Report 9

IMPACT OF DEVELOPING TECHNOLOGY ON INDIRECT LIQUEFACTION

D. Gray
The MITRE Corporation

### SYNOPSIS

The status of commercial technology for indirect liquefaction, as exemplified by SASOL facilities in South Africa, is reviewed. The impact of substituting more advanced gasifiers and synthesis systems is then investigated.

Slagging/BGC/Lurgi, Westinghouse, and Shell gasifiers were substituted for the dry ash Lurgi units used at SASOL. SASOL Synthol synthesis units were replaced by slurry phase Fischer-Tropsch units employing technology pioneered by Kolbel.

The advanced systems were found to have a highly favorable impact on plant efficiency, product distribution and gasoline cost. If all the projected technical improvements can be realized for indirect liquefaction, the yields of refined transportation fuels per ton of coal will approach those anticipated for direct liquefaction processes.

# INTRODUCTION

The analysis described in this paper was undertaken at the request of DOE to assist in their coal liquefaction R&D planning. Conversion of coal to liquid fuels via Fischer-Tropsch remains an important option representing the only modern commercially demonstrated technology. The basic SASOL process is over 25 years cld. While significant improvements have been made by SASOL during SASOL I operation and incorporated in SASOL II and III, many of the limitations of the technology still persist in these latest plants. Progress has been made in the development of coal gasifiers,

advanced synthesis processes and improved product upgrading
methods. While these improved versions are in the pilot-plant stage
and have not been integrated into operating Fischer-Tropsch units,
the effect of such integration into hybrid Fischer-Tropsch processes
can be evaluated by analysis.

This paper first investigates the potential of a full-scale U.S. plant employing proven commercial technology as implemented in South Africa. These findings are then used as a basis for evaluating the potential of more advanced technology gasifiers and synthesis systems to improve technical and economic performance of indirect coal conversion processes. The gasifiers were selected on the basis of their advanced stage of development; all have had successful large pilot plant operation.

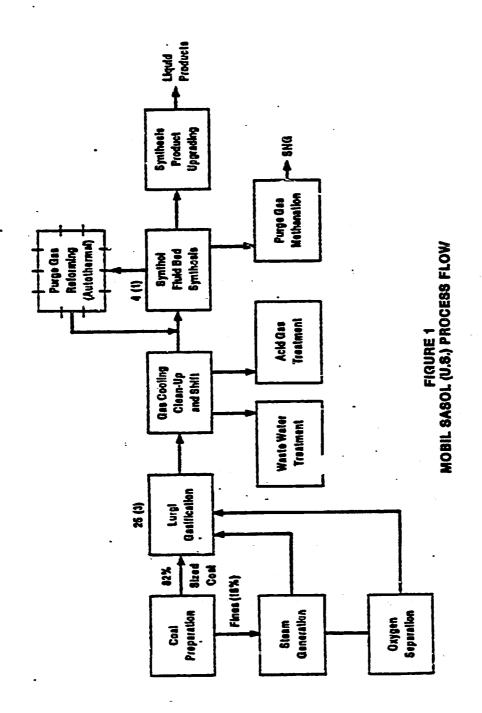
### SASOL TECHNOLOGY

SASOL II employs dry ash Lurgi gasifiers of German design, and fast fluid (entrained recirculating) bed Synthol Fischer-Tropsch synthesis reactors developed by SASOL and Kellogg U.S. The Lurgi gasifiers at SASOL II have been considerably improved because of the extensive operating experience at SASOL I. The Synthol reactors, initially developed by Kellogg, have been redesigned and greatly improved by SASOL because of extensive problems with the original design. The combination of Lurgi dry ash gasifiers with Synthol synthesis reactors is capable of delivering clean fuels and petrochemicals with an efficiency approaching 60 percent. However, 19

methane. When the H<sub>2</sub> and CO in the synthesis gas are reacted in the Synthol units, about 25 percent of the output is methane. Additional light gases are formed when the synthesized liquids are upgraded to specification fuels. When operating at peak efficiency the dry ash Lurgi/Synthol combination yields over 50 percent of its thermal output as Synthetic Natural Gas. At SASOL II, these gases are reformed by partial oxidation to yield additional CO and H<sub>2</sub>, which is then synthesized to yield an all-liquid output. As a result, the overall thermal efficiency of the SASOL II plant is less than 40 percent.

The output of the Synthol reactor in the gasoline boiling range  $(C_5 - 180^{\circ}\text{C})$  has a low octane number and requires substantial refining to meet U.S. fuel standards.

In a study conducted for the U.S. Department of Energy in 1978, Mobil Research and Development Corporation (MRDC), with the assistance of Lurgi, prepared a preliminary design of a U.S. plant employing SASOL technology. This design has been used as the Base Case for the present study. The flow chart for the SASOL (U.S.) Base Case is shown in Figure 1. The flow chart shows two alternative processing modes; one in which light ends from the Synthol unit are methanated to produce SNG, and one in which they are autothermally reformed to produce additional synthesis gas for recycle to the Synthol reactor. The two modes of operation are further



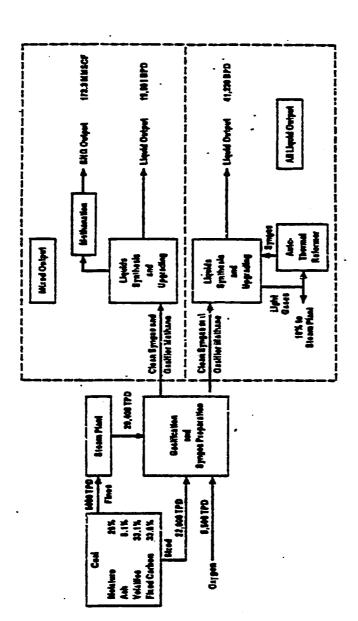
described in Figure 2. When operated in the all-liquid mode, about 10 percent of the recycle stream must be purged to prevent buildup of inert products (principally methane) in the Synthol reactor.

These gases are burned in the boiler to generate the additional steam required to produce oxygen for the autothermal reformer. Only about 61 percent of the energy in the SNG produced in the mixed product case is recovered as liquid output in the all-liquid case. The Base Case plant includes a sophisticated upgrading system, incorporating virtually every process used in a modern petroleum refinery, to maximize the yield of specification motor fuels from the Synthol products.

Table 1 shows pertinent data for the Base Case plant when operated to produce liquid fuels and SNG as coproducts, and when operated to produce an all-liquid output. In the mixed product mode, the daily plant output is 4.91 M Nm<sup>3</sup> for SNG and 19,591 barrels\* of liquid fuels from 25.22 metric tons of coal. Thermal efficiency (HHV) is 57 percent. Operation in the all-liquid mode more than doubles the liquid yield to 41,320 B/Day, but efficiency is reduced to 44 percent.

Economic assessments are based on a 20-year plant life and 100 percent equity financing with a 12-percent Discounted Cash Flow (DCF). The required selling price (i.e., cost) for gasoline

<sup>\*1</sup> barrel is equivalent to 42 U.S. gallons = 159 litres.



BASELINE PLANT INPUT/OUTPUT FOR MIXED PRODUCT AND ALL-LIQUID CASES

TABLE 1 SUPPARY DATA FOR BASE CASE PLANTES

White a second

All-Liquid Output	28,090 41,320 33,652			43 2.14	1, 181 2, 199 0.40 0.51
			1,051 189 862 771 208		
Mixed Output	, 4,91 13,580 19,591 44,950			57 1.01	1,186 1,887 0,35 0.46
Output	BNG (HRM <sup>3</sup> /D) Gasoline (Bb1/D) Total Liquid Fuels (Bb1/D) Total FOR <sup>A</sup>	Input (Ma/hr)	Total Plant Coal (de received) Coal to Steam (de received) Coal to Gasifier (de received) Steam to Gasifier Oxygen to Gasifier	. Efficiency (BMV) X Liquid Yield (Bbis $G_4^{+}/\mathrm{tonne}$ dry coal)	Plant Construction Gost (M 1977 \$) Copital Cost (M 1977 \$) Gasoline Cost (1977 \$/Litre)** Gasoline Cost (1980 \$/Litre)

Prices of Puels Other than Casoline

SHO + CJ

G - Gasoline Price

Diesel G = 9. Fuel Oil G = 5. Alcohols

> \*POE = Fuel Oil Equivalent assuming 6.33 GJ/Bbl. \*\* Prices for Products other than Gasoline Shown in Inset.

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reported in Table 1 has been computed under the assumption that the products other than gasoline are priced in accordance with the schedule indicated in this table.

The data show that the mixed output plant produces cheaper gasoline than the all-liquid (0.46 \$/litre versus 0.53 \$/litre). However, the cost of gasoline from the mixed output plant is profoundly affected by the price of SNG. MRDC derived a price of \$5.85 per GJ (1977\$) from a design study which showed that SNG could be produced for this cost from a single product SNG plant using dry ash Lurgi technology. The cost of gasoline from the mixed output plant would be greater than the allliquid plant cost of 0.53\$/litre if the SNG price fell below \$5.12/GJ. We therefore believe that the all-liquid gasoline costs are more realistic.

The coal used in the postulated SASOL-U.S. plant is a 28-percent moisture Wyoming subbituminous having an assumed cost of \$7.72/MT and a higher heating value of 19,792 kJ/kg. The coal cost is thus 39¢ per GJ. At this price, coal accounts for only 9 percent of the product cost. Coal costs could more than double without raising the product cost by more than 10 percent.

Capital charges account for 65 percent of the product cost.

The remaining 26 percent of cost is dominated by maintenance costs and other factors which are proportioned to plant construction cost.

Thus, the gasoline price is approximately linearly related to plant construction cost; e.g., a 10-percent increase in construction cost

would result in an increase in the gasoline selling price of almost 10 percent.

The estimates of construction cost given in Table 1 are from the MRDC report. An independent verification of these estimates is beyond the scope of this study. In using the estimations, which are highly detailed in Reference 1, we have formed the judgment that the costs determined by MRDC are soundly derived, and provide a sound basis for estimating the incremental costs associated with the modified plants considered in this study. While we caution against the use of any absolute cost data, we feel the comparative ranking of the processes is valid.

# ADVANCED GASIFIERS

The dry ash Lurgi gasifiers are the only large-scale pressurized gasifiers which have extensive commercial experience. Their
major disadvantages in an indirect liquefaction complex are the
relatively high quantities of methane which they produce, and a high
process steam requirement which results in a low overall thermal
efficiency. Other disadvantages include inability to process coal
fines and reduced efficiency when modified to process highly caking
coals.

There are alternative gasifiers now in late stages of development which circumvent some of the limitations of the dry ash Lurgi. The impact on plant output and product cost resulting when these advanced gasifiers are substituted for the dry ash Lurgi has been evaluated in this study. Gasifiers considered include a slagging modification of the dry ash Lurgi design developed by the British Gas Corporation (BGC) and Lurgi, an agglomerating—ash fluidized bed gasifier developed by Westinghouse, and an entrained flow gasifier under development by Shell (Koppers).

The performance predicted for the Westinghouse unit was specifically generated by Westinghouse for the assumed coal. Performance for the BGC/Lurgi and Shell gasifiers with the assumed coal was generated by making minor thermochemical adjustments to published data from tests with similar coals. The Westinghouse projections are somewhat more conservative, relative to theory, than are the other two units.

Outputs of the dry ash Lurgi are compared with the outputs of the three advanced gasifiers in Table 2. The higher efficiencies of the advanced systems are evident. It is also evident that the advanced systems produce a synthesis gas having an H<sub>2</sub>/CO ratio of about 0.5, as compared to 2.1 for the dry ash Lurgi. Conventional Pischer-Tropsch synthesis reactors, such as the Synthol reactor, require an H<sub>2</sub>/CO ratio of about 2.5. The output of the advanced gasifier must thus undergo considerable external water-gas shift as part of the gas preparation step. Our analysis reveals that this penalty is small compared to the efficiency gains of the advanced gasification systems.

TABLE 2 CASIFIER PERFORMANCE COMPARISONS

	Dry-Ash Lurat	BGC Lural	West inghouse?	Shelf
Ossifler Pressure (MPs)	2.40	2.40	2.76	87.4
Exit das Temparature (°C)	.540	<b>6</b>	086	1675
Inpute Malix	•			
Coal (DAP)	577	628	703	703
Oxygen	208	262	263 559	21 282 287
Total Plant Coal (DAF)	703	, <b>60</b> 2	703	703
Raw Gas Composition (Hol X)				
#25	23.0	21.9	24.9	30.9
<b>1</b> 15	11.1	63.6	32.7	4.4
02	0	0.3	-	• •
H20	9.6	2.1	16.6	2.4
Misc.	0.0	0.3	20.0 0.0	4.0
n2/CU Retio	2.07	0.5	0.76	0.48
Freegettes 01/hr LAV				•
Total Plant Coal	20,003	20,003	20,003	20,003
Outputs		•		
CO + H2	7,583	11,689	12,057	16,609
Maphtha	131	3,236 360	2,656	<b>-</b>
Tare + Oile + Phenole	1,736	1,990	0	
Total Output	13,035	15,285	14,743	16,609
		· •		

Mat included in totals - used for steam generation.

Additional comparisons of gasifier output are shown in Figure 3. The bars show the composition and energy content of each stream as a percent of total coal input including coal used for steam production. Note that tars, oils and phenols, as well as coal, are used for steam production for the dry ash and BGC Lurgi gasifiers. When the Westinghouse or Shell gasifiers are used, most plant steam requirements are met by waste heat boilers which capture the high sensible heat of the product gas. Very efficient waste heat recovery systems are assumed. Achieving the required high efficiency of heat recovery from exit gases containing molten slag is one of the major developmental challenges of high temperature entrained flow gasifiers.

Figure 4 is a graphical presentation of the impact of the advanced gasifiers on piant construction cost. Steam plant costs for the Westinghouse and Shell systems are reduced because the waste heat recovery system serves as the main steam boiler, and is charged to the gasifier. Flue gas desulfurization systems are also eliminated. The potential saving is largely absorbed by the requirement for substantially larger oxygen plants. On balance, all of the all-liquid plants fall within a construction cost range of 5 percent.

The plants are similar to the SASOL-U.S. Base Case except for minimal changes in process flows and equipment size required to accommodate the advanced gasification systems. Plants fully optimized to take advantage of the advanced gasification system

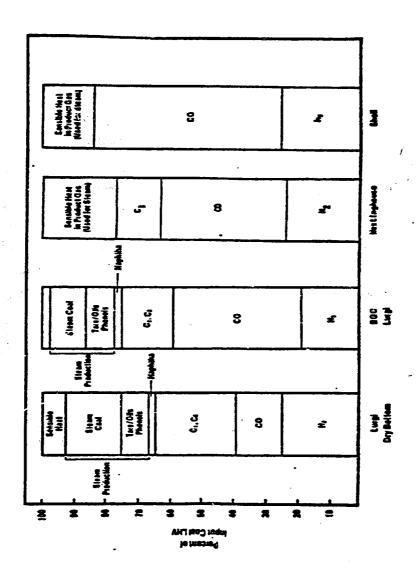


FIGURE 3 GASIFIER OUTPUT COMPARISONS

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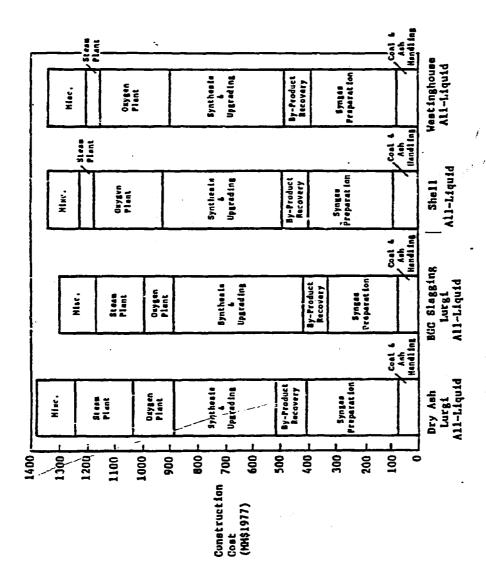


FIGURE 4
PLANT CONSTRUCTION COST COMPARISONS

would be expected to offer slightly higher technical and economic performance. Table 3 shows partinent data for indirect liquefaction plants employing the advanced gasification systems to produce an all-liquid product output.

This table shows that the reduction in gasoline cost resulting from the use of advanced gasifiers is quite substantial, amounting to about 18 percent in the case of Westinghouse and BGC gasification, and about 23 percent for Shell.

All cost estimates produced in this report are in October 1977\$ in order to maintain consistency with baseline data from Reference 1. August 1980 product prices shown in Tables 3 and 5 are approximations which were calculated by applying Nelson Refinery cost indices to the computed 1977\$ results. Capital costs are escalated by 1.26. Operating costs, including coal, were escalated by 1.38. This results in an adjusted 1980 coal price of \$10.67/MT, which is believed to be reasonable for the coal assumed.

In arriving at the capital costs for plants using Kolbel reactors, MITRE assumed that the construction cost of the slurry reactor system would be 20 percent higher than the Synthol reactor system for equal syngas throughput. Because of lower catalyst costs, lower catalyst preparation plant costs, and lower throughput resulting from less reformed methane, the costs for Slurry Phase and Synthol systems were approximately equal.

TABLE 3

(All-Liquid Output)  Base Case BGC Lurgi Westinghor	All-Liquid Output Base Case	) BGC Lurgi	Westinghouse	Shell.
Outpute (Bk1/B)  Gaeoline  Diesel  Ga + G <sub>k</sub> Fuel Oil  Alcoholm  Total Liquids	28,090 5,078 2,757 1,369 4,026 41,320 33,652	31,514 9,706 9,706 1,538 4,538 46,381	30,805 3,886 3,192 1,584 4,672 46,138	34,455 6,579 3,574 1,774 5,204 51,586 41,996
Efficiency (HNV) & Liquid Yield (Bble C4/tonne dry coal) Economics  Plent Construction Coat (M 1977 8) Capital Cost (H 1977 8) Gasoline Cost (H 1977 8) Gasoline Cost (H 1977 8)	43.0 2, 14 2, 14 1, 383 2, 199 0, 40 0, 53	48.0 2.40 1,289 2,050 0.33 0.44	47.6 2.38 1.305 2,076 0.34 0.45	53.0 2.67 1,347 2,142 0,31 0.41

A bbl m 42 U.S. Gallons w 159 Libres.
Ad For - Fuel Oil Equivalent assuming 6.33 QJ/Bbl.

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Subsequent work by UOP/SDC<sup>5</sup> has shown Slurry Phase reactor systems to have substantially lower construction costs than the Synthol reactor system.

## ADVANCED SYNTHESIS

One purpose of this study is to analyze the combination of Kolbel synthesis with advanced gasifiers to determine if this coupling has significant economic and technical impact on the indirect lique-faction process. Although no commercial Kolbel synthesis units are in operation, there are sufficient data from the operation of a demonstration Kolbel plant at Rheinpreussen, Germany from 1938-1953 to analyze the system in some detail. There are also data confirming the experience of the Rheinpreussen work from other investigators using bench scale equipment.

The second generation advanced gasifiers discussed in this report all produce a synthesis gas with a  $\rm H_2/CO$  molar ratio very much lower than that produced by the dry ash Lurgi gasifier. The conventional Synthol reactor requires a gas having a  $\rm H_2/CO$  ratio of 2.5. The gas from the advanced gasifiers will therefore require considerable water—gas shift to make it compatible with Synthol operation requirements. The Kolbel reactor, using a three—phase liquid slurry process, can synthesize liquid hydrocarbons from a gas having a low  $\rm H_2/CO$  ratio. This means that little or no external water—gas shift will be required for synthesis gases produced from advanced gasifiers if they are coupled to a Kolbel synthesis unit.

The most significant advantage of the Kolbel reactor is the product distribution. Product selectivities (Table 4) show that the Kolbel unit produces much higher fractions in the gasoline/diesel range, and substantially lower fractions in the  $C_1$ ,  $C_2$  range than does the Synthol unit. Both units produce relatively high conceptrations of  $C_3$ . These are of lesser consequence since 80 percent are unsaturated and can be combined by polymerization and alkylation to yield products for gasoline blending.

TABLE 4

PRODUCT SELECTIVITY FOR SYNTROL AND KOLBEL
FISCHER-TROPSCH SYNTHESIS REACTORS

PRODUCT WI Z OF TOTAL HYDROCARBONS	KOLBEL	SYNTHOL
c <sub>1</sub> + c <sub>2</sub>	6.8	22.8
C <sub>3</sub>	22.6	. 15.3
C4	5.1	10.6
C <sub>5</sub> - 320°C	63.6	46.6
320°C	1.9	4.6

An additional advantage of the Kolbel unit is a conversion per pass of about 90 percent compared with about 50 percent for Synthol. With Synthol, a recycle to fresh feed ratio of 2:1 is required to achieve the 85 percent conversion assumed in the Rase Case. With the Kolbel unit, an overall conversion approaching 99 percent can be

achieved by recycling only the purge gases which remain after hydrocarbon recovery.

The impact of Kolbel synthesis on the overall process scheme is shown in Figure 5. The upper bars show the composition and energy content of streams at several points in a plant employing Shell gasification and Synthol synthesis. Note that the Synthol output contains 15 percent H<sub>2</sub> and CO, and about 20 percent C<sub>1</sub> and C<sub>2</sub>. SNG produced from these constituents make up about 40 percent of the refined output in the mixed product case. High losses incurred when these products are further processed to yield an all-liquid product reduce the overall plant efficiency from 59.8 percent to 51.5 percent when the plant is operated in the all-liquid mode.

The lower bars in Figure 5 show similar data for a plant employing Kolbel synthesis. The Kolbel output contains less energy because of the higher synthesis gas conversion (98 percent versus 85 percent). However, the Kolbel output is far more suitable for the production of liquid fuels. The resulting refined output of the mixed product plant has an energy content comparable to the corresponding Synthol plant output, and is primarily liquid. Additional losses in the Kolbel case to produce an all-liquid product are small. The overall efficiency of the all-liquid Kolbel plant is thus higher (58.7 percent), and the yield of liquid fuels is 14 percent greater than the yield of the Synthol plant.

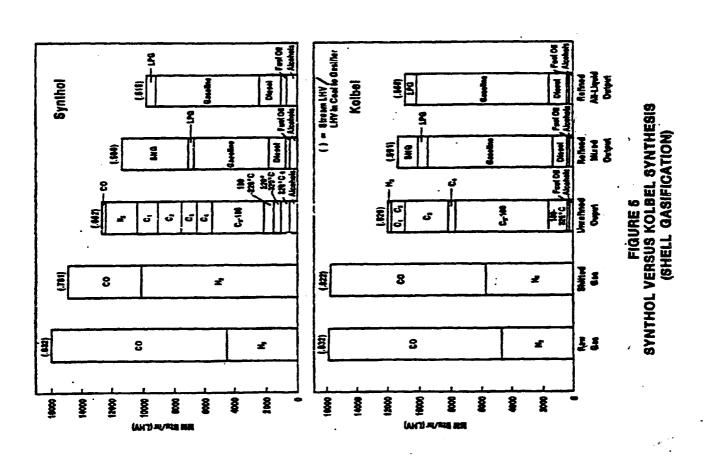


Table 5 summarizes the results of the analyses for the combination of Kolbel synthesis reactor and advanced gasifiers in plants producing an all-liquid output. The most significant features of the analyses are the higher gasoline yields obtained using the Kolbel reactor, the higher overall thermal efficiencies of the plant and the lower capital cost and hence, gasoline costs. The lo-percent increase in thermal efficiency from the SASOL-U.S. Base Case to the Shell/Kolbel plant is highly significant and demonstrates the efficiency advantages obtained by both gasifier and synthesis substitution. A comparison of the Shell/Synthol plant, with an overall efficiency of 53 percent, shows that the further increase attributable to the Kolbel synthesis unit is 5.6 percentage points, which equates to an output increase of 11 percent. As noted in the discussion of Figure 5, this thermal efficiency increase originates from the lower selectivity to lighter gases and the higher selectivity to gasoline boiling range hydrocarbons obtainable with Kolbel synthesis.

The 57-percent increase in the yield of gasoline for the Shell/Kolbel case over the Base Case is a considerable process advantage. The increase in product output, combined with an overall decrease in capital cost for the Shell/Kolbel case, accounts for the low cost of gasoline (32 cents/litre).

TABLE 5

SUMPLARY DATA FOR PLANTS USING KOLBKL SYNTHESIS AND ADVANCED GASIFIERS (A11-Liguid Output)

	Base Case	BGG Lurai	West Inghouse	Blell
Outputs (6b1/v)				
enitosep	28,090	39,945	38,848	44,166
	5.078	5,025	5,093	5,792
- C	2,757	4,055	4,112	4,675
10 January	1,369	523	531	909
Atcolota	4.026	613	823	916
Total Monida	41,320	50,361	49,407	56,178
Total FUSA	33,652	41,506	40,700	46,272
M (ARI) Sura July M	43.0	52.5	51.6	58.7
Liquid Yield (Bble Ca+/tonna dry coal)	2.14	2.55	2.49	2,83
Kconenice				
Plant Construction Cost (H 1977 \$)	1,383	1,180	1,205	1,194
Capital Cost (# 1977 \$)	2,199		1,916	7,0
Gasoling Gost (1977 \$/Litre)	0,40		0.19	0.25
Gasuline Cost (1980 \$/1.itre)	0.53		0.38	

1.5bl m 42 U.S. Callons m 159 Litres.
APUR - Fuci Oil Equivalent assuming 6.33 G3/8bl.

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### CONCLUSIONS

This paper has investigated advanced gasification systems and the Kolbel liquid slurry phase reactor as alternatives to dry ash Lurgi gasification and fast fluid bed Synthol reactors used at SASOL. This combination has shown in concept the potential for significant advantages in output, product cost, plant construction cost, liquid product selectivity and overall plant thermal efficiency. Performance data for the advanced components have been derived from pilot scale operations.

If the assumed level of component performance is achieved in a plant designed for all-liquid output, advanced gasifiers offer an increase in output with no increase in capital costs. This performance translates to an 18-percent decrease in gasoline production cost. Advanced gasifiers plus Kolbel synthesis offer an increase in output averaging 36 percent, resulting in a decrease in gasoline production cost approaching 33 percent.

Much recent R&D in coal gasification has been directed toward the production of fuel gas and SNG. Gasifier R&D for the Synthame, Hygas, CO<sub>2</sub> Acceptor, Bi-Gas, and Exxon Catalytic processes has been directed toward maximizing the methane content of the product gas. Methane production in gasification for liquid synthesis is a disadvantage since it must subsequently be reformed if only liquid products are to be produced. Gasifiers optimized for SNG production are thus not well suited for indirect liquefaction.

The slight advantage of the Shell gasifier over the other advanced gasifiers stems primarily from the absence of methane in the product gas. This advantage is lost in plants designed for a combination of liquid products and favorably priced SNG. It is also notable that the Shell unit, because of its high operating temperature, is the unit most likely to be compromised by technical problems related to liner integrity and heat recovery.

We would recommend that all three gasifier types (slagging, fixed bed, fluidized-bed, and entrained) be thoroughly evaluated before making a final selection of gasifiers for a commercial plant. The status of development of candidate gasifiers would undoubtedly be a major consideration in the final selection, as it has been at SASOL.

The efficiency advantages offered by advanced gasifiers in plants employing conventional Fischer-Tropsch reactors can be further improved by combining the advanced gasifiers with an alternative synthesis system such as the slurry phase Kolbel reactor. This additional improvement stems partly from a synergism which results from the ability of the Kolbel reactor to accept the low H<sub>2</sub>/CO ratio synthesis gas produced by the advanced gasifiers. However, the most significant advantage of the Kolbel reactor stems from its greater selectivity toward the synthesis of gasoline.

These advantages are clearly worth pursuing by supporting R&D in the synthesis area in slurry phase reactors, slurry compatible

catalysts, scaling characteristics and modifications in poduct output towards diesel and jet fuels. The successful demonstration of this slurry technology would confirm the attractiveness of this Fischer-Tropsch option.

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