

## 8.0 SENSITIVITY ANALYSES

### 8.1 Introduction

Several sensitivity analyses have been performed to determine the extent to which results are affected by alternative analysis assumptions. These results are presented and discussed in the paragraphs below.

### 8.2 The Sensitivity of Gasoline Prices to SNG Value

All plants considered in this study are least expensive and most efficient when operating in the mixed product mode. However, the price which must be charged for gasoline produced from these plants is profoundly influenced by the value of the SNG co-product; particularly in the cases where SNG production is high. Also, since it is possible to reform the SNG to yield additional synthesis gas and additional liquid products, the relative values of SNG and gasoline will be the determining factor in the selection between the mixed output and all-liquids plants.

MRDC (Reference 1) determined \$6.17/MMBtu as an SNG base price for comparison from a study which showed that this product could be produced and sold at this price from an SNG plant employing the corresponding Lurgi SNG technology. The price thus represents a reasonable upper limit for the value of coal derived SNG. However, prices of less than one-half that amount (in \$1977) would be relatively high in the market place. Use of the \$6.17/MMBtu SNG price may tend to obscure advantages of the advanced systems.

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The sensitivity of gasoline prices to SNG prices lower than \$6.17/MMBtu can be determined from the data presented in Figure 8-1, which shows the required gasoline price (Market Basis) for mixed and all-liquid plants as a function of the price at which SNG can be sold. Plants illustrated in Figure 8-1 are the SASOL-U.S. Base Case and the SK/Kolbel combination. These plants represent the extremes of highest and lowest SNG production when operating in the mixed product mode. These data confirm that the price of gasoline from the SASOL-U.S. plant producing a mixed output is extremely sensitive to SNG price. The all-liquid SASOL-U.S. plant configuration is seen to result in lower priced gasoline than its mixed product counterpart for all SNG prices less than \$5.40/MMBtu.

For the SK/Kolbel combination, the break even price for SNG is seen to be about \$4/MMBtu. However, gasoline prices show no more than a  $\pm 5\text{¢}/\text{gal}$  sensitivity to SNG prices ranging from \$2/MMBtu to \$6/MMBtu.

It is also evident that the price of SNG influences the gasoline price advantage which the SK/Kolbel combination holds relative to the SASOL-U.S. Base Case. Should the price of SNG exceed \$8/MMBtu, then the SASOL-U.S. plant could produce cheaper gasoline. In this situation, however, an all SNG plant would yield income 30 percent in excess of DCF requirements. No liquids would be produced unless excess profits of similar magnitude could be made.

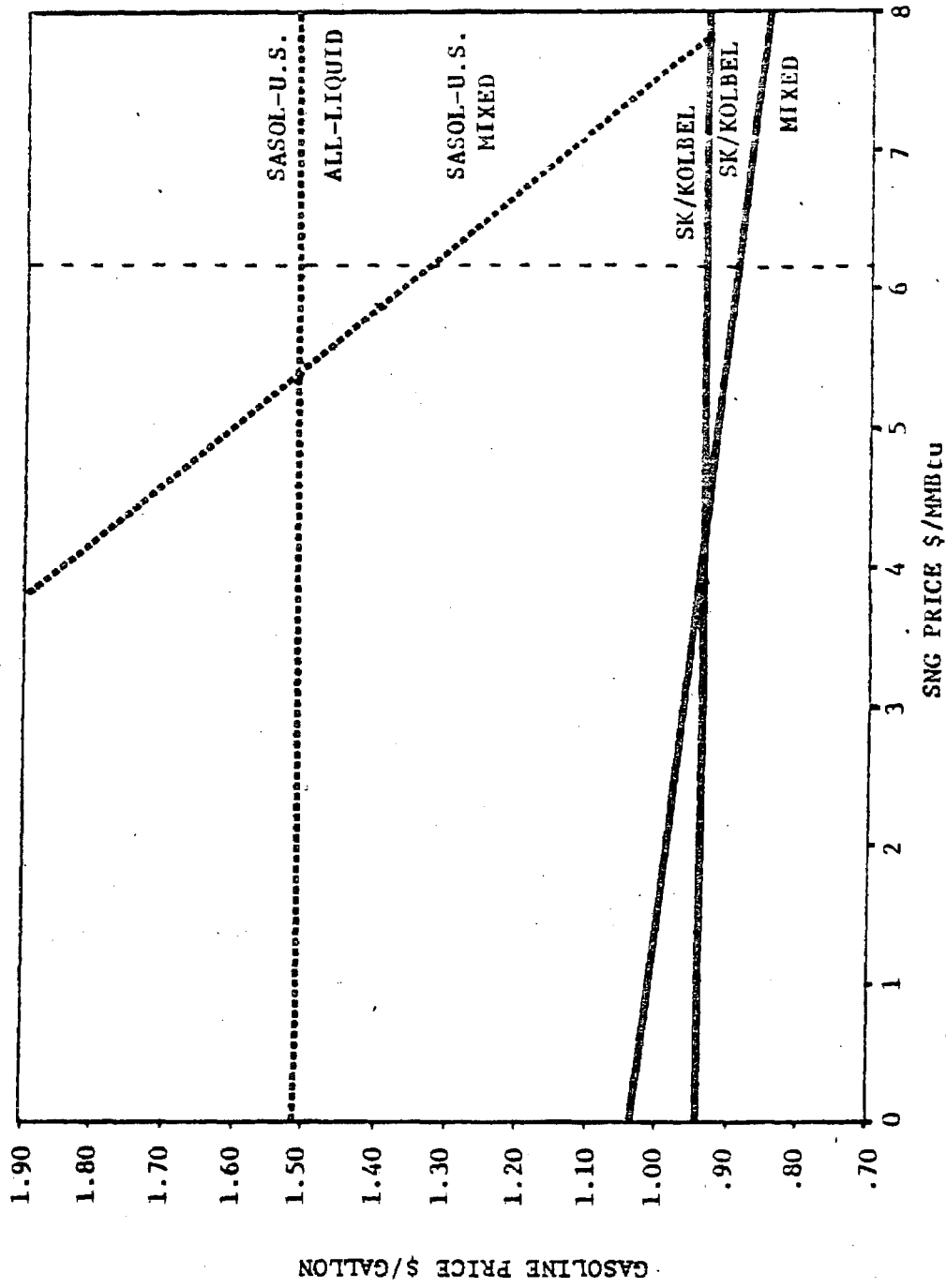


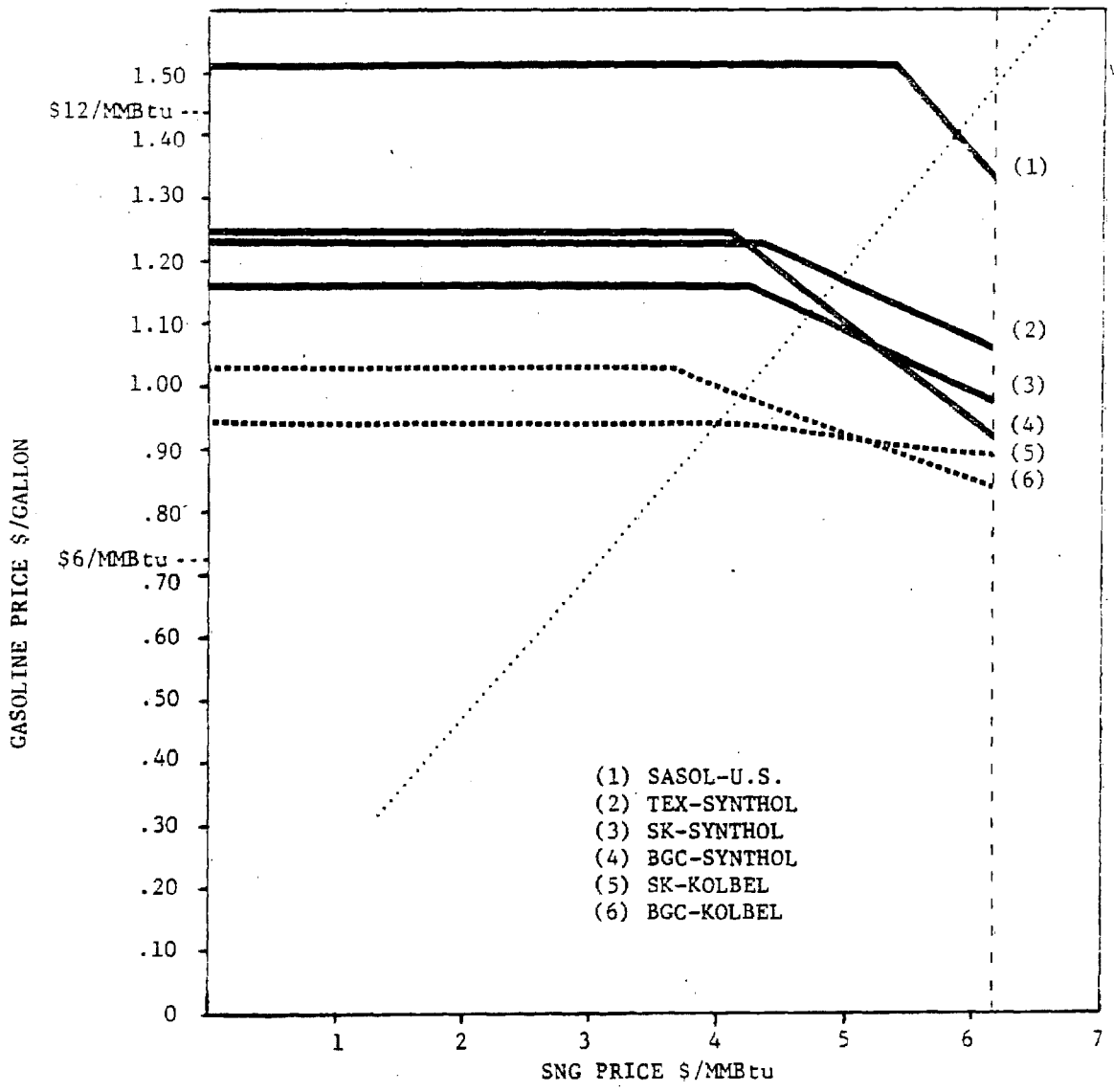
FIGURE 8-1  
SENSITIVITY OF GASOLINE PRICE WITH VALUE OF SNG

Comparison of the alternative plants over a wide range of SNG prices can be made from data provided in Figure 8-2. The figure shows the lowest gasoline price, from either an all-liquid or mixed product plant, as a function of SNG value.

The general relationship between the advanced system and the SASOL-U.S. Base Case is not affected by SNG price. Advanced gasifiers permit gasoline price saving on the order of 25¢ per gallon. The combination of advanced gasifier and Kolbel synthesis permits further savings. However, the relative performance of the advanced gasifiers is influenced by SNG price. The BGC gasifier offers lowest gasoline prices when the price of SNG is \$6.17/MMBtu, but requires higher gasoline prices than either SK or Texaco if SNG price falls below \$4.15/MMBtu. Kolbel synthesis, which provided savings of only 8¢ per gallon when used in a mixed output plant selling SNG for \$6.17/MMBtu, is seen to offer greater savings if SNG prices are lower.

There is no historical precedent and little basis for a future expectation of SNG prices greater than 50% of gasoline prices on a \$/Btu basis. If this relationship, represented by the dotted diagonal line on Figure 8-2, is taken as the upper limit of SNG prices, then the following observation can be made.

1. The relative ranking of the system considered is unchanged by SNG price consideration.
2. Savings in gasoline price resulting from SNG co-production are marginal. All liquid plants would probably be preferred except in special



**FIGURE 8-2**  
**SENSITIVITY OF GASOLINE PRICE WITH VALUE OF SNG FOR ALL**  
**CASES CONSIDERED**

situations where transportation to nearby premium SNG markets was already established.

3. Kolbel synthesis provides gasoline cost savings of 17¢/gallon or more in all cases of interest.

### 8.3 Sensitivity of Entrained Flow Gasifier Performance to Excess Moisture in the Gasification Reaction

#### 8.3.1 Introduction

In the analyses presented in Section 5.3, performance of the Texaco and Shell-Koppers entrained flow gasifiers were computed on the basis of an assumption that the wet western coal was dried to 5% moisture prior to gasification. In the case of the Texaco gasifier, it was further assumed that a 70/30 coal/water slurry could be achieved. The impact of less complete coal drying, and/or less dense slurries on gasifier performance is considered here.

#### 8.3.2 Theoretical Consideration

The moles of hydrogen plus carbon monoxide produced in an entrained flow gasifier are maximized when the gasification reaction occurs under conditions that preclude formation of methane and when the heat of reaction is provided solely from the partial oxidation of carbon to CO. The amount of H<sub>2</sub>O that is required to meet thermal equilibrium and stoichiometry requirements under these conditions of maximum syngas output is only a few percent of the DAF coal feed.

Additional moisture introduced to the reaction has the effect of increasing the mass which must be raised to the reaction temperature of about 2000°F, thereby increasing the oxygen which must be supplied and the amount of carbon which is burned to

completion. The excess moisture will have the further effect of changing the equilibrium in the gasifier in favor of additional  $\text{CO}_2$  formation by the consumption of  $\text{CO}/\text{H}_2\text{O}$  to form  $\text{H}_2/\text{CO}$  in the water/gas shift reactions. The extent to which this shift occurs at the gasification temperature may be influenced by the catalytic properties of the coal ash. Examination of data from various entrained flow gasifiers (Reference 13 and 20) indicated that about one-third of the excess moisture is consumed in shift. However, the degree of shift is not of great consequence since the heat released by the reaction is small, and the number of moles of syngas present is not changed.

The larger mass of products which results from excess moisture increases the sensible heat which can be recovered from the output stream, partially offsetting the loss in syngas production. However, as a result of quench requirements for particulates removed prior to heat recovery, and the inability to recover the heat of condensation from the steam present in the exit gas, only about one-half of the additional heat released in the gasifier is recoverable. Heat recovered in excess of that needed to produce the additional oxygen required is likely to be minimal. The reduction in syngas output which results from excess moisture is thus a very good approximation of the reduction in net gasifier efficiency.

The reduction in the moles of syngas for each mole of moisture present may be approximated by computing the number of moles of CO which must be burned to CO<sub>2</sub> in order to release the heat necessary to raise the excess moisture to reaction temperature of 2500°F.

$$\begin{aligned}\Delta h_{\text{H}_2\text{O}} \quad 100\text{F} \rightarrow 2500^\circ\text{F} &= 2290 \text{ Btu/lb} \\ &= 41,220 \text{ Btu/lb-mole}\end{aligned}$$

Assume 1/3 of H<sub>2</sub>O reacts with CO to form H<sub>2</sub> + CO<sub>2</sub>

$$\Delta h_{\text{shift}} = \frac{16,542 \text{ Btu/lb-mole}}{3} = 5,415 \text{ Btu/lb mole}$$

Heat required from CO + O<sub>2</sub> → CO<sub>2</sub> is thus 41,220 - 5,415 = 35,805 Btu/lb-mole of excess H<sub>2</sub>O

Heat released for CO +  $\frac{1}{2}$  O<sub>2</sub> → CO<sub>2</sub> is 122,044 Btu/lb-mole  
CO reacted

$$\begin{aligned}\text{Moles CO lost per mole excess H}_2\text{O required is thus } &\frac{35,805}{122,004} = \\ .293 \frac{\text{Moles CO}}{\text{Mole H}_2\text{O}}\end{aligned}$$

In the analysis of the Shell-Koppers gasifier presented in Section 5.3, coal was dried to 5% moisture and fed to the gasifier by a dry coal feeder. Moisture per pound of DAF coal is:

$$\frac{\text{moisture/coal}}{\text{DAF coal/coal}} = 0.05/.883 = 0.057 \text{ (The minor addition of steam (.03 lb/lb DAF) is ignored since it absorbs little heat in reaching reaction temperature)}$$

The moles of syngas produced from a flow of 1550 M lb/hr DAF coal was shown in Section 5.3 to be 135.92 M lb mole/hr.



Texaco performance was based on use of a coal containing 5% moisture in a 70/30 slurry. Water in the mixture per pound of DAF coal was thus  $\frac{(.05 \times 70 + 30)}{.883 \times 70} = .542$  lb/lb

Moisture in excess of Shell-Koppers was thus:

$$.542 - .057 = .485 \text{ lb/lb DAF coal or}$$

$$\frac{.485 \times 1550 \text{ lb/hr DAF coal}}{18 \text{ lb H}_2\text{O/lb-mole}} = 41.8 \text{ lb-moles}$$

The analysis presented above would indicate that the resulting reduction in the moles of syngas produced would be:

$$41.8 \text{ M lb moles H}_2\text{O} \times .293 = 12.22 \text{ M lb-moles syngas}$$

The gasifier analysis presented in Section 5.3 shows that the Texaco gasifier yields 123,675 lb-moles of syngas, which is almost precisely the quantity which would have been predicted by adjusting the Shell-Koppers data for additional moisture. We thus conclude that the effect of excess moisture can be approximated by assuming that each lb mole of excess water reduces syngas production by .293 lb-moles.

### 8.3.3 Results and Discussion

Figure 8-3 shows the moles of syngas produced as a function of the quantity of water introduced to the gasifier. Results are shown for two coal feed rates. The solid line represents the 1550 M lb/hr DAF, which was assumed to be gasified in the analysis presented in Section 5.3. The dashed line shows the output if the 124 M lb/hr DAF coal used for coal drying had been gasified.

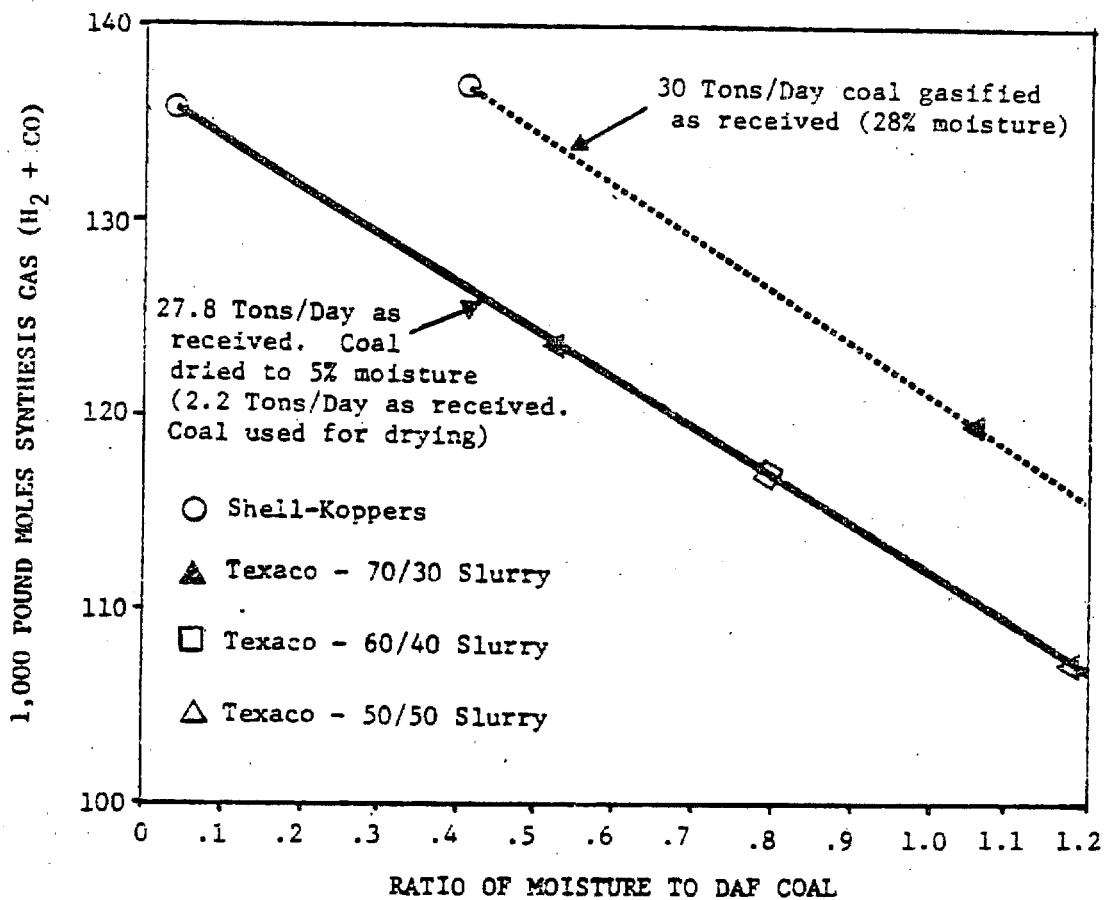


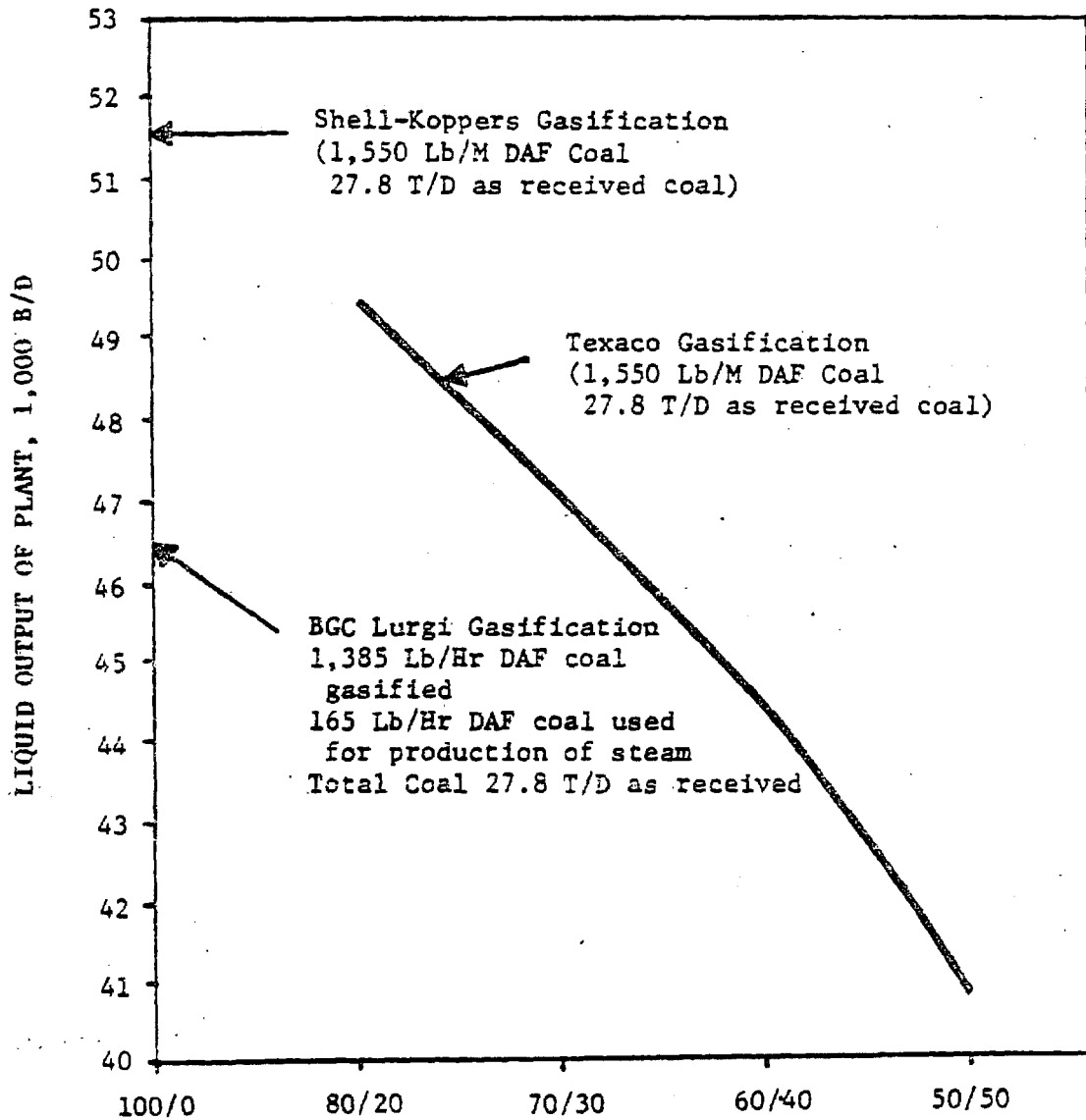
FIGURE 8-3  
EFFECT OF MOISTURE ON SYNGAS PRODUCTION FROM ENTRAINED  
FLOW GASIFICATION

The most striking result of the analysis is the indication that more syngas would have been produced by the Shell-Koppers gasifier if the 8% of total coal assumed to be required for coal drying had been gasified. However, as was noted in Section 5.3, the assumption that 8% of the coal is required for drying is very conservative since it makes no account of the possibility that some or all of the energy for coal drying might be available from waste heat sources. Nonetheless, the results of Figure 8-3 do imply that the decision to dry western coal for Shell-Kopper gasification must be carefully considered in view of the overall plant heat balances.

The Texaco gasifier, operating with a 70/30 slurry and coal dried to 5% moisture produces about 8% less syngas than does the Shell-Koppers gasifier. Operation at 60/40 slurry with 5% moisture coal would reduce the quantity of syngas an additional 6500 moles. A much larger decrement would result if a 50/50 slurry were used.

The figure also shows the Texaco syngas production with a 70/30 slurry of as-received coal. The loss of output relative to the dried coal case is not large. However, the previously discussed caveats regarding comparisons of performance with dried and as-received coal apply in the Texaco case also.

Figure 8-4 shows the effect of Texaco slurry concentration on the product output of an all-liquid plant. Outputs with Shell-Koppers and BGC gasification are shown for references. These data show that the Texaco gasifier ceases to be competitive with the BGC



**FIGURE 8-4**  
**OUTPUT OF ALL-LIQUID TEXACO PLANT VS. SLURRY CONCENTRATION**

gasifier unless slurry concentration near the 70/30 ratio assumed  
in this study can be achieved.

## 9.0 CONCLUSION AND RESEARCH AND DEVELOPMENT RECOMMENDATIONS

### 9.1 Advanced Gasifiers

#### 9.1.1 Conclusion

The dry ash Lurgi gasification system used at SASOL has significant limitations when used in plants designed primarily to produce liquid fuels from coal by indirect processes. These limitations stem from an inherently low thermal efficiency resulting from a high process steam requirement, and the high rate of methane production. The production of tars, oils and phenols is also detrimental if the output of premium liquid fuels is to be maximized.

All of the advanced gasification systems considered in this study circumvent the limitation of the dry ash Lurgi to a significant degree. When combined with conventional gas clean up and Synthol synthesis processes used at SASOL-II, the advanced gasifiers offer large improvements in liquid output and substantially lower gasoline prices, as is illustrated in Table I-3. The advanced gasifiers result in a lower overall plant investment. The capital cost reduction stems from higher throughputs (e.g., less gasifier required) plus lower steam requirement and lower waste water generation. However, the lower gasoline prices projected for the system employing advanced gasifiers stem primarily from their better technical performance; not lower capital cost.

The advantages of the BGC design relative to its dry ash counterpart are a lower methane production and substantially

higher efficiency. The Shell-Koppers entrained flow gasifier, which incorporates a dry coal feed system, offers a net thermal efficiency comparable with the BGC Lurgi, with methane, phenols, tars and oils virtually absent from the raw gas. The Texaco gasifier also produces a raw gas virtually free of unwanted hydrocarbons, although an efficiency slightly less than the other two advanced gasification systems. However, its overall performance is comparable with the BGC if an all liquid product is desired.

The low  $H_2/CO$  ratio of advanced, high efficiency, gasifiers has frequently been identified as a disadvantage. Our analysis, based on overall plant costs and energetics, has shown that the penalty imposed by the requirement of having a water gas shift reactor downstream of the advanced gasifier is small compared to the efficiency advantages they offer. Advanced synthesis systems obviating the need for shift further enhance their performance relative to the dry ash lurgi.

#### 9.1.2 R&D Recommendations

9.1.2.1 Shell-Koppers. From the standpoint of thermochemistry, the Shell-Koppers gasifier is an ideal system for the production of methane-free synthesis gas from coal. If the dry feeder proves reliable, and virtually complete carbon utilization is achieved as claimed, then the attainment of ideal performance will be impeded only by the difficulties associated with the recovery of sensible heat from the gasifier output. Areas most deserving of R&D

attention are those related to the dry coal feeder, and waste heat boilers capable of efficient recovery of heat from a raw gas containing molten ash.

Dry coal feed systems offer significant advantages over slurry feed systems, particularly if high moisture coals are used. R&D directed toward improved coal feed systems is ongoing under DOE sponsorship.

Other potential problem areas, including the development of improved heat recovery systems, are difficult to address at the component scale. There is a need therefore to acquire pilot scale experience with entrained pressurized gasification systems employing dry feed so that problems associated with safety and control, suitability of various coal types, life of refractory linings and other problems can be addressed. The dry feed concept is not unique to Shell-Koppers and little is known of the details of their implementation of the concept. A design and demonstration competition might yield equal or superior implementation from U.S. firms.

9.1.2.2 Texaco. The Texaco gasifier is thermochemically similar to the Shell-Koppers except that moisture is introduced as a carrier for the coal. This moisture required is excess to the quantity needed for efficient generation of synthesis gas, and must necessarily reduce the efficiency below that which can be obtained with a dry feed. This observation is contrary to



the conclusion of Reference (7) wherein it was concluded that there were no incentives for development of a dry coal feeder for a Texaco gasifier designed to produce medium Btu gas for use in a combined cycle power system. However, in the Fluor analysis the quantity of steam plus moisture introduced to the "dry" feed Texaco system was substantially higher than the total moisture introduced to the 65/35 slurry feed system to which the dry feed system was compared. Operation with very low total moisture, as has been demonstrated with the Shell-Koppers system, was not considered.

Concern has been expressed about the susceptibility of the dry feed system to catastrophic over pressurization in the event of an interruption in the coal feed. The slurry-fed Texaco gasifier has an important role as a backup to the dry feed systems in the event that this and other problems of the dry feed system cannot be solved.

The component development needs discussed previously (feed and waste heat recovery) would be pertinent to the Texaco as well as to the Shell-Koppers gasifier.

9.1.2.3 BGC. The BGC gasifier provides excellent performance, especially if a plant producing a combination of liquid products and SNG is envisioned. Continued tests of this gasifier under various operating conditions and with additional coal types, including low ash, high moisture western coal is recommended.

Tests of the Grand Forks Slagger<sup>(37)</sup> affirm that low rank coals can be efficiently gasified in slagging units. However, the ability to gasify excess coal fines and tars, oils and phenols with these coals has not yet been demonstrated.

Experience to be gained in the operation of the gasifier to high Btu gas manufacture should serve as a source of operability data for indirect liquefaction applications.

## 9.2 Synthesis Processes

The severe selectivity limitations associated with conventional Fischer-Tropsch synthesis reactors have provided an incentive for research into alternative methods of converting synthesis gas into liquid fuels. The Advanced Synthesis reaction of this report has incorporated an alternate F-T system by substituting the Kolbel liquid slurry phase bubble column reactor for the fast fluid bed Synthol system. The combination of this Kolbel unit with the advanced gasifier system has shown significant advantages in product cost, capital investment, liquid product yield and overall thermal efficiency.

The following points are the key to this advantage:

- the Kolbel ability to accept low  $H_2/CO$  ratio synthesis gas produced by advanced gasifiers
- its high selectivity to gasoline boiling range hydrocarbons
- its low production of light gases especially methane and  $C_2$  hydrocarbons

- its high single pass conversion of synthesis gas
- its low production of oxygenates and alcohols

Conventional F-T systems are unable to accept the low  $H_2/CO$  ratio syngas from advanced gasifiers. The synthesis gas must be shifted considerably from the initial ratio to the 2.54 required for the Synthol process. The Kolbel reactor requires a minimal shift when using synthesis gas from the BGC-Lurgi and the Shell-Koppers gasifier. No shift at all is required when coupling with a Texaco unit. The minimization of this shift is reflected in savings in construction cost because of smaller shift units and less expensive by-product recovery systems.

The Kolbel system has a high selectivity to gasoline in the raw liquid product. Fifty-three wt. % of the total hydrocarbon product is in the range  $C_5-180^\circ C$ . This raw naphtha has an IOR of 73 compared to an octane number of 55 for the SASOL raw gasoline. (38) This quality advantage has not been exploited in this report, but could result in less liquid product refining for the Kolbel case.

The production of light gases in Synthol, while being desirable for a mixed output plant, are a disadvantage for plants producing all liquids. For a gasifier producing no methane in combination with a Synthol unit, 38% of the thermal output of the plant is SNG. For an all liquid output this SNG would have to be reformed back to synthesis gas and recycled to the F-T unit. This process is inefficient and results in low overall thermal efficiencies for all

liquid plants. Kolbel produces few light gases and for the Shell-Koppers/Kolbel combination, only 11% of the thermal output is SNG. This enables a higher thermal efficiency to be obtained for a plant making an all liquid product.

Single pass conversions of 89% of the synthesis gas are reportedly possible using the Kolbel synthesis. Single pass conversions for Synthol are much lower than this (~50% conversion/pass) and require recycle to fresh feed ratios of 2.

The low concentration of oxygenates and alcohols produced by Kolbel is an advantage for a plant optimizing its output of a transportation fuel product slate.

While the Kolbel slurry phase F-T synthesis represents one alternative approach, other systems are currently being investigated. The Mobil MTG process overcomes the poor gasoline selectivity problem by first converting the synthesis gas to methanol. The methanol is then dehydrated and aromatized over zeolite catalysts to produce high octane gasoline with very high selectivity. Light olefins are a co-product and are alkylated to produce more gasoline blending stock.

Upgrading the raw product from the MTG process would only require alkylation of the C<sub>3</sub> and C<sub>4</sub> hydrocarbons followed by blending this with the gasoline fraction obtained from the zeolite. This contrasts with the complete refining required for the raw F-T products obtained from both Synthol and Kolbel. Substantial savings in capital investment should result from the elimination of these refinery units.

However, the initial methanol synthesis process is not without its limitations. The Cu-Zn based methanol synthesis catalyst has an extremely low sulfur tolerance level. The five ppm range obtainable in synthesis gas by using Selexol and Rectisol units must be further reduced to approximately the 20 ppb range.<sup>(59)</sup> Current methanol synthesis achieves very low conversions per pass (2-10%) and thus requires very considerable recycle gas streams (~20:1). Also, the pressure of even the low pressure methanol synthesis reactors is around 50 atmospheres which is generally considerably higher than gasification systems. This necessitates a high compression requirement. In addition to the fixed bed methanol synthesis systems available commercially, Chem Systems is experimenting with three-phase methanol synthesis using a Kolbel type system, although the oil slurry is pumped from the reactor through heat exchangers and then recirculated to the bottom of the bed. The catalyst remains in the ebullating bed reactor. This system is claimed to have the advantage of higher conversions per pass, but there are problems in producing catalysts that are resistant to attrition under reaction conditions.<sup>(39)</sup>

To overcome the problems associated with the production of methanol, Mobil has investigated systems not requiring methanol as an intermediate step. Use of zeolite catalysts for upgrading raw F-T products have been tested and high octane gasoline and high diesel index fuel oil have been produced.<sup>(40)</sup> The two-stage combination of

a F-T system and a zeolite process has the advantage of producing high octane gasoline with good selectivity without the complex refinery scheme.

A one-stage process using bifunctional catalysts composed of ruthenium and zeolite in the same reactor is another approach. The ruthenium forms F-T reaction intermediates that are converted (in situ) via acid catalyzed hydrogen transfer by the zeolite to aromatics and branched paraffins. (38)

#### Research and Development Recommendations

Kolbel synthesis when coupled with advanced gasifiers could represent an improvement in indirect liquefaction technology if the previously documented performance of the Rheinpreussen plant can be confirmed. An R&D program would then seek to establish the following:

- confirmation of the Kolbel product distribution in its high selectivity to gasoline boiling range hydrocarbons and the low light gas make
- activity of the precipitated iron promoted catalyst system and studies of catalyst aging and ease of regeneration
- establishment of a regime where chemical rate control predominates unlimited by diffusional effects from the gas/liquid boundary to the catalyst surface
- the ability of the Kolbel slurry phase reactor to be scaled up to a commercial size unit by overcoming potential problems of uniform gas distribution in the suspension for large cross sectional area reactors
- the ability of the Kolbel reactor to handle the low  $H_2/CO$  ratio synthesis gas feeds from the Shell-Koppers gasifier without shift

When the operating characteristics of the Kolbel reactor have been determined it would then be of interest to combine the reactor with a zeolite upgrading process to refine the raw F-T products. The combination of advanced gasifier, Kolbel synthesis and zeolite upgrading to gasoline may well prove to be a very beneficial indirect liquefaction system.

The principal thrust of this study has been directed to maximizing gasoline production by combining advanced gasifiers with a Kolbel type synthesis reactor. This is entirely proper since gasoline is the major liquid transportation fuel today and for the foreseeable future. However, growth in truck and airplane population will result in a significant increase in the demand for jet and diesel fuel. Investigation of the conversion of  $C_3$  olefins using zeolite type catalysts to convert these light hydrocarbons into higher boiling jet and diesel fuel fractions is a desirable longer term goal in an R&D program for liquid fuels by indirect liquefaction.