgCat h)	3.327120987	3.350308065	3.357447125	
53	Catalyst - kg	38809.12888	38540.53558	38458.58546	
54	Catalyst Loading kg/m^3	245.4985397	243.7994739	243.2810743	
55	Reaction Enthalpy - kJ/gmol -CH2-	214.6	214.6	214.6	
56	kgmol/h of H2+CO Conv (=3* -CH2-)	4608.756862	3990.982608	3800.415403	
57	Heat Release - kW	91577.70579	79302.30256	75515.66161	
58	Heat Release - kW/m^3	579.3016665	501.6499991	477.69649	
59	Heat Release - Btu/(h ft^3)	56010.64541	48502.77817	46186.79742	
60	Mass Transfer Resistance - %	9.33345928	9.077400021	9.001285911	
61	DL - cm2/s	31544.71453	31935.37053	32053.85093	

Table 4.14

SLURRY FISCHER-TROPSCH BAFFLED 80% CONVERSION

DIMENSIONS	5 Reactors	6 Reactors	Max Capacity
Cooling Tubes	External	Internal	Internal
Diameter, m	4.8	4.8	4.8
Straight Length of Bed, m	8.50	9.03	9.30
Xsect, m2	18.10	18.10	18.10
Head Vol, m3	28.95	28.95	28.95
Head Volume Effectiveness - %	15.00	15.00	15.00
Tube OD, mm	NA	38.1	38.1
Tube ID, mm	NA	34	34
Tube Length, m	NA	8.53	8.80
No. of tubes	NA	3401	3391
Tube Area (OD), m2/tube	NA	1.021	1.054
Tube Xsect (OD), m2/tube	NA	0.001140	0.001140
Tube Area (ID), m2/tube	NA	0.000908	0.000908
Net Xsect of Reactor, m2	18.10	14.22	14.23
Total Cooling Surface, m2 (OD)	NA	3471.3	3572.5
Reaction Volume, m3 (Effective)	158.07	132.71	136.70
Reaction Volume, m3 (Total)	182.68	157.32	161.31
CONDITIONS - PER REACTOR			
Feed Gas Temp., oC	149	149	149
Operating Temp, oC	257	257	257
Operating Pressure, atm	28.3	28.3	28.3
Slurry Concentration, wt%	35	35	35
Gas Holdup, %	23.0	23.8	24.1
Liquid Density, kg/m3	675	675	675
Particle Density, kg/m3	3000	3000	3000
Slurry Density, kg/m3	926.2	926.2	926.2
Catalyst Loading, kg/m3	249.6	247.0	246.1
Catalyst Weight, kg (Effective)	39457.0	32782.0	33636.6
Catalyst Weight, kg (Total)	45600.2	38861.4	39692.1
FF - kgmph	4608.4	3840.3	3952.3
TF - kgmph	5826.8	4855.7	4997.3
TF - m3/h	8959.4	7466.2	7683.9
TF - Nm3/h	130603	108836	112010
R/FF Ratio	0.2644	0.2644	0.2644
MW of TF	20.90	20.90	20.90
MW of Effluent	38.04	38.04	38.04
Syngas in TF - %	90.8	90.8	90.8
Syngas Conversion/Pass - %	80	80	80
'-CH2-Production, MTPD	474.9	395.8	407.3
Heat Duty, MW	78.8	65.6	67.6
Inlet Superficial Velocity, m/s	0.138	0.146	0.150
GHSV, Nm3/h kgCat	3.31	3.32	3.33
Mass Velocity, kg/h m2	121781	101485	104444
Space Velocity, Nm3/h m3	826	820	819
STY - kg -CH2-/(h kgCat)	.502	.503	.505
STY kg -CH2-/(h m3)	125	124	124
Heat Flux, kW/m2	NA	18.912	18.912

Table 4.15

SLURRY FISCHER-TROPSCH BAFFLED HIGH CONVERSION

DIMENSIONS	4 Reactors	5 Reactors	Max Capacity
Cooling Tubes	External	Internal	Internal
Diameter, m	4.8	4.8	4.8
Straight Length of Bed, m	12.42	12.10	13.30
Xsect, m2	18.10	18.10	18.10
Head Vol, m3	28.95	28.95	28.95
Head Volume Effectiveness - %	15.00	15.00	15.00
Tube OD, mm	NA	38.1	38.1
Tube ID, mm	NA	34	34
Tube Length, m	NA	11.60	12.80
No. of tubes	NA	2926	2893
Tube Area (OD), m2/tube	NA	1.389	1.532
Tube Xsect (OD), m2/tube	NA	0.001140	0.001140
Tube Area (ID), m2/tube	NA	0.000908	0.000908
Net Xsect of Reactor, m2	18.10	14.76	14.80
Total Cooling Surface, m2 (OD)	NA	4063.6	4433.0
Reaction Volume, m3 (Effective)	229.09	182.95	201.19
Reaction Volume, m3 (Total)	253.70	207.56	225.80
CONDITIONS - PER REACTOR			
Feed Gas Temp., oC	149	149	149
Operating Temp, oC	257	257	257
Operating Pressure, atm	28.3	28.3	28.3
Slurry Concentration, wt%	35	35	35
Gas Holdup, %	23.3	23.0	24.1
Liquid Density, kg/m3	675	675	675
Particle Density, kg/m3	3000	3000	3000
Slurry Density, kg/m3	926.2	926.2	926.2
Catalyst Loading, kg/m3	248.7	249.6	246.1
Catalyst Weight, kg (Effective)	56963.6	45669.0	49503.1
Catalyst Weight, kg (Total)	63082.9	51812.3	55558.5
FF - kgmph	5954.6	4763.7	5196.8
TF - kgmph	5954.6	4763.7	5196.8
TF - m3/h	9155.8	7324.8	7990.6
TF - Nm3/h	133466	106774	116481
R/FF Ratio	0	0	0
MW of TF	20.90	20.90	20.90
MW of Effluent	38.04	38.04	38.04
Syngas in TF - %	90.8	90.8	90.8
Syngas Conversion/Pass - %	95.5	95.5	95.5
-CH2-Production, MTPD	579.4	463.5	505.6
Heat Duty, MW	96.1	76.9	83.8
Inlet Superficial Velocity, m/s	0.141	0.138	0.150
GHSV, Nm3/h kgCat	2.343	2.338	2.353
Mass Velocity, kg/h m2	124450	99562	108613
Space Velocity, Nm3/h m3	583	584	579
STY - kg -CH2-/(h kgCat)	.424	.423	.426
STY - kg -CH2-/(h m3)	105	106	105
Heat Flux, kW/m2	NA	18.912	18.912

4.7 Superficial Velocity and Catalyst Concentration

As discussed above, Bechtel has chosen to design the slurry reactors in all cases for 35wt% slurry concentration and up to 0.15 m/s superficial inlet velocity. This represents current liquid phase methanol design practice, although it is understood that Air Products is designing the reactor for the Great Plains Clean Coal 3 Demonstration Project for a superficial velocity of 0.25 m/s (personal communication). On the other hand, Bechtel's design conditions are well beyond anything that has been demonstrated to date in Fischer-Tropsch pilot plant operations . For this reason an alternative design has been prepared for more conventional Fischer-Tropsch design conditions of 0.7 m/s and 20 wt% slurry.

The results of this effort are shown in Tables 4.16 and 4.17. Basically, as superficial velocity is decreased with no change in other conditions, the reactor capacity decreases but the reactor can become shorter. Mass transfer becomes more limiting but the decrease in GHSV is slight since surface kinetics predominate. Decreasing the slurry concentration, as well, decreases the rate of reaction since the amount of surface is reduced. This brings the relative contribution of mass transfer back to the original level, the allowable GHSV is reduced and the reactor stays about the same in height. Halving the superficial velocity and halving the slurry concentration would double the number of untubed reactors for the same capacity without changing their dimensions. This can be seen by comparing the first columns of Figure 4.6 and Figure 4.17. The number of reactors has increased from 5 to 10. The bed length is slightly shortened since the slurry concentration has not quite been halved, decreasing from 35 wt% to 20 wt%.

Because the heat removal requirement has not been changed, the number of internal tubes required per reactor is reduced and the space available for reaction is increased. As shown in the middle columns of Figures 4.6 and 4.17, the number of reactors of the internal tube design increases from 6 to 11 and the reactors can be about one meter shorter in height.

Air Products uses the higher superficial velocity in the Great Plains once-through methanol design to reduce the diameter of the reactor, increasing the height. This is beneficial from a cost standpoint since the wall thickness of the shell and heads is reduced.

Table 4.16

	A	B	C	D	E
1	CASE	ALTERNATIVE DESIGN - LOW VELOCITY LOW CONCENTRATION			5/25/90
2	uGo - cm/s		7.5		
3	alpha		-0.5658		
4	I		2.2317		
5	U		2.5604		
6	alpha*		-0.623348182		
7	T - oC		257		
8	Wt.% Slurry		20		
9	Vol.% Solids		5.132521834		
10	dR - cm		480		
11	L - cm		1123		
12	dp - micron		26		
13	rhoS - g/cm^3		3.1		
14	muL - poise		0.02474214		
15	rhoL - g/cm3		0.670865		
16	sigmaL - dyne/cm		16.5		
17	DA - cm2/s		0.00053911		
18	muSlurry - poise		0.029706009		
19	rhoSlurry - g/cm^3		0.795540884		
20	kLa Correction Factor		0.808602596		
21	REACTOR MODEL	MODEL 1	MODEL 2	MODEL 3	
22	epsilonG - Bukur's Model	0.154595362	0.160202376	0.160967831	
23	kLa - s^-1 (uncorr) for H	0.630505221	0.6557049	0.659152012	
24	kLa - s^-1 (corr) for H	0.509828159	0.530204685	0.532992028	
25	kH - (s*kgCat/m3)^-1		0.000507903	3.3e^9*exp(-130/RT)	
26	kH- s^-1		0.052563367	With pressure correction	
27	kH*epsilonL - s^-1	0.044437314	0.044142591	0.044102356	
28	He - (kPa cm^3)/mol		20064929.63		
29	RTL/(uGo*He) - s^-1		32.88264484		
30	kA - s^-1	0.040874626		0.040731992	
31	Stanton No. - target	1.344065819		1.339375638	
32	H2 Conversion	0.879178047		0.704955101	
33	Stanton No. - result	1.344064032		1.339372189	
34	Average uG - cm/s	5.44487236		5.852128198	
35	Stanton No. - reaction		1.45152513		
36	StantonM - target		17.43453233		
37	H2 Conversion		0.726174448		
38	n		0.500283759		
39	Y		0.726174449		
40	StantonM - result		17.43279639		
41	Average uG - cm/s		6.802526792		
42	Pressure - kPa		2600		
43	Reactor Xsect - m^2		18.09557368		
44	Reactor Vol. - m^3		203.2132925		
45	Feed Rate - m^3/h		4885.804895		
46	Feed Rate - Nm^3/h		64561.33359		
47	SV - Nm^3/(m^3 h)		317.7023156		
48	H2+CO Conversion	0.968600278	0.800034603	0.776656912	
49	CO Conversion	1.008669387	0.833130374	0.808785697	
50	STY - Nm^3/(h*m^3)	307.7265513	254.1728143	246.7456993	
51	STY - Nm^3/(kgCat h))	2.287746207	1.902225313	1.848325605	
52	GHSV - Nm^3/(kgCat h)	2.361909509	2.377679094	2.379848267	
53	Catalyst - kg	27334.38066	27153.08965	27128.34028	
54	Catalyst Loading kg/m^3	134.5107907	133.6186689	133.4986788	
55	Reaction Enthalpy - kJ/gmol -CH2-	214.6	214.6	214.6	
56	kgmol/h of H2+CO Conv (=3* -CH2-)	2789.958315	2304.421096	2237.084231	
57	Heat Release - kW	55437.50504	45789.70068	44451.69223	
58	Heat Release - kW/m^3	272.8045216	225.3282751	218.7440186	
59	Heat Release - Btu/(h ft^3)	26376.51195	21786.20026	21149.5916	
60	Mass Transfer Resistance - %	8.017333992	7.685696884	7.642139131	
61	DL - cm2/s	24760.23863	25269.47681	25338.39994	

Table 4.17

SLURRY FISCHER-TROPSCH ALTERNATIVE DESIGN

DIMENSIONS	10 Reactors	11 Reactors	Max Capacity
Cooling Tube Design	External	Internal	Internal
Diameter, m	4.8	4.8	4.8
Straight Length of Bed, m	10.97	10.95	12.07
Xsect, m2	18.10	18.10	18.10
Head Vol, m3	28.95	28.95	28.95
Head Volume Effectiveness - %	15.00	15.00	15.00
Tube OD, mm	NA	38.1	38.1
Tube ID, mm	NA	34	34
Tube Length, m	NA	10.95	12.07
No. of tubes	NA	1444	1431
Tube Area (OD), m2/tube	NA	1.311	1.445
Tube Xsect (OD), m2/tube	NA	0.001140	0.001140
Tube Area (ID), m2/tube	NA	0.000908	0.000908
Net Xsect of Reactor, m2	18.10	16.45	16.46
Total Cooling Surface, m2 (OD)	NA	1893.4	2066.8
Reaction Volume, m3 (Effective)	202.93	184.48	203.06
Reaction Volume, m3 (Total)	227.54	209.09	227.67
CONDITIONS - PER REACTOR			
Feed Gas Temp., oC	149	149	149
Operating Temp, oC	257	257	257
Operating Pressure, atm	28.3	28.3	28.3
Slurry Concentration, wt%	20	20	20
Gas Holdup, %	15.3	15.3	16
Liquid Density, kg/m3	675	675	675
Particle Density, kg/m3	3000	3000	3000
Slurry Density, kg/m3	798.8	798.8	798.8
Catalyst Loading, kg/m3	135.3	135.3	134.2
Catalyst Weight, kg (Effective)	27460.6	24963.7	27250.4
Catalyst Weight, kg (Total)	30790.8	28293.9	30553.0
FF - kgmph	2304.2	2094.7	2286.5
TF - kgmph	2913.4	2648.5	2891.1
TF - m3/h	4479.7	4072.4	4445.4
TF - Nm3/h	65301	59364	64801
R/FF Ratio	0.2644	0.2644	0.2644
MW of TF	20.90	20.90	20.90
MW of Effluent	38.04	38.04	38.04
Syngas in TF - %	90.8	90.8	90.8
Syngas Conversion/Pass - %	80	80	80
-CH2-Production, MTPD	237.5	215.9	235.6
Heat Duty, MW	39.4	35.8	39.1
Inlet Superficial Velocity, m/s	0.069	0.069	0.075
GHSV, Nm3/h kgCat	2.378	2.378	2.378
Mass Velocity, kg/h m2	60890	55354	60424
Space Velocity, Nm3/h m3	322	322	319
STY - kg -CH2-/(h kgCat)	.360	.360	.360
STY - kg -CH2-/(h m3)	49	49	48
Heat Flux, kW/m2	NA	18.912	18.912