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COSTS OF SYNTHESIS GASES AND METHANOL

PART II

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4 SYNGASES, HYDROGEN, AND METHANOL FROM THE STEAM REFORMING OF NATURAL GAS

Steam reforming of hydrocarbons is a highly refined technology which has for long been the established way of generating syngas for the large scale production of ammonia, hydrogen, and methanol. It has also frequently been used to provide syngas and hydrogen for smaller operations such as oxo alcohols manufacture. The preferred feedstock for steam reforming has generally been a methane-rich natural gas, when it was readily accessible at a competitive price. In the pre-1973 era of cheap oil, a naphtha feedstock was frequently chosen when either natural gas was not available or a lower H_2:CO ratio was specifically desired. The low differential between natural gas and naphtha prices justified such a choice. With current and projected price differentials we may expect that the use of C_2-naphtha range hydrocarbon feedstocks will become increasingly unattractive in steam reforming, opposite natural gas. This is because of their higher value in other uses, e.g., in making ethylene and (in the case of naphtha) gasoline.

As discussed in Section 3, the present work is aimed at projecting costs of syngas feedstocks for the anticipated new generation of processes for many other bulk chemicals. In general, the latter call for syngas feedstocks with a lower H_2:CO mol ratio than is inherently produced by steam reforming of natural gas (i.e., approaching 3:1 when CO_2 is recycled to the reformer). In addition, by the time some of these proposed syngas routes are expected to approach commercial status (i.e., the latter half of the 1980s), it could well be that in places with relatively cheap coal, production of syngas from coal may be more economic than production from natural gas.

However, natural gas reforming currently stands as the most widely used, best developed, and normally still the cheapest way to generate syngas. We therefore consider that natural gas reforming economics must still provide the reference basis, or calibration, for cost comparisons and projections relating to syngas.

Most of the proposed syngas routes to bulk chemicals require ratios of 2:1 or less, or sometimes methanol and carbon monoxide. However, because of the shift reaction following reforming, the actual ratio of H_2:CO in the product from steam reforming of natural gas is typically well above the stoichiometric 3:1 for methane and normally closer to 5:1. To produce the lower ratios one can either separate or "skim" off some hydrogen from the reformer product, or feed carbon dioxide to the reformer, or both. The carbon dioxide could be recycled from the reformer product and under conditions of "total recycle" a H_2:CO ratio close to the stoichiometric 3:1 for methane can be attained. To obtain ratios lower than this, additional carbon dioxide is required to supplement the recycle and this could be recovered from reformer flue gas or, when practical, it could be imported from an ammonia or hydrogen facility. Such technology has typically been practiced in connection with oxo syngas production in relatively small operations. However, little has been published on the comparative economics of these options.

The thrust of the present section is in examining means for production of syngases with H_2:CO ratios below 3:1 by steam reforming. Methanol economics are also briefly reviewed because of the central position of methanol in many of the proposed syngas routes. Similarly, an updated review of hydrogen economics is presented because the value of hydrogen as a coproduct is a key determinant in the economics of "skimming" and CO production.

To this end the steam reforming of natural gas has been examined in full flow sheet detail for the following cases:

A. Refined syngas (98 vol% H_2 + CO, dry basis) with H_2:CO ratio $\simeq$ 3. This is achieved by a total CO_2 recycle system, i.e., CO_2 is recovered from the crude syngas and fed with natural gas to the reformer.

B. Refined syngas ($\sim$98 vol% H_2 + CO, dry basis) with H_2:CO ratio = 2. To obtain such a mixture by reforming, it is necessary to have imported CO_2 available in addition to recycle CO_2 for the reformer feed. The effect on costs of providing this extra CO_2 by flue gas scrubbing compared with cheap or free CO_2 coproduced from an adjacent NH_3 or H_2 facility is also included in the estimate.

C. Chemical grade H_2 (97 vol% H_2, dry basis). The conventional process consisting of reforming, high and low temperature CO shift, CO_2 separation and methanation was evaluated. However, some estimates are presented for a proposed variant entailing high temperature shift plus PSA (pressure swing adsorption).

D. Chemical grade methanol. The ICI low pressure process is taken as the basis, with natural gas serving both as a feedstock and as the fuel for the reformer furnace.

E. Crude syngas from a methanol plant reformer. The gas mixture considered is the cooled effluent from a reformer which is operated at conditions typically used in methanol production. This case was included to provide a cost figure for the unpurified crude stream which could be used in miscellaneous downstream applications, e.g., small scale CO production for acetic acid when it is integrated with large scale methanol manufacture.

Production of syngas with a ratio of H_2:CO lower than 2:1 (by increased CO_2 import) was not examined in full flow sheet detail. The reasons are discussed later. An estimate, based on extrapolation, is presented for illustration. The scale of operation taken for these basic cases is the "equivalent" of the largest single-train methanol unit that is considered feasible with current engineering experience. This was quoted by industry experts to be in 2,500-3,000 metric tons/day. For the syngas and hydrogen cases we selected the lower end of this bracket and output rates for Cases A-E were based on a fixed natural gas feedstock rate that corresponds to a 2,500 metric tons/day methanol unit. As shown later, this calls for a somewhat larger reformer in Cases A and B than the methanol Case D. However, this is considered well within the single-train limits. In Case C, viz, hydrogen, the output corresponds to 479 million lb/yr (100% H_2 basis), which is much larger than typical size steam reforming facilities geared for the production of hydrogen alone. The cost estimates in this case represent a minimum from which costs at more realistic capacities have been derived.

Although details of separation systems for CO production and their economics are presented in Section 7, cost estimates for the adjustment of H_2:CO ratios by the use of these systems are also presented here for comparison.

Chemistry of Steam Reforming

In the reaction of hydrocarbons with steam (catalyzed by Ni in industrial reformers), a wide range of gas mixture compositions can be produced, depending on the operating conditions, viz, temperature, pressure, steam/hydrocarbons ratio, etc. In the simplest case with methane the basic reactions are:

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \qquad (4.1)$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad (4.2)$$

A mixture containing H_2, CO, CO_2, H_2O, and CH_4 is obtained whose composition is determined by the thermodynamic equilibria for reactions 4.1 and 4.2.

When C_2-and-higher hydrocarbons are present, the primary reaction is the conversion of these hydrocarbons to methane and CO_2 as follows:

$$C_nH_{(2n+2)} + \frac{n-1}{2}H_2O \longrightarrow \frac{3n+1}{4}CH_4 + \frac{n-1}{4}CO_2 \qquad (4.3)$$

There is evidence (415029, B-1516) that, with hydrocarbons within the naphtha range, the above reaction goes to completion under conditions used in commercial reformers. Therefore, as with methane, the composition of the product mixture is defined by the equilibria for reactions 4.1 and 4.2, with the proviso that the reacting hydrocarbon mixture is first totally consumed according to the stoichiometry of reaction 4.3.

The actual mechanism by which the conversion of hydrocarbons takes place is complex and possibly includes free radicals. It is postulated (B-1516, 472175, 472180) that there are three basic steps:

(1) The breakdown of the hydrocarbons to primary intermediates.

(2) Direct reaction of steam with these intermediates, leading to hydrogen, carbon oxides, and methane.

(3) An equilibration stage between H_2, steam, CO_2, CO, and CH_4.

Although the above mechanism is probably an oversimplification, kinetic equations based on such a sequence are satisfactory in the interpretation of experimental data (B-1516, 472180). However, under conditions used in industrial reformers the approach to equilibrium is close. Therefore, thermodynamic models based on equations 4.1, 4.2, and 4.3 are usually adequate to predict product compositions when other side reactions do not take place to any significant extent (415029).

The main side reactions are those which lead to the formation of carbon. Since this is undesirable in industrial reformers, considerable research has been devoted to understanding the conditions under which it can occur (415131, 415133, 472156, 472161, 472164, B-1514). From this knowledge, reformer designs and catalyst formulations have been evolved to eliminate or minimize the incidence of carbon formation. With the simplest methane molecule, possible reactions which lead to carbon deposition are:

$$2CO \rightleftharpoons C + CO_2 \qquad (4.4)$$

$$CO + H_2 \rightleftharpoons C + H_2O \qquad (4.5)$$

$$CH_4 \rightleftharpoons C + 2H_2 \qquad (4.6)$$

When higher hydrocarbons are present in the feedstock there is the additional possibility of cracking and carbon deposition from the breakdown of the products of cracking, e.g.,

$$C_nH_m \xrightarrow{\text{cracking}} \text{olefins and polymers} \longrightarrow C \qquad (4.7)$$

Kinetic studies (B-1516, 30983, 472176, 472181, 472182) have shown that the water gas shift reaction 4.2 is always virtually at equilibrium. Since reaction 4.5 is equivalent to reaction 4.4 minus reaction 4.2, it follows that reaction 4.5 is on the same side of equilibrium as reaction 4.4. Also these kinetic data have shown that the rates of reactions 4.4 and 4.5 are considerably greater than that for reaction 4.6.

The thermodynamics of reaction 4.4, the "Boudart reaction," are frequently used for a preliminary examination of conditions for carbon deposition. Thus carbon deposition can occur when:

$$\frac{[CO]^2}{[CO_2]} > \frac{K_{p(4)}}{P} \qquad (4.8)$$

where: $K_{p(4)}$ = equilibrium constant for reaction 4.4 (atmospheres abs.)

P = total pressure (atmospheres abs.)

$[CO]$, $[CO_2]$ = vapor phase mol fractions of CO and CO_2.

The steam/carbon ratio (defined as the ratio of mols of steam to atoms of carbon in the reformer feed) at which the equality of equation 4.8 occurs has been defined as the thermodynamic minimum ratio for the avoidance of carbon deposition (B-1516).

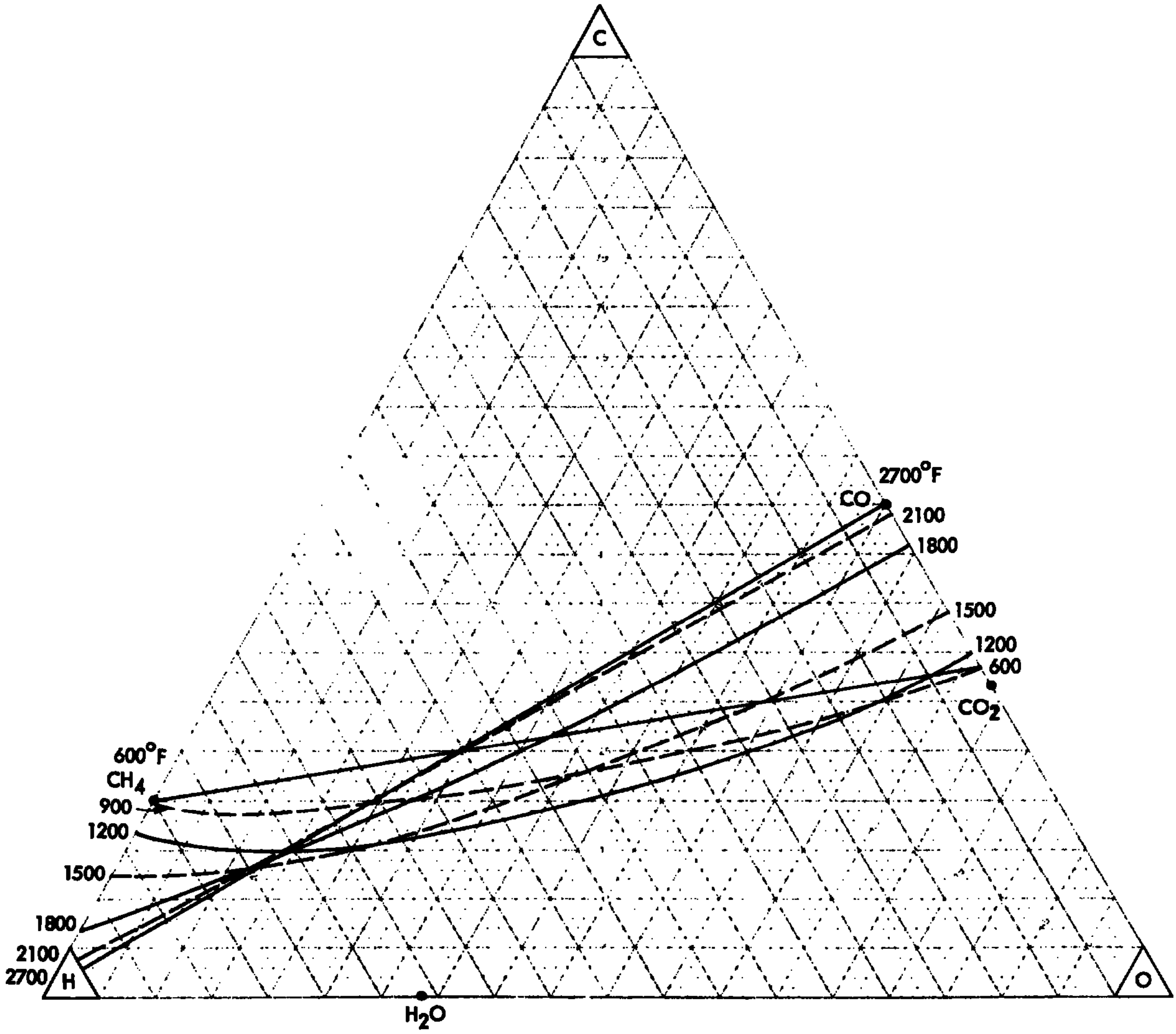
For a more complete analysis of carbon formation conditions, it is necessary to calculate the thermodynamic equilibria for all the three simultaneous reactions 4.4, 4.5, and 4.6. Cairns and Tevebaugh (472118) have proposed a novel graphical presentation of calculated equilibria data, that uses the triangular coordinates shown in Figure 4.1. The gas phase compositions are represented in terms of the atom percentages of the constituent elements carbon, hydrogen, and oxygen. The curves shown in the illustrative Figure 4.1 (called carbon isotherms) represent the carbon formation boundaries for a range of temperatures at a constant pressure of 400 psia. Mixtures of the elements which lie above the curves are in the carbon forming zone. The utility of this approach in defining carbon formation boundaries has been stressed in several subsequent publications (472156, 472161, 472174, 472177).

However, the equilibrium situation alone is not sufficient to predict conditions under which carbon deposition may be significant. Kinetic considerations may be overriding, particularly with a tailored catalyst design which enhances reforming reactions and suppresses

Figure 4.1

CARBON FORMATION

Equilibrium Isotherms (°F) at 400 psia Total Pressure



Source: 472177.

carbon formation. ICI have shown that the inclusion of alkalies in the nickel catalyst support prevents carbon deposition in naphtha reforming even at conditions close to the carbon forming boundaries (415132).

The values of the equilibria constants for the principal reactions 4.1, 4.2, and 4.4 are shown in Figure 4.2 as a function of temperature. From the nature of the variations depicted in this figure, the following observations may be deduced for the steam/methane system:

(1) Temperature: Increasing the temperature gives greater methane conversions and higher $CO:CO_2$ ratios (hence also lower $H_2:CO$ ratios). Within the temperature range that is used in steam reforming, the latter effect is very marginal.

(2) Pressure: Because of the increase in the number of molecules from reaction 4.1, enhanced pressures tend to lower the methane conversion but have little effect on the $CO:CO_2$ or $H_2:CO$ ratios.

(3) Steam/carbon ratios: An increase in steam/carbon ratios leads to higher methane conversions but could tend to lower the $CO:CO_2$ ratios (and thereby raise the $H_2:CO$ ratios).

The optimum combination of the above three variables depends on the end use for the reformer product stream. However, a low methane slippage is a dominant requirement. Figure 4.3 illustrates how methane slippage depends on these variables.

Discussion of the Assumed Technical Basis

The operating conditions were chosen to furnish a syngas stream containing at least 98 vol% ($CO + H_2$), dry basis, the rest being essentially unconverted methane plus some nitrogen and inerts. As shown earlier, methane slippage can be reduced by increasing reformer temperatures or the steam/carbon ratio and by decreasing the pressure. In a real situation the combination of conditions chosen for the reformer would be determined by the end use for the syngas. In most applications of syngas, the main reactor is operated at enhanced pressures and pass conversions are substantially incomplete. This necessitates a recycle loop and a purge. Thus, while a higher purity lowers the amount of purge gas and hence saves on feedstock, the use of lower reforming pressures necessary to obtain this purity imply that additional capital

Figure 4.2

EFFECT OF TEMPERATURE ON THE REACTION EQUILIBRIUM CONSTANTS IN STEAM METHANE REFORMING REACTIONS

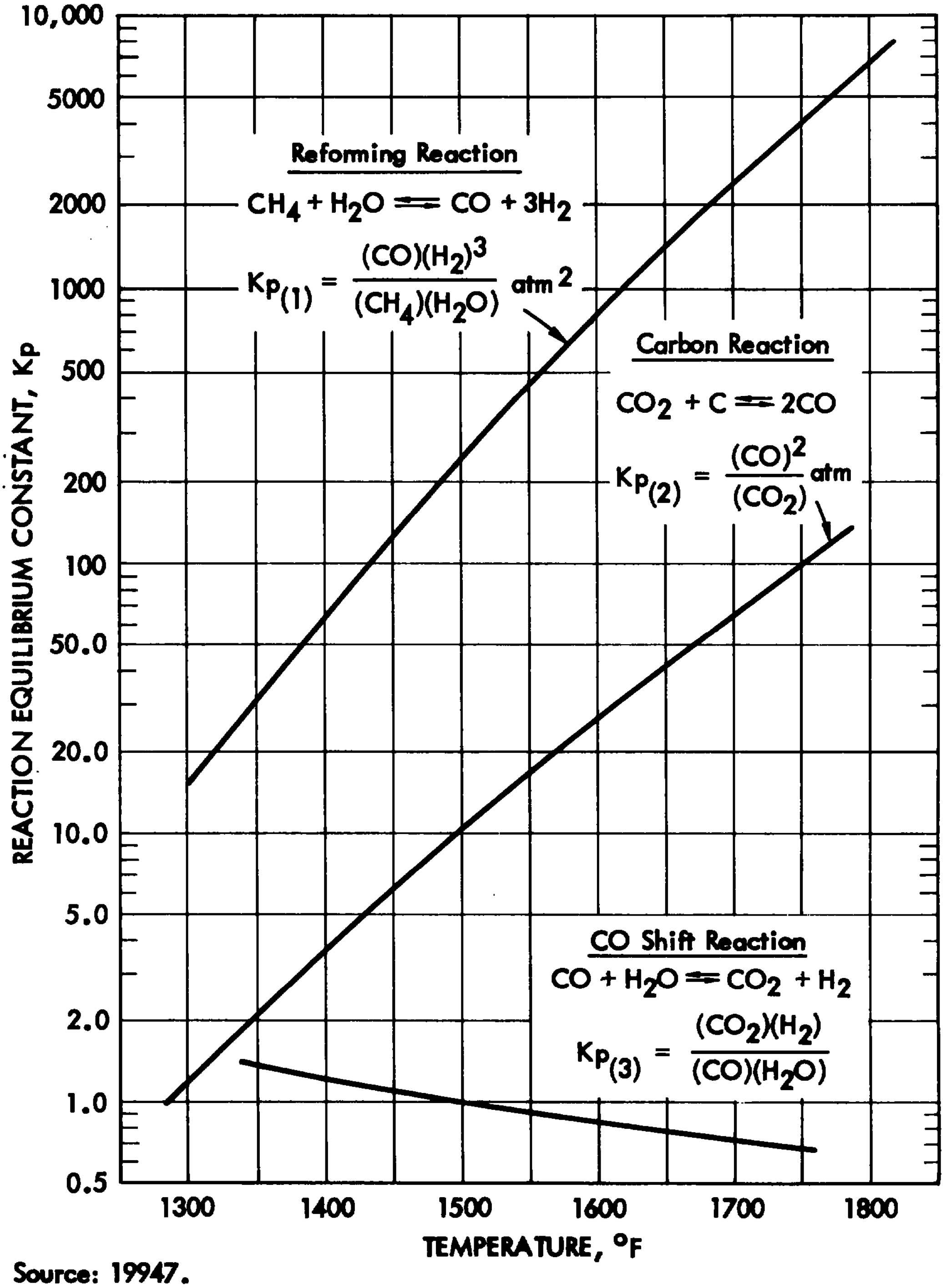


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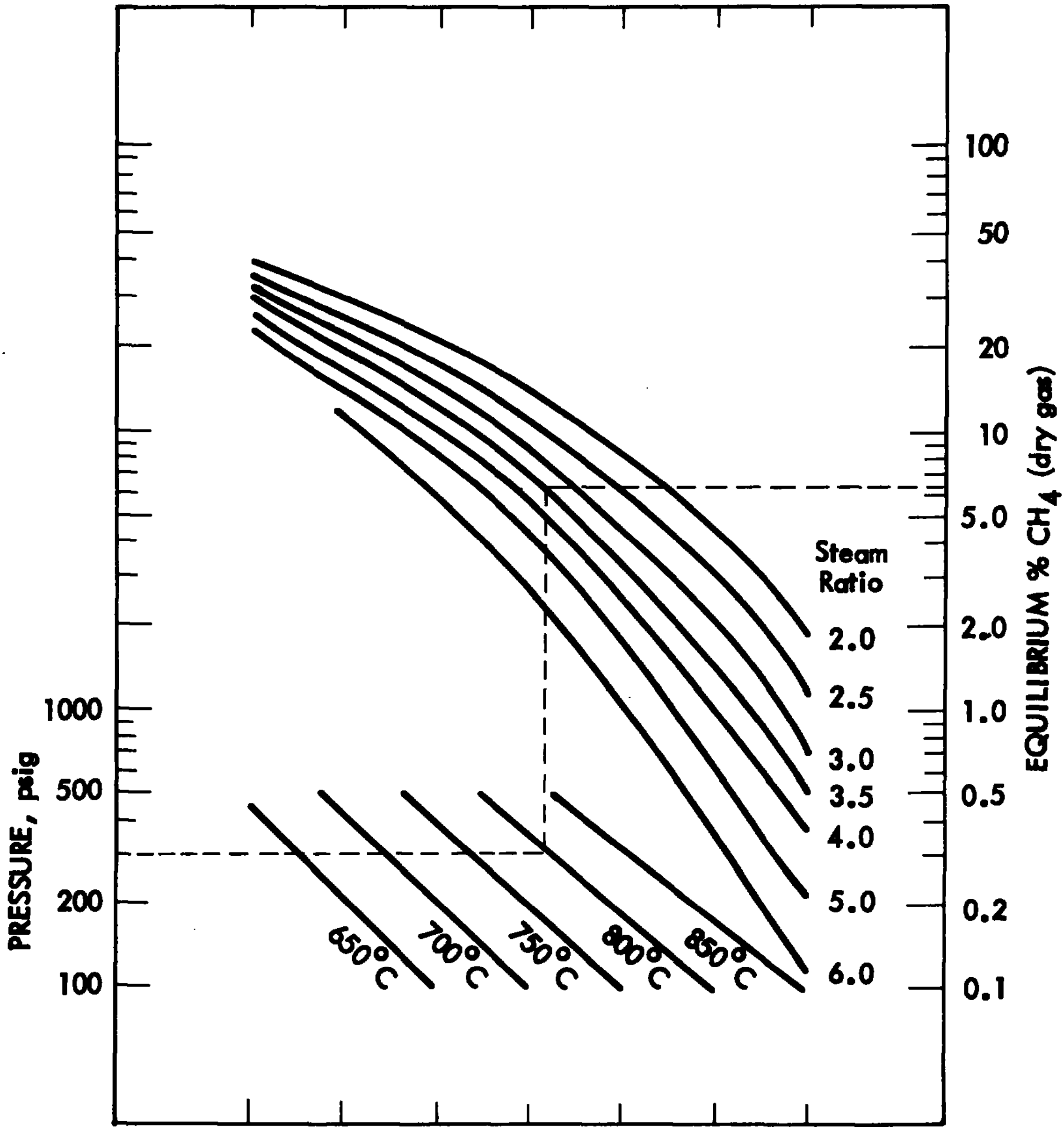
Figure 4.3

EQUILIBRIUM CONCENTRATION OF METHANE AS A FUNCTION OF TEMPERATURE, PRESSURE, AND STEAM RATIO FOR METHANE IN A STEAM METHANE REFORMER



Source: B-1516

and energy costs are incurred in compression. An optimum, therefore, needs to be defined for each case. On the U.S. Gulf Coast, for instance, natural gas is available at pressures up to 1000 psia but steam reforming pressures used in ammonia and methanol production are typically 275-450 psia. (For methanol the lower end of the range is generally applied and for ammonia the pressures are nearer the upper end of the range.) For syngas generation we chose reformer conditions similar to those used in methanol plants, but with somewhat higher steam carbon ratios (see Table 4.1). We consider that these provide a reasonable balance between syngas pressure and purity. A discussion of the main technical aspects of our design basis is presented under the following headings.

Steam Reforming Stage

From the earlier discussion of the chemistry of steam reforming it has been shown that the equilibrium crude product composition depends on temperature, pressure, and "total" reformer feed composition (i.e., including steam and, where applicable, carbon dioxide). In examining the effects of these key parameters, we used a computer program available to SRI (472173). The natural gas composition assumed (for the desulfurized methane-rich stream) is shown in Table 4.2 and is representative of a typical pipeline gas in the U.S. Gulf Coast area. For the syngas Cases A and B we selected a reformer exit temperature of 1625°F, a pressure of ~20 atmospheres (~295 psia), and a fixed steam:carbon ratio of ~4:1. (The feed steam:carbon ratio used here is defined as the number of molecules of steam per carbon atom contained in hydrocarbons in the reformer feed, i.e., excluding carbon dioxide). The use of CO_2 addition to the reformer feed (at these conditions and a constant steam:carbon ratio) and its effect on crude product H_2:CO ratios was calculated for a "20°F approach to equilibrium," i.e., the compositions refer to equilibrium at a temperature 20°F less than indicated for the reformer exit. The main data are shown in Table 4.3 and illustrated graphically in Figure 4.4. These data demonstrate the thermodynamic feasibility of lowering H_2:CO ratios by CO_2 addition, but

Table 4.1

STEAM REFORMER CONDITIONS

	Case A	Case B	Case C	Case D
Product	Syngas (H_2/CO ratio ≃ 3)	Syngas (H_2/CO ratio = 2)	Hydrogen	Methanol
Temperature (°F) at radiant section inlet	1000	1000	1000	1000
Temperature (°F) at reformer exit	1625	1625	1600	1600
Exit pressure (psia)	295	295	295	295
Steam/carbon ratio*	4.0	4.0	4.0	3.0
Natural gas rate (lb-mols/hr)	8,078	8,078	8,078	8,078
Radiant section thermal duty (MM Btu/hr)	1,132	1,236	993	921
Assumed heat flux (Btu/ft^2)	20,000	20,000	20,000	20,000

---

*Defined as mols steam/atom carbon in natural gas feed. The natural gas composition assumed in this study is given in Table 4.2.

give no indication of possible kinetic constraints. It will be further observed that as the H_2:CO ratio is lowered below the stoichiometric ~3:1 level, there is a progressive increase in the total and imported CO_2 rates (hence also in total reformer feed rates) and in the thermal load. However, the methane slippage falls only slightly and this results in a corresponding small change in the total rate of (CO + H_2) in the reformer product.

Table 4.2

ASSUMED COMPOSITION OF NATURAL GAS FEEDSTOCK

	Volume Dry Basis (%)
Methane	94.49
Ethane	2.70
C_3+	1.49
Carbon dioxide	0.54
Nitrogen + inerts	0.78
Total	100.00

HHV of above mixture = 1,045 Btu/scf

Carbon dioxide addition to the reformer feed is practised in oxo syngas generation from natural gas to provide the desired lower H_2:CO ratios. It has also been applied to methanol synthesis from natural gas, where it permits the utilization of some of the surplus hydrogen in the syngas feed to make methanol, viz,

$$CO_2 + H_2 \longrightarrow CO + H_2O$$

$$CO + 2H_2 \longrightarrow CH_3OH$$

$$CO_2 + 3H_2 \longrightarrow CH_3OH + H_2O$$

Table 4.3

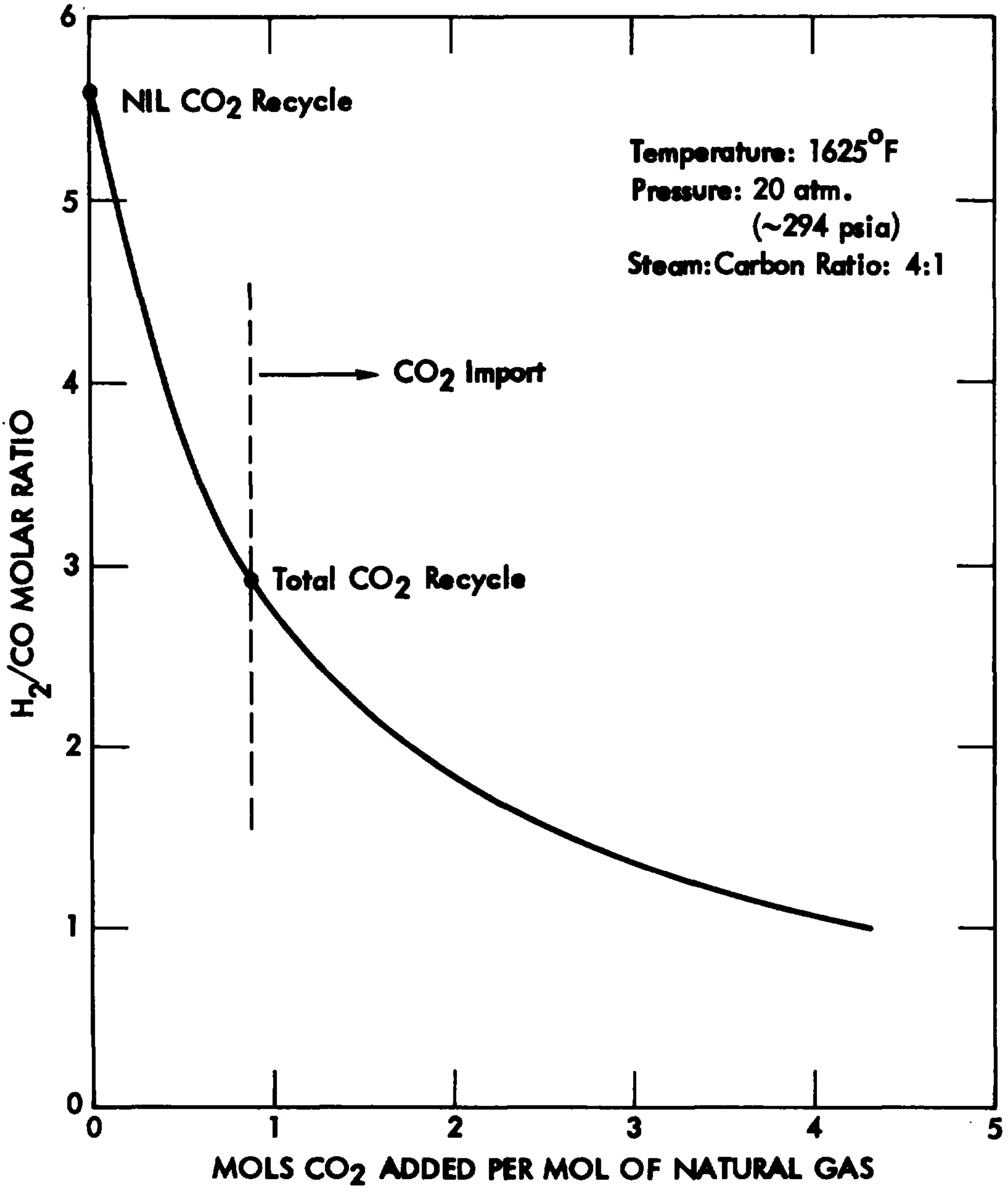
EFFECT OF CO_2 ADDITION TO REFORMER FEED

Basis: (1) Constant reformer feed rate = 8,078 lb-mols/hr (equivalent to 2,500 metric tons/day methanol plant)
(2) Constant steam rate = 34,855 lb-mols/hr
(3) Reformer temperature (at exit) = 1625°F
(4) Reformer pressure (at exit) = 295 psia

CO_2 Addition Rate (lb-mols/hr)	Total Reformer Product Rate (lb-mols/hr, wet basis)	Component Rates in Reformer Product (lb-mols/hr)					H_2/CO Ratio	CO + H_2 Rate (lb-mols/hr)	Radiant Section Heat Load (MM Btu/hr)
		CO	H_2	CO_2	H_2O	CH_4			
Nil	58,742	4,590	26,450	3,359	23,636	645	5.76	31,040	993
7,000	62,296	8,066	23,834	7,094	26,810	430	2.95	31,900	1,132
10,850	70,144	9,628	22,521	9,445	28,119	367	2.34	32,149	1,191
13,930	73,622	10,770	21,579	11,432	29,460	318	2.00	32,349	1,236
23,880	83,625	13,926	19,001	18,404	31,969	263	1.36	32,927	1,374
35,000	94,763	16,525	16,644	26,912	34,506	114	1.01	33,169	1,506

Figure 4.4

H_2/CO RATIO AS A FUNCTION OF CO_2 ADDITION TO REFORMER FEED



However, full and conclusive information is not available in the published and patent literature on the extent to which such addition of carbon dioxide is technically feasible. Industry sources suggested that some units designed to provide syngas for oxo synthesis have been operated satisfactorily with "high" CO_2 rates to give "low H_2:CO ratios." The primary oxo reaction for the formation of aldehyde from olefin demands a 1:1 ratio, e.g., as in:

$$C_3H_6 + CO + H_2 \longrightarrow \underset{\substack{\text{Butyraldehydes} \\ \text{(normal and iso-)}}}{C_3H_7CHO}$$

Because of side reactions leading to the hydrogenation of the olefin (to paraffin) and the aldehyde (to the alcohol) the actual H_2:CO consumption ratio tends to be somewhat greater than 1:1. It is therefore believed that actual industrial operating experience does not go below a 1:1 ratio and probably stops at 1.1-1.2:1, even though some limited pilot scale studies are reported for lower ratios (472129, 472130).

The main problems that are likely to be encountered at high CO_2 addition rates are:

- A slower rate of approach to equilibrium. This is because there is a net consumption of CO_2 by the slower reverse shift reaction (see Table 4.3) i.e.,

$$CO_2 + H_2 \longrightarrow CO + H_2O$$

- Carbon deposition by the disproportionation of CO (i.e., the Boudart reaction: ($2CO \longrightarrow CO_2 + C$). The tendency for this reaction to occur is increased because of the higher CO levels in the mixture that arise at the lower ratios. As discussed before carbon deposition can occur if

$$\frac{[CO]^2}{[CO_2]} > \frac{K_{p(4)}}{P}$$

We believe that these problems are soluble by a careful design of the reformer. The slower approach to equilibrium can be dealt with by designing for a lower heat flux rate across the reformer tubes to prevent possible "hot-spotting." Also, because at the lower temperatures the critical carbon deposition regime can be encountered, the feed gas must be raised to a sufficiently high temperature (~1400°F) before it contacts the catalyst. This is accomplished by inserting inert material in front of the catalyst. To prevent carbon deposition during cooling of the reformer product a rapid-quench system must be used, e.g., a low-residence-time waste heat boiler.

It may be anticipated that, while low H_2:CO ratios (approaching 1:1) are technically feasible, the higher capital and energy costs (both in the reforming and the CO_2 separation stages) plus the additional cost of imported CO_2 would make it uneconomic. (Table 4.4 compares the main features of a 1:1 case with the 3:1 and 2:1 cases and illustrates this point.) For this reason we did not examine the 1:1 case in full flow sheet detail. Indicative economics were worked out from detailed mass/energy balances and by extrapolation of capital costs.

Table 4.4

EFFECT OF SYNGAS H_2:CO RATIO ON REFORMER DESIGN PARAMETERS

	H_2:CO Ratio		
	3:1	2:1	1:1
Molar reformer feed rates (relative)	100	114	156
Number of tubes (relative)	100	110	178
Total CO_2 feed to reformer (relative)	100	199	500
CO_2 recycle rate (relative)	100	161	380
Radiant section heat load (relative)	100	110	134
Natural gas feed usage (mscf/mscf syngas)	0.249	0.247	0.242
Natural gas fuel usage (mscf/mscf syngas)	0.151	0.178	0.219
CO_2 import (lb/mscf syngas)	Nil	8.86	28.32

The question of steam balance is an important aspect of reformer design. The total quantity of steam that is raised and its quality, with regard to pressure and degree of superheat, can be varied within wide limits without any significant loss in energy efficiency. Energy for raising this steam comes partly from the heat recovered in cooling the reformer product, and a convection section within the reformer furnace provides the balance by heat transfer from flue gases leaving the radiant section. The considerable degree of flexibility available to the designer permits steam production at rates that are different from the norm of a "match" (i.e., when steam production equals steam consumption). Thus steam can be either imported into or exported from the system when necessary. The flexibility is achieved by an appropriate design of the furnace radiant and convection sections for varying proportions of the total heat load and by including, if required, "auxiliary firing" in the flue gas duct (415137). The auxiliary burners can be fired independently from the radiant section burners. An illustration of the flexibility available is provided in the designs that are used commercially for methanol, hydrogen, and ammonia manufacture, where the steam production patterns can be widely different.

For cases corresponding to H_2:CO ratios of 3:1 and 2:1 in the present syngas study, we matched the steam quality to the respective different turbine needs for CO_2 compression. In each case the exhaust steam from the turbine was at conditions close to that needed for reformer feed. Since the same steam:carbon ratio (with respect to natural gas feed) is employed, the quantity of steam is the same in both cases. In Case C, viz, hydrogen, the steam quality is designed to meet the needs of hydrogen compression to 750 psia. The compression stage was not included in the flow sheet battery limits because the objective was to furnish a product value for hydrogen at the lower pressure of a conventional plant for use in the economic examination of "skimming schemes," discussed later. The production costs of hydrogen and crude syngas were calculated by showing the high pressure steam generated as an export and regarding the medium pressure reformer steam as an import to which different prices (as discussed later) have been assigned. For Case D, viz, methanol, the design is on a "matching" basis with no export steam. The values assigned to the different grades of steam in Cases C and E are discussed later.

We have assumed the furnace efficiencies in all cases to be in the 85% region, based on the higher heating value of the fuel gas, i.e., where:

$$\text{Furnace efficiency} = \frac{\text{Total heat absorbed (radiant + convective)}}{\text{Total heat released (on higher heating value basis)}}$$

Though no precise published data are available, specifically, on reformer furnace efficiencies, the assumed figure is consistent with the overall energy efficiencies reported for the production of methanol (415329, 472158, 472159, 472160).

It should be appreciated that the choice of steam balance configurations is somewhat arbitrary for the syngas and hydrogen cases (Cases A, B, and C) as it is without defining the end use for the syngas or hydrogen stream. When these streams are required at higher pressures and additional steam is needed for compression and other downstream duties, it would be possible to provide this in an integrated reformer furnace design.

Carbon Dioxide Separation

The reformer catalyst is poisoned by sulfur compounds and the necessary inclusion of a desulfurization stage (e.g., activated carbon beds assumed in this study) ensures that an acid gas removal stage has to deal solely with CO_2. Several proprietary processes are available for acid gas removal (B-1517). A selection of these is displayed in Table 4.5, highlighting their main features. In the present syngas cases, the CO_2 removal requirements are basically similar to those for ammonia or hydrogen manufacture by natural gas steam reforming. For the latter two, the most commonly employed systems are those based on

Table 4.5

SOME SELECTED ACID GAS REMOVAL PROCESSES AND THEIR MAIN FEATURES

Process (licensor)	Solvent	Absorber Pressure (psia)	Range of Acid Gas Partial Pressure (psia)	Typical Process Use	Process Limitations	Utilities Required (scale 1 to 10)
Chemical Solvents: Alkanolamines						
Ucar (Union Carbide)	Monoethanolamine + corrosion inhibitors	25-1000	<100	CO_2 removal at low pressure or sweetening natural gas with low partial pressure of acid gases. When only CO_2 is to be removed reduction to 100 ppm can be achieved in single stage column. Reclaimer system can be used to purge accumulated salts, e.g., formates.	Mercaptans not removed. COS and CS_2 react with and degrade MEA. Not competitive at high partial pressures of acid gases.	10
DEA (SNPA)	Diethanolamine and additive	<1000	>30	Removal of acid gases, from natural gas down to pipeline specifications. (Removes mercaptans, COS, and CS_2.)	Solution foaming occurs with higher concentration of DEA in solution.	9
ADIP (Shell)	Di-isopropanolamine	<1000	<60	Refinery gases with H_2S and low CO_2 contents.	Less complete CO_2 removal. High solvent costs.	7
DGA (Fluor)	Diglycolamine	<1000	>60	Best use is on high partial pressures of H_2S to meet natural gas pipeline specifications.	COS and CS_2 react with and degrade DGA. High solvent cost.	8
Chemical Solvents: Alkaline Potassium Salts						
Benfield (Benfield)	Potassium carbonate and amine plus corrosion inhibitors	100-1000	10-120 (higher if CO_2 only)	CO_2 removal in hydrogen and ammonia manufacture; acid gas removal in natural gas.	CO_2 removal to levels below 0.1-0.2% would require a two stage absorber. A reclaimer system cannot be used to purify contaminated solvent.	7
Catacarb (Eickmeyer)	Aq potassium salts and additives	100-1000	10-80 (higher if CO_2 only)	As for Benfield.	As for Benfield.	8
Giammarco-Vetrocoke (Giammarco)	Potassium carbonate plus arsenic trioxide	200-1000	<10 for H_2S with high CO_2 partial pressure	As for Benfield.	As for Benfield.	7
Physical Solvents						
Rectisol (Lurgi)	Methanol	300-2000	>60	Purification of crude syngas from coal or heavy oil when selective removal of H_2S from CO_2 is required. Can produce separately an H_2S stream for Claus plant feed and a CO_2 stream.	Volatility of solvent requires refrigeration to reduce losses.	2
Selexol (Norton)	Dimethylether of polyethylene glycol	300-1000	>60	As for Rectisol (but gives more selective H_2S removal than Rectisol).	CO_2 removal less complete than for Rectisol.	1

Table 4.5 (Concluded)

SOME SELECTED ACID GAS REMOVAL PROCESSES AND THEIR MAIN FEATURES

Process (licensor)	Solvent	Absorber Pressure (psia)	Range of Acid Gas Partial Pressure (psia)	Typical Process Use	Process Limitations	Utilities Required (scale 1 to 10)
Combined Physical-Chemical Solvents						
Sulfinol (Shell)	Sulfolane (tetrahydrothiophene dioxide) plus diisopropylamine.	<1000	>80 (when CO_2 is present)	Purification of crude syngas from coal or heavy oil when selective separation of H_2S is not required.	Cannot selectively remove H_2S from stream containing CO_2.	5

absorption in alkaline potassium salts and the ones in which alkanolamines are used as solvents. In both these types of processes the absorption of CO_2 proceeds by an exothermic chemical reaction which is reversible, and a stripping stage regenerates the solvent by dissociation of the chemical compound. Compared with processes based on physical solvents, desorption, being endothermic, leads to a higher energy usage but this is adequately compensated for by greater solvent capacities at the relatively low CO_2 partial pressures obtained in steam reforming. For this reason physical solvents such as Rectisol® and Selexol® are not considered economic for use in syngas generation by natural gas steam reforming (see Table 4.5). They are more relevant for schemes based on the partial oxidation of resid or coal gasification, as discussed in Sections 5 and 6.

With the two major types of chemical absorption solvents, i.e., alkaline potassium salts and alkanolamines, the dominant processes in use are Benfield® (based on aqueous K_2CO_3) and Union Carbide Corporation's Ucar® Amine Guard (based on aqueous monoethanolamine). The applicability of K_2CO_3 to the removal of CO_2 was reported in the published literature as early as 1904. However, the actual process was first developed much later (early fifties) by the U.S. Bureau of Mines, and in recent years several improvements were made by Benson and Field, and hence "Benfield" was coined as the name for the process and its licensing corporation. (Benfield Corporation is now a wholly owned UCC subsidiary.) The improvements relate (1) to enhanced solvent capacities and absorption rates by the addition of proprietary activators, (2) to the elimination of corrosion problems by the use of inhibitors, and (3) to the evolution of a process design which minimizes energy usage (472168, B-1517).

As in the case of K_2CO_3, the commercial use of alkanolamines for acid gas absorption followed much later after the original discovery in 1930. The two amines that have proved to be of principal commercial interest are monoethanolamine (MEA) and diethanolamine (DEA). The former is preferable for systems requiring the removal of CO_2 alone, owing to its higher capacity. The latter has been chosen when sulfur compounds, particularly COS and CS_2, are present in appreciable amounts. MEA forms irreversible reaction products with these compounds. DEA on the other hand is much less reactive with these compounds. The most serious operating problem with ethanolamine systems was corrosion until UCC's development of the Ucar® Amine Guard process, which incorporates the corrosion inhibitor system (472178, 472179). Inhibitor systems were also developed by other companies, e.g., Dow Chemical Corporation and Drew Chemical Corporation. The composition of these materials is proprietary; they are commercially available under trademarks. Since their original work UCC have made further improvements to both the corrosion inhibitor system and the process design package which is offered in conjunction (472172).

To arrive at a choice between these two leading processes (Benfield® and Ucar® Amine Guard) we made a detailed examination of their individual features. From data available to SRI there did not appear to be a significant difference in capital costs. The Benfield process showed lower overall energy costs but in the present context Ucar® appears to have some advantages in that:

- The CO_2 slippage is lower, with 100 ppm CO_2 easily attainable with a single absorber column instead of 0.1-0.2 vol% with Benfield®.
- The presence of high CO levels in the syngas can lead to the formation of formic acid and subsequently its salts. With K_2CO_3 systems this would necessitate a higher level of purge (and hence greater K_2CO_3 makeup) than is usually necessary with non-CO systems (e.g., in NH_3 manufacture). With UCC's MEA-based system, the higher volatility of the amine permits its separation from the salt by a reclaimer which takes a small slipstream of the hot lean solvent.

Therefore despite some energy advantages claimed on behalf of Benfield®, we used Amine Guard in our syngas designs. Both processes use low temperature energy (205-225°F) and, apart from a small deficit in the hydrogen case, for the syngas cases, sufficient energy of this quality is available as "waste heat."

Flue Gas Scrubbing

In Case B (syngas with H_2:CO ratio = 2:1) the import of CO_2 is necessary for adjusting the H_2:CO ratio in the reformer product to the desired level. When surplus CO_2, e.g., from an NH_3 or H_2 facility, is not available the cost of obtaining CO_2 from reformer flue gas was examined. We assumed that the furnace is fired by desulfurized natural gas; therefore, the recovered CO_2 stream contains virtually no sulfur and is acceptable for reformer feed. We selected UCC's MEA system for this duty because of the low partial pressure of CO_2 in the flue gas stream for which the alternative K_2CO_3 systems are not suitable. At these conditions MEA systems exhibit much greater solvent capacities. There is a further advantage in using identical systems for CO_2 removal for both the reformer product and flue gases. It is then possible to integrate the two by having a common stripper.

In our evaluation the cost of scrubbing flue gases is worked out to furnish a unit cost of CO_2 for use as a materials cost input.

Hydrogen Production

When hydrogen is produced by the steam reforming of natural gas, the conventional process includes high and low temperature CO shifts, a CO_2 removal, and finally methanation. In the previous SRI study on hydrogen (PEP Report 32A, December 1973) we examined such a process. The technology basis employed was representative of industrial practice at that time. Since then, significant advances have been introduced both in the general area of steam reforming and its more specific application to hydrogen production (472163, 472164, B-1513). Most of the innovations center on achieving higher energy efficiencies by more complete heat recovery with closer temperature approaches. The introduction of the preheating for combustion air by enhanced flue gas cooling was one of the key features. Others relate to improvements in reformer design, and reformer catalyst performance. Also, there has been some progress in the evolution of longer-life materials for reformer tubes and furnace insulation (472163). For hydrogen production the most notable development is the suggested use of pressure swing adsorption (PSA) to replace the low-temperature CO shift, CO_2 removal, and methanation stages (472171). The unadsorbed H_2-lean gas is recycled as reformer fuel. It is claimed that, with rising costs of natural gas feedstock, this approach would become more economic than the conventional method.

For the present, we considered a comprehensive update of hydrogen costs, in the traditional PEP manner, to be beyond the scope of the overall syngas study. The flow sheet design used is thus based on the conventional process but it incorporates several energy saving features which now form a standard part of current industrial practice, viz, the use of air preheating, more extensive heat recovery, and adiabatic operation of the low-temperature CO shift reactor, i.e., without the water injection used in earlier designs. While no detailed flow sheet examination has been carried out for the process variant with PSA, some economic data available to SRI (472171) were used to provide an indication of its likely merits.

Methanol Production

The introduction of the "Low Pressure" (LP) process by ICI in 1967 represented a step change in the development of methanol technology from syngas. Compared with the prevailing "High Pressure" (HP) processes there were significant savings in operating and capital costs. Most notably, there was a major reduction in the consumption of feedstock plus fuel, about 15%-20% (58150, 415329). Following ICI's breakthrough LP processes for methanol were also developed in the early seventies by other companies, e.g., Lurgi, Haldor Topsoe, and Mitsubishi. The HP processes are now obsolete, insofar as installation of new capacity is concerned. There were still a few HP plants in operation during 1981 but most of these are either being converted to the LP process or due to be phased out.

Following the energy crisis of 1973 and the consequent escalation in feedstock prices, the main effort in the evolution of improved designs for the LP process was directed toward further reductions in the consumption of feedstock plus fuel. Besides the advances that were developed in the general area of steam reforming (discussed earlier under Hydrogen Production), many design innovations have been introduced which are more specific to methanol.

In SRI's PEP Report 43B, July 1981, we updated the economics of methanol production. Among natural gas based routes the two leading processes--those licensed by ICI and Lurgi--were examined. However, the process flow sheet versions assumed in the update did not correspond to the highest energy efficiency designs that are now claimed to be practical for these processes (58149, 58150). For the present syngas study we specifically selected the ICI process for a reappraisal. We have used a flow sheet concept corresponding to the latest "high efficiency design," which incorporates the numerous energy-saving features that have come about from a program of continuing development. We therefore consider that the data presented give a realistic picture, not only for the specific process chosen for illustration but for methanol technology in general. This is because the economics of the other leading process (Lurgi) are believed to be very similar. A recent Lurgi publication (472157) claims a slight edge on feedstock plus fuel costs (3%-5%) but this is at the expense of some additional capital that is needed for their more complex synthesis reactor design.

The main developments in the ICI technology have been described in recent ICI and Davy-McKee papers (58111, 58144, 58145, 58150, 415329). The progress toward reduction in energy consumption is briefly reviewed here and is summarized in Table 4.6. The main energy losses in methanol production occur in the reforming section. In the original 1967 version of the process, substantial quantities of heat energy were rejected into cooling water and air (via air coolers) and in the flue gases leaving the reformer.

The first step in the evolution of higher efficiency design was marked by the introduction in late 1974 of a "Reduced Energy Concept" for the ICI process. In its earlier form the design changes introduced consisted of:

Table 4.6

ICI METHANOL PROCESS TREND TOWARD ENERGY REDUCTION

	Pre-1967, HP Process	1967, LP Process	1974, "Reduced Energy Concept"
Added design features	MeOH synthesis pressure 250 atm. Use of reciprocating compressors.	Low pressure (50-100 atm) MeOH synthesis. Use of centrifugal compressors.	Reformer gas heated reboilers. Boiler feedwater heating against reformer gas and in synthesis loop. Air preheating against flue gases. Purge gas turbine expanded for power recovery.
Feedstock and fuel [MM Btu/metric ton MeOH (HHV)]*			
With CO_2 addition	45.2	37.5	35.5
No CO_2 addition†	n.a	n.a	n.a

	1977, Improved Distillation	1979, "High Efficiency Design"
Added design features	Four column MeOH purification instead of conventional two column system—using overhead energy from one column for reboil in others.	Feedstock water saturator using low grade energy. Enhanced heat recoveries from reformer and synthesis sections and from flue gases.
Feedstock and fuel [MM Btu/metric ton MeOH (HHV)]*		
With CO_2 addition	32.0	30.9
No CO_2 addition†	34.7	32.6

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*Sources: 415329, 472158.

†Published data are not available for all the cases; as an approximation a 10% increment above the usages with CO_2 addition may be assumed.

- Replacement of LP steam reboilers in the distillation train by ones that were heated by reformer process gas.
- Inclusion of a boiler feedwater heating system in the reformer gas cooling system and in the methanol synthesis loop to recover energy which had been discarded in the original 1967 design.

In later versions of the Reduced Energy Concept process, further energy savings were effected by:

- Enhanced heat recovery from flue gases by the introduction of an air preheater in the reformer convection section.
- The use of purge gas expanders (linked to generators) to utilize the energy which is available in the high pressure purge gas from the synthesis loop. Previously, this gas was let down unproductively across a pressure reducing valve.

The "Improved Distillation" design was added to the design package by Davy-McKee in 1977. Instead of the conventional two-column system, a four-column arrangement was deployed. The earlier conventional system consisted of a light ends removal column and a methanol refining column. The latter, which produced chemical grade methanol overhead and rejected water in the bottoms stream, also removed higher alcohols as a sidestream a few trays from the bottom. The essential features of this system are described in an ICI patent (58074). The energy consumption of such a system has been quoted as 960 metric ton calories (3.8 million Btu) per metric ton of product methanol. The Davy-McKee four-column system uses a light ends column as before, with the main methanol purification being effected in the next two columns. The first of these is operated under pressure. This permits the condensation of overhead vapor at a sufficiently high temperature for use as reboil energy in the next column, which operates at near atmospheric pressure. The pressure column produces slightly impure methanol (~99.5% w/w), rejects water that is virtually methanol free and removes most of the higher alcohols as a sidestream. The atmospheric pressure column does the final refining. The reduction in energy is obtained through the use of lower reflux ratios. A system similar to that of Davy-McKee (but using three columns) is described in an ICI patent (58097), where the potential savings in energy is indicated to be about 37%-40%. The fourth column in the Davy-McKee system is a relatively small one which further recovers methanol from the bottoms of the atmospheric pressure column.

In the High Efficiency Design (1979) version of the process the additional energy saving features introduced were:

- The use of a "feedstock saturator." This consists of a contacting device such as a packed column where the natural gas feed is scrubbed countercurrently with hot water (472134, 415230). Energy for heating the water is low grade and comes mainly from the methanol synthesis loop. It is claimed that (when no CO_2 addition is used) about 50% of the reformer steam can be transferred to the natural gas feed in this way (415329).
- A greater extent of heat recovery from the reformer product, flue gas, and synthesis product streams. The useful heat recovery from these three streams was extended down to temperatures near 150°F, 120°F, and 180°F respectively (instead of 200°F, 180°F, and 250°F, which were typical of earlier designs).

As stated before, in our reappraisal of the ICI process we have endeavored to formulate a design basis which incorporates all the energy saving features that are now considered representative of the present state of art. The mass and energy balances and the detailed design are as for a case where no CO_2 is available for addition (to either reformer or methanol synthesis feed). The reformer conditions (295 psia and 1600°F at exit and a steam:carbon ratio of 3:1) are typical of current practice. For the methanol synthesis we selected a pressure of 1500 psia and an exit temperature of 520°F. In their published data ICI indicate (58144) that the optimum pressure is probably 1050–1250 psia—however, they recommend 1500 psia for larger plants so that a single methanol reactor can be used and a single-stream operation is maintained. For these conditions a "carbon efficiency" of 96% is considered attainable (58144).

$$\text{Carbon efficiency} = 100 \times \frac{\text{Mols of methanol produced}}{\text{Mols of CO} + \text{CO}_2 \text{ in makeup syngas}}$$

We assumed a recycle/makeup gas ratio of 5.25 with a methanol level of 4 mol% in the crude converter product. This agrees with published data (472165, 472167). The purge stream under these conditions corresponds to about 27% (volume basis) of the makeup syngas.

For the purification section our flow sheet follows the Davy-McKee concept; guidance was taken from the ICI patent (58097) for details on design and energy consumption. The latter was assumed to be 2.38 million Btu/metric ton methanol (600 metric ton-calories/metric ton methanol).

The overall natural gas usage (feedstock plus fuel) was calculated to be 32.77 million Btu/metric ton methanol (based on HHV). This agrees closely with published data (See Table 4.6).

H_2:CO Ratio Adjustment by Separation Processes

From the discussion of syngas uses, which we dealt with earlier, it has been emphasized that the ratios of greatest interest lie in the bracket 1:1-2:1, except for the few cases cited where pure CO is required in the synthesis. Thus, from a natural gas source it would be possible to make a syngas stream in the desired ratio bracket by merely skimming off the surplus H_2 from a 3:1 or a 2:1 stream, instead of importing CO_2. Such an approach could be attractive if there is a use for the skimmed H_2, allowing it to be credited at chemical value. The main processes available for the skimming are as follows:

(1) Cryogenic separation

Several versions of cryogenic processes are used industrially for the separation of hydrogen from $CH_4/H_2/CO$ mixtures. The process examined here is based on Union Carbide's liquid methane wash system. The syngas stream is scrubbed countercurrently with liquid methane to yield a 98.5 vol% H_2 (less than 10 ppm CO) stream as unabsorbed gas. The liquid stream is fractionated in a two-column train to give a purified CO stream (99 vol% purity), a purge fuel stream (which contains most of the CH_4 impurity), and a liquid methane stream for recycle. The cryogenic effect is produced by the compression of a recycle CO stream and its subsequent isentropic expansion.

(2) Pressure swing adsorption (PSA)

The approach here is to selectively adsorb compounds other than hydrogen on a zeolite system and subsequently release them by lowering the pressure. This technique yields hydrogen of very high purity (99.99%+) but its main disadvantage in the present context is that the pressure of the desorbed hydrogen-lean stream is lowered considerably (to approximately 20 psia), necessitating recompression.

(3) Tenneco's Cosorb® (CO absorption process)

This process uses a proprietary solvent which selectively absorbs CO. As with CO_2 absorption systems, the CO is recovered in a stripping stage. A CO stream of up to 99.9% (dry vol basis) can be produced by the process. On residual CO levels in the H_2 product, the process is capable of restricting these to below 10 ppm. We consider that, when this is necessary, it would be more economic to allow a CO slippage in the H_2 product of about 0.1% at the absorption stage, with final reduction (to less than 10 ppm), being carried out in a methanation stage. Since CO absorption can be carried out at the higher pressures of syngas generation, the unabsorbed hydrogen stream is lowered only slightly in pressure. However, desorption is effected at near atmospheric pressures. Thus, as in the case of PSA, recompression of the CO stream would be necessary.

(4) Monsanto's Prism® separators

These are based on the principle of selective permeation through hollow fiber membranes. An enriched hydrogen stream (approaching 98% vol purity) can be produced by this method. The main impurity is CO and, as with Cosorb®, methanation would be necessary. For obtaining higher purity H_2 a combination with PSA would be used instead. An advantage with this method is that the drop in pressure of the main stream is not large. However, the permeating H_2 stream could drop to about 65 psia.

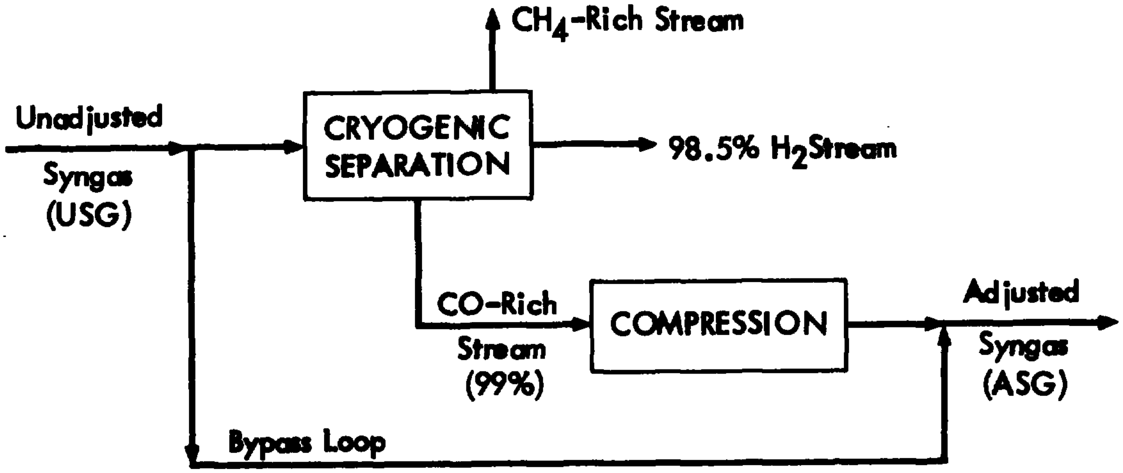
Of these, cryogenic separation of syngas and Cosorb® applied to blast furnace gases, have been previously examined in PEP Report 123 for the production of a refined CO stream. A further examination of these in CO production, with additional feedstock composition cases is presented in Section 7.

Four possible schemes, using the processes listed, were examined and are illustrated by the schematic diagram in Figure 4.5. A detailed description for each of the four systems is given later. With the exception of the scheme using the Prism® separators, in all other

Figure 4.5

SCHEMATIC DIAGRAM FOR H_2 SKIMMING PROCESSES

I CRYOGENIC



II COSORB®

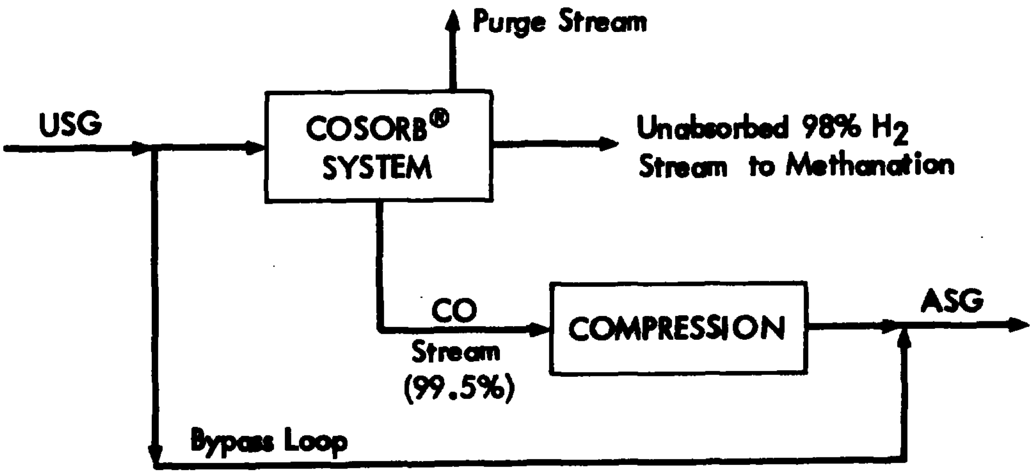
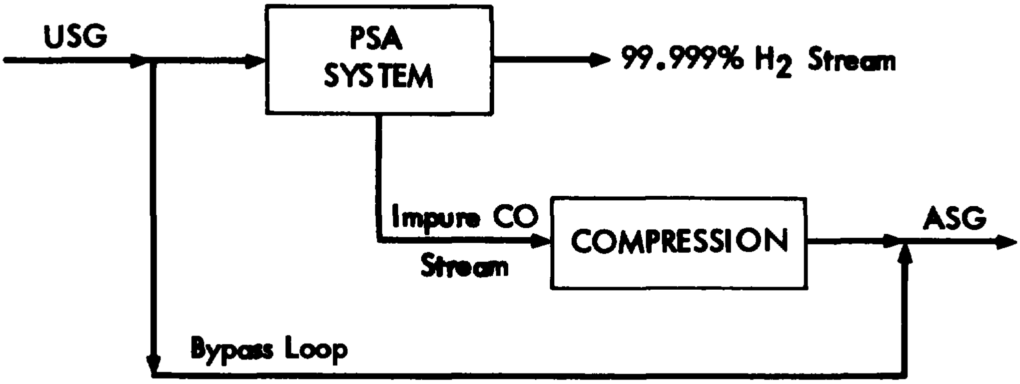
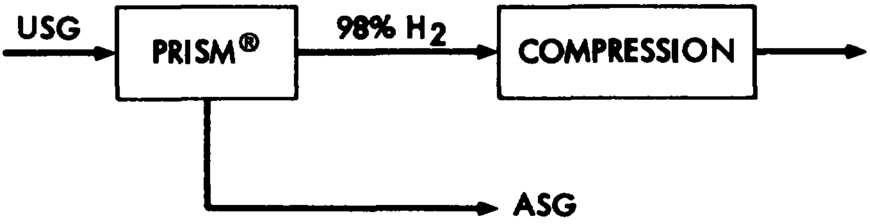


Figure 4.5 (Concluded)

III PRESSURE SWING ADSORPTION (PSA)



IV MONSANTO'S PRISM® SEPARATORS



schemes only a part of the total syngas stream is processed to achieve the desired adjustment in H_2:CO ratios. This is because the specified H_2 purities are possible at high recoveries and the use of a bypass arrangement saves on recompression costs. With the Prism® separator a high H_2 stream purity is not economically attainable at enhanced recoveries and therefore the processing of the whole stream is preferable. Also, unlike the other processes, the recompression is carried out on the enriched H_2 stream and this represents a fixed duty which is not dependent on bypass. In schemes showing bypass, the proportion of the split is determined by the initial syngas ratio and the desired adjusted ratio.

The economics of the four schemes illustrated were examined in a modular way with data made available to SRI by Union Carbide for PSA and cryogenic systems, by Tenneco/Kawasaki Heavy Industries for Cosorb®, and by Monsanto for Prism® separators.

Values Assigned to Steam

In the preceding discussion of reformer steam balances, the design basis for Cases C (hydrogen) and E (crude syngas) was shown to entail the import and export of various grades of steam. The details of steam quality for these cases is tabulated below:

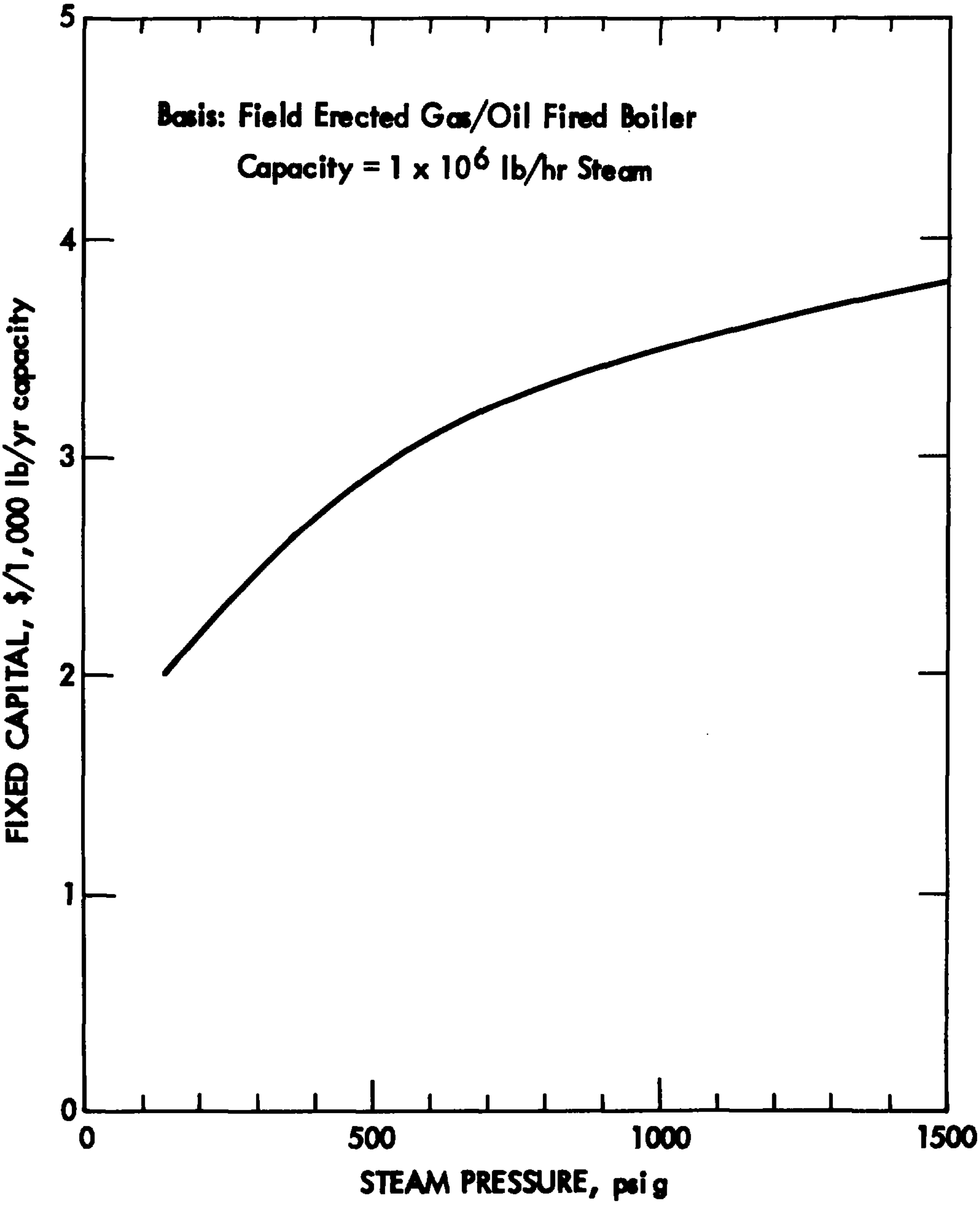
	Export High Pressure Steam			Import Medium Pressure Steam		
	Pressure (psia)	Temp. (°F)	Enthalpy (Btu/lb)	Pressure (psia)	Temp. (°F)	Enthalpy (Btu/lb)
Case C: (hydrogen)	750	900	1,456	310	600	1,315
Case E: (crude syngas)	1100	1000	1,502	350	670	1,348

	Export Low Pressure Steam		
	Pressure (psia)	Temp. (°F)	Enthalpy (Btu/lb)
Case C: (hydrogen)	—	—	—
Case E: (crude syngas)	50	320	1,195

To enable the economic evaluation of these cases it was necessary to assign values to these grades of steam. Reference was made to PEP Report 136 (Plant Utilities Costs, September 1980) in which the economics of steam generation from large, field-erected, gas/oil fired boilers was examined. The fixed capital costs for steam generation equipment were extracted from this report and are shown in Figure 4.6 as a function of steam pressure for a capacity of 1 million lb/hr steam. Since the fuel is a major part of the cost of steam, nonfuel related costs were calculated for the three grades of steam at a constant 30% of the fixed capital. The fuel related charges were based on gas at $4.17/million Btu (HHV) and 85% thermal efficiency (based on HHV of fuel). Owing to the small differences in the enthalpies of similar grades of steam in Cases C and E, a single value was assigned to each of the two grades. The computation is tabulated below:

Figure 4.6

STEAM GENERATION CAPITAL AS A FUNCTION OF PRESSURE



	High Pressure Steam	Medium Pressure Steam	Low Pressure Steam
Pressure assumed for cost (psia)	900	400	150
Temperature assumed for cost (°F)	900	650	380
Fixed capital, PEP Cost Index = 400 ($/1,000 lb/yr capacity)	3.4	2.7	2.1
Net enthalpy requirement (Btu/lb)	1,370	1,250	1,110
Nonfuel costs at 30% fixed capital ($/1,000 lb)	1.02	0.81	0.63
Fuel costs with gas at $4.17/million Btu and 85% efficiency ($/1,000 lb)	6.72	6.13	5.44
Fuel and nonfuel costs ($/1,000 lb)	7.74	6.94	6.07
Rounded steam value ($/1,000 lb)	7.75	6.95	6.10

Process Description

Cases A and B: Syngas Streams with H_2:CO Ratios of 3:1 and 2:1 Obtained by CO_2 Addition to Reformer Feed

The process sequence for both these cases is virtually identical and is illustrated by the flow diagrams in Figures 4.7 and 4.8 (foldouts at end of report). The only differences are:

- Heat exchanger E-105 in the heat recovery train is not required for the 2:1 case.
- The CO_2 compressor K-201 handles the imported gas in addition to the recycle gas for the 2:1 case.
- In the 2:1 case, both the fuel and the feed natural gas are desulfurized to afford a sulfur free flue gas for the CO_2 recovery and import.

The corresponding equipment requirements and the stream flows are presented in Tables 4.7 through 4.10. As discussed before, these refer to a production scale obtained with a natural gas reformer feed rate equivalent to 2,500 metric tons/day of methanol yielding a syngas rate in the region of 300 million scfd.

Natural gas is received by pipeline and reduced to 310 psia at the reformer section inlet before being passed through beds of activated carbon M-101 and M-102 for adsorption of H_2S. The two beds are used alternately, i.e., one on line and the other on the regeneration cycle. (The whole stream is desulfurized in the 2:1 case.) The desulfurized reformer feed gas is mixed with steam and CO_2 and goes to the reformer's (F-101) radiant section via preheating convection bank E-101, which heats the stream to 1000°F. The tubes of the radiant section contain a reforming catalyst such as United Catalyst Corporation's G-56B. Convection tube banks E-102 and E-103 in the furnace are employed for steam superheating and air preheating respectively. Air blower K-101 introduces the air into the furnace (fired by natural gas) and a flue gas extractor K-102 is used for the discharge of flue gases. The crude reformer product leaves the radiant section at 1625°F and 295 psia and is quenched to 650°F in E-104, where the heat is recovered in the generation of steam. The superheated steam from E-102 goes via steam drum V-101 to drive CO_2 compressor K-201. A noncondensing turbine is employed. The quantity of steam generated is the same for both cases but for the 2:1 case, where compression energy requirements are greater (owing to a higher CO_2 rate), the quality of steam is superior. The steam turbine inlet and exit conditions for the two cases are as follows:

	Case A	Case B
Inlet pressure (psia)	640	900
Inlet temperature (°F)	780	980
Exit pressure (psia)	310	310
Exit temperature (°F)	700	640

Further heat recovery from the reformer product takes place in E-105 (not for the 2:1 case), E-201, and E-202. The first of these is used to heat deaerated water and the last provides the preheat before deaeration. E-201 comprises the reboiler in the CO_2 stripping column. Final lowering of the reformer product temperature to 155°F is carried out in E-206 against cooling water. The water condensed in E-201, E-202, and E-206 is removed by condensate drums V-202, V-203, and V-204 respectively.

The cooled reformer stream enters the CO_2 removal system at 155°F and 250 psia. Absorption of CO_2 in MEA solution is carried out in column C-201, which is equipped with sieve trays. The flow of the two phases is countercurrent. Heat transfer surfaces (E-207) in the column remove the heat of solution and maintain the exiting rich solution temperature below 170°F. The rich solution is raised to 190°F by heat from the stripper bottoms in E-205 before it enters flash vessel V-205, where part of the CO_2 is removed. Further heat transfer from the stripper bottoms in E-204 heats it to 210°F before the stream is fed near the top of stripper column C-202. The stripper column (which also has sieve trays) is operated at 20 psia at the top and a base temperature of 225°F. The heat for the stripping is provided by the reformer product, in E-201. A reflux is maintained at the top of the column to minimize the presence of MEA in the stripped CO_2 gas. The lean MEA solution from the bottom of the stripper gives up heat as described before and is further cooled against cooling water in E-203 before being returned to the absorber. The unabsorbed gas, i.e., the product syngas from C-201, is cooled in E-209 to 120°F.

Table 4.7

SYNGAS (H_2:CO RATIO = 3:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 RECYCLE

MAJOR EQUIPMENT

Plant Capacity: 97 x 10^9 scf/yr Syngas
at 0.90 Stream Factor

Equipment Number	Name	Size (bhp)	Material of Construction	Remarks
	Compressors			
K-101	Air blower	5,260	Carbon steel	
K-102	Flue gas extractor	5,940	Carbon steel	Not shown on drawing.
K-201	CO_2 compressor	13,000	Carbon steel	

Equipment Number	Name	Size (sq ft)	Heat Load (MM Btu/hr)	Material of Construction: Shell	Material of Construction: Tubes	Remarks
	Exchangers*					
E-101	Feed preheater	19,400	320	Flue duct	316 ss	
E-102	Steam superheater	17,600	77	Flue duct, carbon steel		
E-103	Air preheater	38,700	105	Flue duct, carbon steel		
E-104	Heat recovery boiler	8,300	560	Carbon steel	316 ss	
E-105	Boiler feedwater heater	16,800	170	Carbon steel	316 ss	
E-201	CO_2 stripper reboiler	34,700	320	Carbon steel	316 ss	
E-202	Demin water preheater	6,200	70	Carbon steel	316 ss	
E-203	Lean amine cooler	35,300	93	Carbon steel	Carbon steel	
E-204	Amine interchanger-I	70,900	80	Carbon steel	Carbon steel	
E-205	Amine interchanger-II	59,000	75	Carbon steel	Carbon steel	
E-206	Absorber feed cooler	12,000	110	Carbon steel	316 ss	
E-207	Absorber intercooler	17,900	250	Carbon steel	Carbon steel	
E-208	Stripper condenser	11,800	240	Carbon steel	Carbon steel	
E-209	Syngas cooler	24,000	35	Carbon steel	Carbon steel	

Equipment Number	Name	Heat Load (MM Btu/hr)	Material of Construction	Remarks
	Furnaces			
F-101	Natural gas reformer	1,930	Ni-Cr alloy	1,350 4 in. by 40 ft long tubes filled with 4,700 ft^3 catalyst.

Equipment Number	Name	Volume (gal)	Material of Construction	Remarks
	Tanks			
T-201	Amine storage	90,000	316 ss	Not shown on drawing.
	Pressure vessels			
V-101	Steam drum	64,000	Carbon steel	
V-201	Reflux drum	20,000	Carbon steel	
V-202	Condensate-I	31,000	316 ss	
V-203	Condensate-II	13,000	316 ss	
V-204	Condensate-III	11,000	316 ss	
V-205	Flash vessel	50,000	Carbon steel	

Equipment Number	Name	Height (ft)	Diameter (ft)	Material of Construction: Shell	Material of Construction: Trays	Remarks
	Columns					
C-201	Amine absorber	70	18.4	Carbon steel	316 ss	30 sieve trays, 24 in. spacing.
C-202	Amine stripper	60	21.5	Carbon steel	316 ss	25 sieve trays, 24 in. spacing.

Equipment Number	Name	Size	Material of Construction	Remarks
	Miscellaneous equipment			
M-101	H_2S adsorber	550 cu ft	Carbon steel	
M-102	H_2S adsorber	550 cu ft	Carbon steel	
M-103	Flue gas stack	6 ft dia x 120 ft high	Carbon steel	Not shown on drawing.

Pumps

100 Section - 2, including 1 operating, 1 spare; 759 operating bhp.
200 Section - 6, including 3 operating, 3 spares; 2900 operating bhp.

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*The heat transfer areas shown represent a total. In our evaluation throughout this report, we have assumed an upper limit of 10,000 sq ft for a single unit with replication as necessary.

Table 4.8

SYNGAS (H_2:CO RATIO = 3:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 RECYCLE

STREAM FLOWS

Plant Capacity: 97 x 10^9 scf/yr Syngas
at 0.90 Stream Factor

	Stream Flows (lb-mols/hr)						
	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Methane	7,634.07	—	—	7,634.07	429.80	4,624.44	—
Carbon dioxide	44.00	—	6,996.06	7,040.06	7,093.50	27.50	—
Carbon monoxide	—	—	—	—	8,066.04	—	—
Hydrogen	—	—	—	—	23,834.37	—	—
Nitrogen + inerts	62.70	—	—	62.70	62.70	38.50	43,313.99
Ethane	217.80	—	—	217.80	—	132.00	—
C_3+	119.90	—	—	119.90	—	71.50	—
Water	—	34,854.91	127.60	34,982.51	26,809.59	—	—
Oxygen	—	—	—	—	—	—	11,503.90
Total (lb-mols/hr)	8,078.47	34,854.91	7,123.66	50,057.04	66,296.00	4,893.94	54,817.89
Total (lb/hr)	139,325	627,388	310,124	1,076,837	1,076,838	84,386	1,580,917

	Stream Flows (lb-mols/hr)						
	(8)	(9)	(10)	(11)	(12)	(13)	(14)
Methane	46.24	429.80	—	—	429.80	—	429.80
Carbon dioxide	5,098.46	7,093.50	—	—	7,093.50	—	7,093.50
Carbon monoxide	46.24	8,066.03	—	—	8,066.03	—	8,066.03
Hydrogen	—	23,834.36	.01	—	23,834.35	—	23,834.35
Nitrogen + inerts	43,352.49	62.70	—	—	62.70	—	62.70
Ethane	2.64	—	—	—	—	—	—
C_3+	1.43	—	—	—	—	—	—
Water	9,894.83	8,563.37	18,246.22	3,684.93	4,878.45	4,233.49	644.96
Oxygen	1,462.41	—	—	—	—	—	—
Total (lb-mols/hr)	59,904.74	48,049.76	18,246.23	3,684.93	44,364.83	4,233.49	40,131.34
Total (lb/hr)	1,665,303	748,406	328,432	66,329	682,077	76,203	605,874

	Stream Flows (lb-mols/hr)				
	(15)	(16)	(17)	(18)	(19)
Methane	429.80	—	—	429.80	—
Carbon dioxide	3.97	7,089.52	—	3.97	93.58
Carbon monoxide	8,066.03	—	—	8,066.03	—
Hydrogen	23,834.35	—	—	23,834.35	—
Nitrogen + inerts	62.70	—	—	62.70	—
Ethane	—	—	—	—	—
C_3+	—	—	—	—	—
Water	515.97	128.99	296.88	219.08	1.70
Oxygen	—	—	—	—	—
Total (lb-mols/hr)	32,912.82	7,218.51	296.88	32,615.93	95.28
Total (lb/hr)	291,613	314,261	5,344	286,269	4,149

Table 4.9

SYNGAS (H_2:CO RATIO = 2:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

MAJOR EQUIPMENT

Plant Capacity: 98 x 10^9 scf/yr Syngas
at 0.90 Stream Factor

Equipment Number	Name	Size (bhp)	Material of Construction	Remarks
	Compressors			
K-101	Air blower	6,250	Carbon steel	
K-102	Flue gas extractor	7,050	Carbon steel	Not shown on drawing.
K-201	CO_2 compressor	26,100	Carbon steel	

Equipment Number	Name	Size (sq ft)	Heat Load (MM Btu/hr)	Material of Construction Shell	Material of Construction Tubes
	Exchangers				
E-101	Feed preheater	23,100	370	Flue duct, 316 ss	
E-102	Steam superheater	50,300	210	Flue duct, carbon steel	
E-103	Air preheater	52,400	130	Flue duct, carbon steel	
E-104	Heat recovery boiler	9,600	645	Carbon steel	316 ss
E-201	CO_2 stripper reboiler	55,900	520	Carbon steel	316 ss
E-202	Demin water preheater	6,200	88	Carbon steel	316 ss
E-203	Lean amine cooler	42,400	110	Carbon steel	Carbon steel
E-204	Amine interchanger-I	116,000	130	Carbon steel	Carbon steel
E-205	Amine interchanger-II	95,000	120	Carbon steel	Carbon steel
E-206	Absorber feed cooler	13,900	135	Carbon steel	316 ss
E-207	Absorber intercooler	28,800	410	Carbon steel	Carbon steel
E-208	Stripper condenser	19,000	390	Carbon steel	Carbon steel
E-209	Syngas cooler	24,000	35	Carbon steel	Carbon steel

Equipment Number	Name	Heat Load (MM Btu/hr)	Material of Construction	Remarks
	Furnaces			
F-101	Natural gas reformer	2,290	Ni-Cr alloy	1,480 4 in. by 40 ft long tubes filled with 5,150 ft^3 catalyst.

Equipment Number	Name	Volume (gal)	Material of Construction	Remarks
	Tanks			
T-201	Amine storage	110,000	316 ss	Not shown on drawing.
	Pressure vessels			
V-101	Steam drum	64,000	Carbon steel	
V-201	Reflux drum	32,000	Carbon steel	
V-202	Condensate-I	33,000	316 ss	
V-203	Condensate-II	13,000	316 ss	
V-204	Condensate-III	13,000	316 ss	
V-205	Flash vessel	60,000	Carbon steel	

Equipment Number	Name	Height (ft)	Diameter (ft)	Material of Construction Shell	Material of Construction Trays	Remarks
	Columns					
C-201	Amine absorber	70	20.2	Carbon steel	316 ss	33 sieve trays, 24 in. spacing.
C-202	Amine stripper	60	27.0	Carbon steel	316 ss	25 sieve trays, 24 in. spacing.

Equipment Number	Name	Size	Material of Construction	Remarks
	Miscellaneous equipment			
M-101	H_2S adsorber	960 cu ft	Carbon steel	
M-102	H_2S adsorber	960 cu ft	Carbon steel	
M-103	Flue gas stack	11.5 ft dia x 120 ft high	Carbon steel	Not shown on drawing.

Pumps

100 Section - 2, including 1 operating, 1 spare; 1012 operating bhp.
200 Section - 6, including 3 operating, 3 spares; 3520 operating bhp.

Table 4.10

SYNGAS (H_2:CO RATIO = 2:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

STREAM FLOWS

Plant Capacity: 98 x 10^9 scf/yr Syngas
at 0.90 Stream Factor

	Stream Flows (lb-mols/hr)						
	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Methane	7,634.00	—	—	7,634.00	317.53	5,501.10	—
Carbon dioxide	44.00	—	13,926.00	13,970.00	11,431.65	31.90	—
Carbon monoxide	—	—	—	—	10,770.02	—	—
Hydrogen	—	—	—	—	21,579.16	—	—
Nitrogen + inerts	62.70	—	—	62.70	62.70	45.10	51,510.81
Ethane	217.80	—	—	217.80	—	157.30	—
C_3+	119.90	—	—	119.90	—	85.80	—
Water	—	34,854.61	299.20	35,153.81	29,460.49	—	—
Oxygen	—	—	—	—	—	—	13,681.80
Total (lb-mols/hr)	8,078.40	34,854.61	14,225.20	57,158.21	73,621.55	5,821.20	65,192.61
Total (lb/hr)	139,324	627,383	618,130	1,384,837	1,384,837	100,380	1,880,121

	Stream Flows (lb-mols/hr)						
	(8)	(9)	(10)	(11)	(12)	(13)	(14)
Methane	55.01	317.53	—	—	317.53	—	317.53
Carbon dioxide	6,067.62	11,431.65	.01	—	11,431.65	—	11,431.64
Carbon monoxide	55.01	10,770.01	.01	—	10,770.01	—	10,770.01
Hydrogen	—	21,579.15	.01	—	21,579.15	—	21,579.15
Nitrogen + inerts	51,555.91	62.70	—	—	62.70	—	62.70
Ethane	3.15	—	—	—	—	—	—
C_3+	1.72	—	—	—	—	—	—
Water	11,775.06	8,692.57	20,767.91	3,749.25	4,943.32	4,222	721.32
Oxygen	1,731.04	—	—	—	—	—	—
Total (lb-mols/hr)	71,244.52	52,853.61	20,767.94	3,749.25	49,104.36	4,222	44,882.35
Total (lb/hr)	1,980,499	1,011,012	373,822	67,487	943,526	75,996	867,530

	Stream Flows (lb-mols/hr)					
	(15)	(16)	(17)	(18)	(19)	(20)
Methane	317.53	—	—	317.53	—	—
Carbon dioxide	6.40	11,425.24	—	6.40	150.81	2,501.40
Carbon monoxide	10,770.01	—	—	10,770.01	—	—
Hydrogen	21,579.15	—	—	21,579.15	—	—
Nitrogen + inerts	62.70	—	—	62.70	—	—
Ethane	—	—	—	—	—	—
C_3+	—	—	—	—	—	—
Water	476.07	245.25	254.69	221.38	3.24	53.90
Oxygen	—	—	-	—	—	—
Total (lb-mols/hr)	33,211.86	11,670.49	254.69	32,957.17	154.05	2,555.30
Total (lb/hr)	360,405	507,125	4,584	355,821	6,694	111,032

Case C: Hydrogen by Conventional Steam Reforming of Natural Gas (Including CO Shift Stages and Methanation)

The process sequence for hydrogen synthesis is similar to syngas cases for the reforming section as illustrated in Figure 4.9 (foldout at end of report). The equipment list and stream flows are given in Tables 4.11 and 4.12. As in the syngas cases, the production scale is equivalent to a reformer feed for 2,500 metric tons/day methanol. This corresponds to a hydrogen output of 479 million lb/yr (100% H_2 basis). There is no recycle CO_2 but reformer conditions used are similar, i.e., 1600°F and 295 psia at the exit of the radiant section.

As before, heat recovery for steam generation is carried out in E-104. The quenched reformer product at 650°F is subjected to a high temperature CO shift in an adiabatic, fixed bed catalytic reactor (C-301) using United Catalyst Corporation's Catalyst G-3A or equivalent. The temperature of the stream rises to 760°F, and approximately 75% of the CO present is shifted. The partially shifted stream is used to provide premethanation heat in E-302 and preheat for deaerated water in E-106 and its temperature is lowered to 410°F before entry to the low temperature shift reactor C-302. As before, this is an adiabatic fixed bed design and is packed with United Catalyst's G-66B catalyst (or equivalent). Further conversion of CO takes place and the CO level in the stream is reduced to 0.4 vol% (dry basis). The temperature rises to 445°F. Heat transfer to boiler feedwater takes place in E-107. This is followed by heat recovery in CO_2 stripper reboiler E-201, exit temperature 280°F. Cooling to 155°F is accomplished in E-105 against cooling water before the stream enters the CO_2 removal system.

The aqueous MEA system is identical in design features to that for the syngas cases. The unabsorbed hydrogen-rich stream contains 100 ppm CO_2 and $\simeq$0.4% CO. It is preheated to 590°F in two stages, in E-301 (against methanation product) and in E-302 (as described before) before methanation in C-303 (packed with United Catalyst's G-65 catalyst), where the residual carbon oxides content is reduced to <10 ppm. The methanated product, i.e., the H_2 product stream after heat recovery in E-301 (as described before) is cooled in E-303 to 120°F.

Table 4.11

HYDROGEN (97%) FROM STEAM REFORMING OF NATURAL GAS

MAJOR EQUIPMENT

Plant Capacity: 479 Million lb/yr
(217,000 Metric Tons/yr) Hydrogen, 100% Basis,
at 0.90 Stream Factor

Equipment Number	Name	Size (bhp)	Material of Construction	Remarks
	Compressors			
K-101	Air blower	4,130	Carbon steel	
K-102	Flue gas extractor	4,670	Carbon steel	Not shown on drawing.

Equipment Number	Name	Size (sq ft)	Heat Load (MM Btu/hr)	Material of Construction: Shell	Material of Construction: Tubes
	Exchangers				
E-101	Feed preheater	14,300	220	Flue duct, 316 ss	
E-102	Steam superheater	42,500	180	Flue duct, carbon steel	
E-103	Air preheater	40,100	95	Flue duct, carbon steel	
E-104	Heat recovery boiler	7,100	470	Carbon steel	316 ss
E-105	Absorber feed cooler	20,400	195	Carbon steel	316 ss
E-106	Boiler feed heater	5,900	130	Carbon steel	316 ss
E-107	Demin. water heater	3,900	88	Carbon steel	316 ss
E-201	CO_2 stripper reboiler-1	19,800	180	Carbon steel	316 ss
E-202	CO_2 stripper reboiler-2	16,700	140	Carbon steel	Carbon steel
E-203	Lean amine cooler	35,300	93	Carbon steel	Carbon steel
E-204	Amine interchanger-I	70,900	80	Carbon steel	Carbon steel
E-205	Amine interchanger-II	59,000	75	Carbon steel	Carbon steel
E-206	Absorber intercooler	17,900	250	Carbon steel	Carbon steel
E-207	Stripper condenser	11,800	240	Carbon steel	Carbon steel
E-301	Methanator preheater-1	13,200	70	Carbon steel	316 ss
E-302	Methanator preheater-2	1,870	34	Carbon steel	316 ss
E-303	H_2 product cooler	9,200	55	Carbon steel	Carbon steel

Equipment Number	Name	Heat Load (MM Btu/hr)	Material of Construction	Remarks
	Furnaces			
F-101	Natural gas reformer	1,650	Ni-Cr alloy	1,190 4 in. by 40 ft long tubes filled with 4,140 ft^3 catalyst.

Equipment Number	Name	Volume (gal)	Material of Construction	Remarks
	Tanks			
T-201	Amine storage	90,000	316 ss	Not shown on drawing.
	Pressure vessels			
V-101	Steam drum	64,000	Carbon steel	
V-201	Reflux drum	16,000	Carbon steel	
V-202	Condensate-I	30,000	316 ss	
V-203	Condensate-II	25,000	316 ss	
V-204	Flash vessel	50,000	Carbon steel	

Equipment Number	Name	Height (ft)	Diameter (ft)	Material of Construction: Shell	Material of Construction: Trays	Remarks
	Columns					
C-201	Amine absorber	70	18.4	Carbon steel	316 ss	30 sieve trays, 24 in. spacing.
C-202	Amine stripper	60	21.5	Carbon steel	316 ss	25 sieve trays, 24 in. spacing.
C-301	High temp CO shift	30	20.4	316 ss clad		6,670 cu ft of G/3A catalyst (Girdler) for high-temp shift.
C-302	Low temp CO shift	28	18.9	316 ss clad		5,300 cu ft of C/18/8/C (United Catalyst Corp.) low-temp shift catalyst.
C-303	Methanator	25	11.0	316 ss clad		1,840 cu ft of G-65 girdler catalyst.

Equipment Number	Name	Size	Material of Construction	Remarks
	Miscellaneous equipment			
M-101	H_2S adsorber	550 cu ft	Carbon steel	
M-102	H_2S adsorber	550 cu ft	Carbon steel	
M-103	Flue gas stack	9.7 ft dia x 120 ft high	Carbon steel	Not shown on drawing.

Pumps

100 Section - 2, including 1 operating, 1 spare; 1012 operating bhp.
200 Section - 6, including 3 operating, 3 spares; 1842 operating bhp.

Table 4.12

HYDROGEN (97%) FROM STEAM REFORMING OF NATURAL GAS

STREAM FLOWS

**Plant Capacity: 479 Million lb/yr
(217,000 Metric Tons/yr) Hydrogen, 100% Basis
at 0.90 Stream Factor**

	Stream Flows (lb-mols/hr)					
	(1)	(2)	(3)	(4)	(5)	(6)
Methane	7,634.12	—	7,634.12	645.08	645.08	645.08
Carbon dioxide	44.00	—	44.00	3,358.73	6,812.80	7,794.05
Carbon monoxide	—	—	—	4,589.51	1,135.45	154.19
Hydrogen	—	—	—	26,449.97	29,904.04	30,885.29
Nitrogen + inerts	62.70	—	62.70	62.70	62.70	62.70
Ethane	217.80	—	217.80	—	—	—
C_3+	119.90	—	119.90	—	—	—
Water	—	34,855.13	34,855.13	23,636.15	20,182.08	19,200.83
Oxygen	—	—	—	—	—	—
Total (lb-mols/hr)	8,078.52	34,855.13	42,933.65	58,742.14	58,742.15	58,742.14
Total (lb/hr)	139,326	627,392	766,718	766,718	766,717	766,718

	Stream Flows (lb-mols/hr)					
	(7)	(8)	(9)	(10)	(11)	(12)
Methane	645.08	—	645.08	—	645.08	—
Carbon dioxide	7,794.05	—	7,794.05	—	4.68	7,789.37
Carbon monoxide	154.19	—	154.19	—	154.19	—
Hydrogen	30,885.28	.01	30,885.28	.01	30,885.27	—
Nitrogen + inerts	62.70	—	62.70	—	62.70	—
Ethane	—	—	—	—	—	—
C_3+	—	—	—	—	—	—
Water	8,575.34	10,625.49	633.47	7,941.86	481.44	152.03
Oxygen	—	—	—	—	—	—
Total (lb-mols/hr)	48,116.64	10,625.50	40,174.77	7,941.87	32,233.36	7,941.40
Total (lb/hr)	575,459	191,259	432,506	142,954	87,037	345,469

	Stream Flows (lb-mols/hr)					
	(13)	(14)	(15)	(16)	(17)	(18)
Methane	803.95	803.95	—	3,971.06	—	39.71
Carbon dioxide	—	—	—	23.10	—	4,378.29
Carbon monoxide	—	—	—	—	—	39.71
Hydrogen	30,403.98	30,403.98	—	—	—	—
Nitrogen + inerts	62.70	62.70	—	31.90	37,190.47	37,222.38
Ethane	—	—	—	113.30	—	2.27
C_3+	—	—	—	61.60	—	1.23
Water	644.99	211.47	433.52	—	—	8,497.66
Oxygen	—	—	—	—	9,878.15	1,254.28
Total (lb-mols/hr)	31,915.62	31,482.10	433.52	4,200.96	47,068.62	51,435.53
Total (lb/hr)	87,037	79,233	7,803	72,418	1,357,434	1,429,853

Case D: Methanol from Natural Gas by ICI Low Pressure Process (High Efficiency Design)

The process sequence is illustrated by the flow diagram in Figure 4.10 (foldout at end of report). The equipment list and material balances are shown in Tables 4.13 and 4.14. The design concepts underlying the flow sheet are based on guidelines indicated in the literature (58144, 58145, 415329). The only energy recovery feature that we have added is the use of the hydraulic turbine for lowering the pressure of the liquid crude methanol stream. There are several examples of such systems in industrial practice (475322) but thus far any possible application to methanol has not been commercialized. Discussions with Davy-McKee revealed that, even though some degassing would occur, this would not constitute a serious design problem. The main problems would be related to materials of construction for the turbine to deal with possible corrosion/erosion effects that may arise from the presence of CO_2 and H_2O.

The reforming section differs from that assumed for syngas and hydrogen cases in one essential respect. A feedstock water saturator (C-101) is employed to furnish 50% of the process reformer steam. As before, the natural gas feedstock is desulfurized in M-101 and M-102 with active carbon. The feedstock is heated to 190°F by reformer product in E-109. The saturation of feedstock is effected by countercurrent scrubbing with water in C-101, a packed column containing 1 inch pall rings. The water comes in at 400°F and exits at 250°F. The column design is for 95% saturation and for a 10°F temperature approach, so that the gas stream leaves at 390°F, before it is blended with additional reformer steam. The latter stream is the exhaust steam from the recycle compressor in the methanol synthesis section, which leaves the turbine at 350 psia and 670°F. Preheating of the reformer reactants to 1000°F takes place in E-101, and the reaction is carried out in the radiant section of reforming furnace F-101. The furnace exit temperature and pressure are 1600°F and 295 psia respectively.

A major proportion of the fuel for the furnace consists of a purge from the methanol synthesis section, the balance being natural gas. The hot flue gases leave the radiant section at 1700°F and provide heat for convective sections E-101, E-102, E-103, and E-104. As described before, E-101 comprises the reformer feed preheater. E-102 and E-103 are part of the steam raising system. Most of the latent heat for the steam is provided by the reformer product, in E-105. Convective section E-103 provides the balance. E-102 superheats the steam which leaves steam drum V-101 at 1100 psia and 1000°F. This steam drives the turbines for compressors K-201 and K-202 in the methanol synthesis section. K-201 (makeup gas compressor is a two-casing centrifugal unit driven by a condensing turbine with an exit pressure of 1.27 psia (2.6 inches Hg). K-202, the recycle gas compressor, is a high efficiency, single-casing centrifugal unit driven by a back-pressure turbine. As mentioned before, the exhaust steam from this turbine (at 350 psia) is used as reformer steam. Convective section E-104 preheats furnace air to 510°F. The flue gases leaving E-104 are cooled to 260°F and are extracted through the flue stack (M-103) by single-stage turbo-blower K-102. A similar machine, K-101, injects air into the furnace. The reformer product, which leaves the furnace radiant section at 1600°F releases heat in exchangers E-105, E-306, E-106, E-107, E-108, and E-109. E-105, as mentioned before, comprises part of the steam generation system. E-306 is the refining column reboiler in the purification section. E-106 heats the circulating water in the saturator loop, and E-107 preheats the demineralized water which forms part of the overall steam system. E-108 and E-109 preheat the reformer fuel and feed respectively. The heat recovery sequence cools the reformer product to 180°F. Final cooling to 100°F is against cooling water in E-110. A major part of the water in the reformer product is condensed. The condensate is removed via drums V-102 to V-105 and returned to the demineralized water system.

A two-casing centrifugal compressor, K-201, with an intercooler, raises the pressure of the makeup syngas from 240 psia to 1500 psia. The recycle gas from methanol synthesis is compressed in K-202, a single-casing machine. The total synthesis feed (makeup plus recycle syngas) is heated to 270°F in E-202, by the synthesis product. Part of the synthesis feed is further heated (against synthesis product) to 455°F in E-203. It is then fed to reactor R-201 via a gas distributor. The methanol synthesis reactor consists of a single-shell vessel packed with ICI's proprietary copper based catalyst. The rest of the synthesis feed, at 270°F, is used as a "cold-shot" for controlling the temperature of the reactor. This is achieved by injecting portions of the gas mixture into the catalyst bed at three levels through specially designed distributor lozenges. The crude synthesis product emerges at 520°F and is split into two streams for heat recovery. Part of the energy, as described before, preheats the direct synthesis feed in E-203. The remainder heats the dimineralized and saturator water streams in E-205 and E-204. The former heats the water to 400°F, and after a part of the heated water is diverted to the saturator, the latter heats the balance of the stream to 510°F before it enters steam drum V-101. The two crude synthesis streams are now combined for the heat transfer in E-202 against total synthesis feed. The temperature of the synthesis product leaving E-202 is 200°F. Further heat recovery to 180°F is effected in E-206, where the energy is used to heat the purge stream during its expansion through power recovery turbine K-204. Finally, the syngas is cooled to 100°F by cooling water in E-207, and most of the water and methanol in the product stream condenses.

The condensate, initially at 1350 psia flows from separator V-201 through hydraulic turbine K-203 to recover 285 kwh of drive-shaft energy. The vapor stream from V-201 is recycled to the reactor after a purge. The purge stream is expanded through turbine K-204, where 5,700 kwh of energy is recovered. The depressurized crude methanol is run into surge vessel V-202. Vent gas from this vessel is scrubbed with water in C-201 for minimizing methanol losses to the purge. Unabsorbed gas leaving C-201 is blended with purge gas in the turbine expander. The exit gas from the expander is fed to the reformer as fuel.

The crude methanol is transferred to intermediate storage T-351 before being purified in a four-column train. It is preheated against methanol product in E-301 before being fractionated in the first column, C-301, the light ends column. The overhead vapor from this column is cooled in E-302, and the condensate, mainly methanol with some light ends, is returned as reflux. The uncondensed vapor comprising light ends (essentially dimethyl ether with some methanol) is removed from reflux drum V-301 to blend with the synthesis section purge. The bottoms product from C-301 is fed to C-302, the refining column, which is operated at 100 psia at the base. The overheads product is slightly wet methanol (99.5 wt% purity) and the bottoms product is essentially water with a trace of methanol. In our assumed flow sheet this bottoms stream is fed into the hot demineralized water loop, which meets the needs of the saturator and the steam systems. The refining column also removes a higher alcohols product as a sidestream a few trays from the bottom. The slightly wet methanol product from the refining column is fed to the third column, methanol finishing column C-303. A high purity methanol product is removed overhead, which meets the U.S. Federal Grade Specification AA. The bottoms product, which contains some methanol with higher alcohols and water, is fed to the final column, methanol recovery column C-304. In this column further methanol product is recovered overhead and the higher alcohols and water present in the feed are rejected in the bottoms stream.

As discussed earlier, the reason for using an enhanced pressure in the refining column is to permit the overhead vapor from this column to provide the reboil energy in the other three columns. Thus reboilers E-303, E-304, and E-305 also act as condensers for the refining column. The reboil energy for the refining column is provided by the reformer product in E-306.

Table 4.13

METHANOL FROM NATURAL GAS BY ICI LP PROCESS (HIGH EFFICIENCY DESIGN)

MAJOR EQUIPMENT

Plant Capacity: 1,819 Million lb/yr
(825,000 Metric Tons/yr) Methanol
at 0.90 Stream Factor

Equipment Number	Name	Size	Material of Construction	Remarks
	Reactors			
R-201	Methanol converter	73,000 gal	316 ss clad	16 ft dia x 43 ft high with 9,600 cu ft catalyst. Quench gas lozenges in at 3 levels.

Equipment Number	Name	Size (bhp)	Material of Construction	Remarks
	Compressors			
K-101	Air blower	3,900	Carbon steel	
K-102	Flue gas extractor	4,400	Carbon steel	
K-201	Syngas compressor	45,000	316 ss	
K-202	Recycle gas compressor	10,600	316 ss	
K-203	Liquid turbine drive	-380	Carbon steel	
K-204	Gas turbine	-7,600	316 ss	

Equipment Number	Name	Size (sq ft)	Heat Load (MM Btu/hr)	Material of Construction Shell	Material of Construction Tubes	Remarks
	Exchangers					
E-101	Feed preheater	18,000	173	Flue duct, 316 ss		Tubes are enclosed by flue gas exhaust duct.
E-102	Steam superheater	33,400	104	Flue duct, carbon steel		Tubes are enclosed by flue gas exhaust duct.
E-103	Flue gas boiler	19,800	70	Flue duct, carbon steel		Tubes are enclosed by flue gas exhaust duct.
E-104	Air preheater	51,000	115	Flue duct, carbon steel		Tubes are enclosed by flue gas exhaust duct.
E-105	Reformed gas steam exchanger	4,200	404	Carbon steel	316 ss	
E-106	Saturator water heater	31,400	96	Carbon steel	316 ss	
E-107	Feed water deaerator	30,200	160	Carbon steel	316 ss	
E-108	Fuel preheater	6,400	7	Carbon steel	316 ss	
E-109	Natural gas feed heater	3,400	8	Carbon steel	316 ss	
E-110	Reformed gas cooler	6,800	18	Carbon steel	316 ss	
E-201	Turbine condenser	77,000	248	Carbon steel	Carbon steel	
E-202	Converter feed preheater	65,000	227	316 ss	316 ss	
E-203	Direct feed interchanger	61,000	170	316 ss	316 ss	
E-204	Converter/wtr exchanger-2	30,000	55	Carbon steel	316 ss	
E-205	Converter/wtr exchanger-1	18,000	80	Carbon steel	316 ss	
E-206	Turbine interstage heater	9,300	20	Carbon steel	316 ss	
E-207	Converter product cooler	76,000	275	Carbon steel	316 ss	
E-208	Reaction start-up heater	14,000	35	Carbon steel	316 ss	Not shown on drawing.
E-301	Methanol crude purf exchanger	3,700	5.50	Carbon steel	316 ss	
E-302	Light ends condenser	2,100	32	Carbon steel	316 ss	
E-303	Light ends reboiler	3,700	45	316 ss	316 ss	
E-304	Finishing reboiler	33,000	165	316 ss	316 ss	
E-305	Recovery reboiler	320	2	316 ss	316 ss	
E-306	Refining reboiler	9,200	247	316 ss	316 ss	
E-307	Finishing condenser	17,600	176	Carbon steel	Brass	
E-308	Recovery condenser	200	2	Carbon steel	Brass	

Equipment Number	Name	Heat Load (MM Btu/hr)	Material of Construction	Remarks
	Furnaces			
F-101	Natural gas reforming furnace	1,565	HK40 alloy	1,080 4 in. by 40 ft 25/20 Cr/Ni tube filled with 3,760 ft^3 ICI 574 catalyst.

Equipment Number	Name	Volume (gal)	Material of Construction	Remarks
	Tanks			
T-351	Crude methanol storage	2,000,000	316 ss	
T-352	Higher alcohols storage	66,000	Carbon steel	Two tanks each 28,000 gal storage for 10 days' output. Not shown on drawing.
T-353	Methanol storage	10,000,000	Carbon steel	Nine tanks each one million gal storage for 10 days' output. Not shown on drawing.

Table 4.13 (Concluded)

METHANOL FROM NATURAL GAS BY ICI LP PROCESS (HIGH EFFICIENCY DESIGN)

MAJOR EQUIPMENT

Plant Capacity: 1,819 Million lb/yr
(825,000 Metric Tons/yr) Methanol
at 0.90 Stream Factor

Equipment Number	Name	Volume (gal)	Material of Construction	Remarks
	Pressure vessels			
V-101	Steam drum	65,000	Carbon steel	
V-102	Condensate drum-1	6,000	316 ss	
V-103	Condensate drum-2	12,000	316 ss	
V-104	Condensate drum-3	1,000	316 ss	
V-105	Condensate drum-4	6,500	316 ss	
V-106	Boiler feed vessel	60,000	316 ss	
V-201	Crude methanol separator	10,000	316 ss/clad	
V-202	Crude methanol surge	42,000	Carbon steel	
V-301	Light ends reflux drum	5,000	Carbon steel	
V-302	Refining reflux drum	25,000	304 ss	
V-303	Finishing reflux drum	25,000	304 ss	
V-304	Recovery reflux drum	500	304 ss	

Equipment Number	Name	Height (ft)	Diameter (ft)	Material of Construction		Remarks
				Shell	Trays	
	Columns					
C-101	Feed saturator	80	14.0	316 ss		60 ft of packing.
C-201	Purge gas scrubber	30	7.0	316 ss		25 ft of packing.
C-301	Light ends column	55	5.9	316 ss	316 ss	32 valve trays, 18 in. spacing.
C-302	Methanol refining column	125	18.0	316 ss	316 ss	76 valve trays, 18 in. spacing.
C-303	Methanol finishing column	130	14.0	316 ss	316 ss	60 valve trays, 24 in. spacing.
C-304	Methanol recovery column	30	1.6	316 ss		25 ft of packing.

Equipment Number	Name	Size	Material of Construction	Remarks
	Miscellaneous equipment			
M-101	Hydrogen sulfide adsorber	550 cu ft	Carbon steel	
M-102	Hydrogen sulfide adsorber	550 cu ft	Carbon steel	
M-103	Flue gas stack	9.0 ft dia x 120 ft high	Carbon steel	Not shown on drawing.

Pumps

100 Section - 4, including 2 operating, 2 spares; 1260 operating bhp.
300 Section - 18, including 9 operating, 9 spares; 107 operating bhp.

Table 4.14

METHANOL FROM NATURAL GAS BY ICI LP PROCESS (HIGH EFFICIENCY DESIGN)

STREAM FLOWS

Plant Capacity: 1,819 Million lb/yr
(825,000 Metric Tons/yr) Methanol
at 0.90 Stream Factor

	Stream Flows (lb-mols/hr)									
	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)
Methane	8,095.84	7,634.03	461.80	—	7,634.03	1,220.68	—	—	8.41	—
Carbon dioxide	46.70	44.00	2.70	—	44.00	2,573.92	—	—	2,052.09	—
Carbon monoxide	—	—	—	—	—	4,917.44	—	—	—	—
Hydrogen	—	—	—	—	—	24,174.98	—	—	14.60	—
Nitrogen + inerts	66.80	63.00	3.80	—	63.00	63.00	—	30,465.13	30,531.93	—
Ethane	230.00	217.00	13.00	—	217.00	—	—	—	0.07	—
C_3+	127.28	120.00	7.28	—	120.00	—	—	—	0.04	—
Water	—	—	—	12,712.06	25,423.26	15,445.98	116,818.80	—	10,832.85	28,154.12
Oxygen	—	—	—	—	—	—	—	8,092.04	868.95	—
Methanol	—	—	—	—	—	—	0.57	—	0.16	—
Dimethyl ether	—	—	—	—	—	—	—	—	—	—
Higher alcohols	—	—	—	—	—	—	—	—	—	—
Total (lb-mols/hr)	8,566.62	8,078.03	488.58	12,712.06	33,501.29	48,396.00	116,819.37	38,557.17	44,309.10	28,154.12
Total (lb/hr)	149,522	140,995	8,528	228,817	598,614	598,613	2,102,756	1,111,969	1,168,158	506,774

	Stream Flows (lb-mols/hr)									
	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)
Methane	7,634.03	—	1,220.68	24,194.11	13,978.13	11,436.65	25,414.79	—	1,220.68	—
Carbon dioxide	44.00	—	2,573.92	2,576.41	2,832.68	2,317.65	2,706.39	—	129.98	—
Carbon monoxide	—	—	4,917.44	2,885.11	4,291.40	3,511.15	3,030.67	—	145.56	—
Hydrogen	—	—	24,174.98	144,674.93	92,867.45	75,982.46	151,974.35	—	7,299.41	—
Nitrogen + inerts	63.00	—	63.00	1,248.71	721.44	590.27	1,311.71	—	63.00	—
Ethane	217.00	—	—	—	—	—	—	—	—	—
C_3+	120.00	—	—	—	—	—	—	—	—	—
Water	12,711.20	15,442.07	3.22	32.00	19.37	15.85	2,488.26	445	45.44	2,855.82
Oxygen	—	—	—	—	—	—	—	—	—	—
Methanol	—	—	—	495.10	272.31	222.80	7,692.72	—	24.98	7,172.65
Dimethyl ether	—	—	—	—	—	—	3.20	—	—	3.20
Higher alcohols	—	—	—	—	—	—	5.90	—	—	590
Total (lb-mols/hr)	20,789.23	15,442.07	32,953.24	176,106.37	114,982.78	94,076.83	194,627.99	445	8,929.05	10,037.57
Total (lb/hr)	369,797	277,957	320,643	921,984	683,445	559,181	1,242,628	8,010	47,306	281,348

	Stream Flows (lb-mols/hr)											
	(21)	(22)	(23)	(24)	(25)	(26)	(27)	(28)	(29)	(30)	(31)	(32)
Methane	—	1,220.68	—	—	—	—	—	—	—	—	—	—
Carbon dioxide	—	129.98	—	—	—	—	—	—	—	—	—	—
Carbon monoxide	—	145.56	—	—	—	—	—	—	—	—	—	—
Hydrogen	—	7,299.41	—	—	—	—	—	—	—	—	—	—
Nitrogen + inerts	—	63.00	—	—	—	—	—	—	—	—	—	—
Ethane	—	—	—	—	—	—	—	—	—	—	—	—
C_3+	—	—	—	—	—	—	—	—	—	—	—	—
Water	—	45.44	2,855.82	37.28	19.78	2,798.76	5.21	32.08	—	32.08	5.21	88,672.50
Oxygen	—	—	—	—	—	—	—	—	—	—	—	—
Methanol	6.48	31.45	7,166.17	7,151.27	14.33	0.57	7,131.24	20.02	18.48	1.54	7,149.73	—
Dimethyl ether	3.20	3.20	—	—	—	—	—	—	—	—	—	—
Higher alcohols	—	—	5.90	1.18	4.72	—	.04	1.14	—	1.14	.04	—
Total (lb-mols/hr)	9.68	8,938.72	10,027.89	7,189.73	38.83	2,799.33	7,136.49	53.24	18.48	34.76	7,154.98	88,672.50
Total (lb/hr)	354	47,660	280,993	229,565	1,032	50,396	228,296	1,270	591	678	228,887	1,596,105

	Stream Flows (lb-mols/hr)						
	(33)	(34)	(35)	(36)	(37)	(38)	(39)
Methane	—	—	—	—	—	—	—
Carbon dioxide	—	—	—	—	—	—	—
Carbon monoxide	—	—	—	—	—	—	—
Hydrogen	—	—	—	—	—	—	—
Nitrogen + inerts	—	—	—	—	—	—	—
Ethane	—	—	—	—	—	—	—
C_3+	—	—	—	—	—	—	—
Water	75,961.30	5,076.94	9,443.50	684.17	111.37	10,239.04	32,981.81
Oxygen	—	—	—	—	—	—	—
Methanol	—	—	—	—	—	—	—
Dimethyl ether	—	—	—	—	—	—	—
Higher alcohols	—	—	—	—	—	—	—
Total (lb-mols/hr)	75,961.30	5,076.94	9,443.50	684.17	111.37	10,239.04	32,981.81
Total (lb/hr)	1,367,303	91,385	169,983	12,315	2,005	184,303	593,673

Separation Processes for Adjusting H_2:CO Ratio

As discussed earlier, four separation schemes were examined for the adjustment of H_2:CO ratios. The following is a brief description for each of the individual processes.

Cryogenic Separation by Liquid Methane Wash (354176, 431024)

The cryogenic process assumed in this study is based on information provided by Union Carbide. In essence it comprises the use of a liquid methane wash system, as shown in Figure 4.11 (foldout at end of report).

The syngas is first passed through molecular sieves in a fixed bed column to reduce the water and CO_2 to about 0.1 ppm. The dried syngas is cooled to about -185°F in the main heat exchanger and scrubbed countercurrently with liquid methane in a plate column (methane wash column) operating at 240 psia at the base. The overheads product is 98.5% H_2 (vol basis) with less than 10 ppm CO. The main impurity is CH_4. The bottoms stream is reduced in pressure to 47 psia by a reducing valve and subjected to a second methane wash in the Inters column. The overheads from this column is a purge stream whose magnitude corresponds to about 2-4% of the total syngas stream and enables the production of a 99% CO stream. The bottoms stream from this column is fractionated in a third column, where the CO product is obtained overhead. The bottoms stream, essentially liquid methane, is recycled to the first two columns via an interchanger, where the feed to the CO/CH_4 separation column is further cooled.

The CO stream from the final column is compressed to 240 psia in a multistage centrifugal compressor. Part of this stream is removed as CO product. (When the purpose of the separation is to adjust the H_2:CO ratio, this CO is blended with the bypassing syngas, as shown in Figure 4.5.) The rest of the stream constitutes a CO recycle which is used to "drive" the cryogenic unit. This is accomplished by its compression to 395 psia and subsequent expansion in two separate streams.

One part of the stream goes through a turbine expander, where it is reduced in pressure to 30 psia before passage through the main exchanger. The other part of the stream goes through the reboiler of the CO/CH_4 separation column before expansion through a reducing valve to provide cooling in the condenser of this column.

As shown in the conceptual diagram (Figure 4.11) all outgoing streams pass through the main heat exchanger, where they contribute to the cooling of the incoming syngas.

Pressure Swing Adsorption (PSA)

The earlier versions of Union Carbide's PSA process consisted of a four-bed system operating in parallel. As described before, the process is cyclical. The use of four programmed beds—one adsorbing, one depressurizing, one purging and one repressurizing—gave an essentially continuous flow of purified hydrogen.

During the early seventies Union Carbide developed an improved version of PSA which they called the "Polybed" system (472155), consisting of 10 beds. Operation entails having three beds in the adsorption cycle at any one time. The remaining seven beds are in various stages of the regeneration cycle. The cycles of the adsorbing beds are programmed such that, when one of them is brought on line, another completes its adsorption step. Depressurization is carried out in two stages. Initially, it is in a direction which is cocurrent with the feed flow. During this stage a major proportion of the adsorbed hydrogen is released for use in repressurizing and purging adsorbers. Also, during this stage most of the other adsorbed components are retained on the bed. The adsorbent bed is then purged with pure hydrogen before the second stage depressurization, which is carried out in a countercurrent direction. During this stage the nonhydrogen components are removed. As before, this is followed by purging with hydrogen.

The adsorber is then repressurized in stages. Initially there is pressure equalization, with the three adsorbers undergoing depressurization. This is followed by pressure buildup with product hydrogen before resumption of the adsorption cycle.

The Polybed system consists of a complex network of valves linked to an electronic programmable controller. Union Carbide claim that compared with the earlier four-bed system, Polybed affords higher hydrogen recoveries, more efficient utilization of the adsorbent, and enhanced capacities for a single-train system to about 50 million scfd hydrogen. As stated earlier, the hydrogen purity from the system is 99.99%+ and hydrogen recoveries for a feed stream containing 65-75% hydrogen are 85-88%.

Tenneco's Cosorb® System (431036, 431126)

Tenneco's Cosorb® process is essentially a solvent absorption process for the removal and recovery of carbon monoxide from gaseous mixtures. A proprietary solvent is used which consists of cuprous aluminum tetrachloride ($CuAlCl_4$) dissolved in toluene at concentrations of about 20-25 mol%.

A schematic flow diagram for the process is presented in Figure 4.12 (foldout at end of report) and is based on information obtained from Tenneco and one of their license holders and approved engineering contractors, Kawasaki Heavy Industries. As with the cryogenic process, it is necessary to remove water present in the syngas by molecular sieves to about 0.1 ppm. Polar compounds such as water react irreversibly with $CuAlCl_4$. The dried syngas is contacted countercurrently with the solvent in the complexing column. The unabsorbed H_2-rich gases are cooled in an interchanger and then in a heat exchanger. A refrigerant is used in the latter. Most of the toluene present is condensed and removed by a disengagement vessel. The cold H_2-rich vapor leaving this vessel provides the first-stage cooling in the interchanger. The liquid phase leaving the bottom of the complexing column contains a high proportion (~99%) of the carbon monoxide present in the feed syngas. The $CuAlCl_4$ forms a complex with the CO in an exothermic reaction. The CO-rich solvent stream is heated against lean solvent returning from the decomplexing column and is reduced in pressure. This causes most of the dissolved gases (mainly H_2) to separate in the flash drum. The flashed gases are purged from the system after being cooled in a refrigerated heat exchanger for toluene recovery. The solution from the drum is fed to the decomplexing column, where the CO-$CuAlCl_4$ complex is thermally dissociated. This column is operated in the same way as the stripper column in the MEA system for CO_2 removal described before. Heat for dissociation of the complex and for the stripping process is provided by the 50 psia steam used in the reboiler. The lean solvent gives off heat to the rich solvent and is cooled further in a heat exchanger against cooling water before being recycled to the complexing column.

The stripped CO leaves the condenser of the decomplexing column via a drum where condensed toluene is refluxed to the column. A makeup toluene stream from the toluene recovery system is added to the reflux to maintain a constant composition in the recycled lean solution. The CO stream leaving the reflux drum contains some recoverable toluene. A system comprising an interchanger and a refrigerated heat exchanger, as for the H_2 stream, is used to remove most of the toluene. Further toluene removal down to 0.1 ppm is accomplished by adsorption on a fixed bed. Tenneco state that the Cosorb® system can be designed for CO purities of 99.9%. The actual specification will clearly depend on the end use for the CO. The major impurity is hydrogen. However, the product would contain some HCl (less than 1 ppm), which is formed by the reaction of water with $CuAlCl_4$ (i.e., from the 0.1 ppm H_2O in the dried syngas stream). For some applications, e.g., acetic acid manufacture--where halogens are used in the catalyst--the presence of HCl at these low levels would not matter.

For CO applications which demand a more rigid specification on HCl content, it would be necessary to interpose a separation system for HCl (e.g., ion exchange) between the refrigerated cooling and the fixed bed adsorption stages. The incremental cost for this is considered to be negligible.

Monsanto's Prism® Separators (472166, 472162, 472170)

The Prism® separators developed by Monsanto employ membranes that have been formed into hollow fibers. Thousands of these hollow fibers are assembled in each separator unit. Depending on the pressure of the gas, the nature of the separation duty, and the scale of operation, a number of separators may be used both in parallel and in series. The gas to be processed is fed to the shell side of the separator module. As the stream flows along the outer surface of the hollow fibers, the gas components permeate selectively. Thus hydrogen of course permeates much more readily than carbon monoxide.

The driving force for the membrane separation is the difference between the component partial pressures on the outer (shell side) of the hollow fiber and the inner (bore side) of the fiber. Pressure drop on the shell side of the fiber bundle is minimal. For a syngas initial pressure of 250 psia, the adjustment of H_2:CO ratios from 3:1 and 2:1 to 2:1 and 1:1 respectively can be effected with a 20 psi pressure drop on the shell side. On the basis of information from Monsanto the pressure of the enriched hydrogen streams would be reduced to 65 psia. For the two adjustment cases cited, the quoted hydrogen purities are 98% and 97% (vol., dry basis) respectively. The main impurity is CO and to make the hydrogen suitable as chemical grade, we assumed the use of a methanation stage operating at 590°F, which is similar to that described earlier for hydrogen production. A product/feed heat interchanger with a 40°F temperature approach was also included in our evaluation and due allowance was made for the balance of heat required.

From data made available to SRI by Monsanto, the capital requirement for the Prism® process can be significantly reduced if the syngas is compressed to a higher pressure. However, compression costs are justifiable only when the syngas is needed at the higher pressures. Monsanto state that Prism® separators operate satisfactorily with as much as 1600 psi pressure differential across the hollow fiber membranes.

Cost Estimates

Basic Cases

Detailed capital and production cost estimates for the five basic cases examined are presented in Tables 4.15 through 4.24. In all these cases the production scale corresponds to a fixed reformer feed rate equivalent to a 2,500 metric tons/day methanol plant. Production rates are shown in million scfd for syngas and in lb/yr for methanol and H_2. The product values are expressed in cents/1,000 scf for the syngas cases and in cents/lb for H_2 and methanol.

The unit cost for CO_2, 4.4¢/lb, as applied to Case B (which requires CO_2 import) is the product value obtained from the process economics of flue gas scrubbing. The details which are presented in Tables 4.25 through 4.28, were worked out from data provided by Union Carbide for their MEA based system. The process flow, shown in Figure 4.13 (foldout at end of report) is essentially similar to that depicted for syngas and H_2 production, with the difference that a flash stage is not applicable because of the lower solvent loading that results from the relatively low CO_2 partial pressure in the flue gas.

The data for Case E (crude syngas) were derived from Case D, methanol by the ICI low pressure process. It was assumed that the product stream comprises the crude syngas product from the reformer cooled to 100°F. In the methanol process high pressure steam is generated (by heat recovery and by heat absorption in the convection section of the furnace) for driving the compressor. The uncondensed steam from the turbine is used in the reformer feed. For the crude syngas case the costs were calculated by assigning different values to the high and medium pressure steam. (These values have been tabulated earlier.) This procedure was also adopted for the hydrogen case. Further, in the methanol process a purge gas stream (from methanol synthesis stage) is used as fuel for the reformer furnace. For the crude syngas case it is assumed that this is replaced by natural gas fuel.

For reasons discussed earlier, the possible production of a syngas stream with a H_2:CO ratio of 1:1 was not examined in full flow sheet design. However, we estimated production cost from detailed mass and energy balances. Extrapolations of the capital information obtained for Cases A and B, are shown in Table 4.29. A large import of CO_2 is required, 28.32 lb/1,000 scf syngas. This is not only in excess of the CO_2 available in the flue gas (i.e., 26.49 lb/1,000 scf on a 100% recovery basis) but corresponds to by-product CO_2 output from over 3,000 metric tons/day NH_3. Thus, large scale production of a 1:1 syngas would present obvious logistics problems on the question of CO_2 availability. Relatively small scale production, e.g., for oxo, may nevertheless be practical with by-product CO_2 from an NH_3 or H_2 facility. The cost data in Table 4.30 are therefore somewhat academic for large operations, as they assume full CO_2 availability. The CO_2 recoverable from flue gases would permit a minimum H_2:CO ratio of about 1.2:1.

The key numbers from the syngas cost tables (Tables 4.15 to 4.24) are summarized in Table 4.30. Also shown are the estimated H_2 costs from a scheme (see Figure 4.14, foldout at end of report) which replaces low temperature CO shift, CO_2 removal, and methanation, with PSA. Compared with the conventional process for H_2 the costs shown for this scheme (Table 4.30) are substantially lower. The slightly higher capital costs are more than offset by the combined effect of lower natural gas usage and enhanced production of MP steam for export. However, because the data for the PSA scheme were derived from outside information (472173) and (unlike the conventional H_2 process) not based on a detailed SRI flow sheet appraisal, the comparison should be regarded only as an approximate guideline owing to a possible lack of consistency. For this reason, in our subsequent evaluations of the skimming processes and CO production modules we have used H_2 costs from the conventional process.

Note that the adjustment of H_2:CO ratio by CO_2 addition imposes a penalty which becomes increasingly severe as the ratio of 1:1 is approached. This is illustrated graphically in Figure 4.15. If the CO_2 imported were available in the quantities required as a cheap by-product (of either NH_3 or H_2 manufacture) at 1.5¢/lb*, the costs for the 2:1 and 1:1 cases would be lowered to $2.84/1,000 scf and $4.04/1,000 scf respectively.

For Case D, methanol, the battery limits capital and total fixed capital costs for 2,500 metric tons/day is $155 and $213 million respectively (PEP Cost Index = 400). The corresponding product value (including 25% ROI) works out at 11.70¢/lb, when the coproduct higher alcohols mixture is credited at the fuel value of $4.17/million Btu. These figures refer to the production of chemical grade methanol which is well within U.S. Federal Government Grade AA. The purification section capital costs (and associated off-plots excluding tankage) amount to about $15.0 million. If the product specification corresponded to fuel grade material (containing 1,000-1,500 ppm water and allowing inclusion of light ends and higher alcohols with the methanol) purification can be effected in a single column. The corresponding fixed capital requirement for the purification section would be reduced to $8.0 million. This roughly represents a cost saving of 0.18¢/lb when no value is attached to the saving in low grade energy used in distillation. The amount of energy saved is 270 Btu/lb methanol.

If crude methanol (ex-synthesis section) is directly usable for further downstream processing, the reduction in capital (allowing for less tankage capacity) would be $21.0 million. The cost of crude methanol (81.6% by weight) would be 11.24¢/lb—expressed on a 100% basis. As before, no credit is attached to savings in low grade energy used in purification, which corresponds to 1,077 Btu/lb methanol. It will thus be observed that the incremental costs for methanol purification are almost negligible.

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*Considered to be the value of CO_2 gas for its present outlets, e.g., liquid CO_2 for refrigeration. It is an estimate of a maximum transfer price for atmospheric pressure gas that would still justify investment in a liquefaction plant with realizations, currently in the region of $50-$60 ton (2.5¢-3¢/lb).

Syngas H_2:CO Ratio Adjustment by H_2 Skimming

As discussed before, the removal or "skimming" of surplus hydrogen from syngas mixtures derived from natural gas may be used to adjust the H_2:CO ratios instead of CO_2 injection in the reformer feed. The relative economics of the two approaches would depend on the realizations that can be obtained for the H_2 coproduct compared with the cost of imported or flue-gas-scrubbed CO_2.

As previously described, SRI evaluated four schemes for the skimming. Economic data for these schemes are presented in Table 4.31, where the cases examined are the skimming of 3:1 and 2:1 syngas streams to produce adjusted ratios of 2:1 and 1:1 respectively. Under the assumed relativities in the contributions of energy and capital to the costs, Monsanto's "Prism®" separator system has the lowest overall cost. It is also the least capital intensive of the four schemes and, apart from PSA, demands less energy than the other two. PSA requires the highest capital but uses the least energy. However, the skimming costs for all four schemes constitute a relatively minor proportion of the total syngas cost. In an actual situation the choice among the four could be dictated by other considerations such as H_2 product purity and the ability of Cosorb® and cryogenic separation to furnish a carbon monoxide coproduct.

In our evaluation of the economics of adjusting syngas H_2:CO ratios by skimming, we chose Prism® as the basis for illustration. The calculated data are presented in Tables 4.32 through 4.35, showing the costs for syngas with H_2:CO ratios of 2:1 and 1:1. For the 2:1 case the skimming of syngas with an initial ratio of 3:1 is compared with the alternative based on CO_2 import. For the 1:1 case, skimming was examined with two initial syngas ratios, 3:1 and 2:1. The costs are compared, as before, with the nonskimming option which relies solely on CO_2 import. The effect of H_2 coproduct realizations and CO_2 unit costs has been illustrated by taking two extreme levels for both materials. For hydrogen the upper level (50¢/lb) is equivalent to "chemical value" and the lower level (24¢/lb) corresponds to a fuel credit consistent with the \$4.17/million Btu used for natural gas feedstock. In the case of CO_2 the upper level (4.4¢/lb) represents flue gas scrubbing costs and the lower level (1.5¢/lb) is a value related to CO_2 refrigeration outlets.

A graphical representation of the data in Table 4.35 is given in Figure 4.16. Skimming is clearly the preferred method when H_2 coproduct realizations approach chemical value. When hydrogen realizations fall well below chemical value and approach fuel value, CO_2 import could be the economic way. A graphical plot in terms of H_2-CO_2 break-even values is given in Figure 4.17. In the case where syngas with an H_2:CO ratio of 2:1 is required, fuel grade H_2 would break even with 3.3¢/lb CO_2 (plot I, Figure 4.17). Flue gas scrubbing which yields 4.4¢/lb CO_2 would thus not be economic. If cheap CO_2 is available at 1.5¢/lb, the required break-even point for H_2 is 34¢/lb. Thus, an average realization equivalent to 68% of chemical value would be necessary for the skimming case to be competitive. Since three options have been examined for the production of 1:1 syngas, the break-even relationships are shown by plots II, III, and IV in Figure 4.17. These represent the three combinations of two for each of the plots. Some trends that can be discerned from these plots and from those in Figure 4.16 are illustrated as follows:

- When coproduct hydrogen can realize only fuel value, the skimming of 3:1 gas to produce 1:1 product is still more economic than ratio adjustment by CO_2 import alone, unless the unit cost of such an import is below 1.5¢/lb, i.e., much less than that for recovery from flue gas.
- When full chemical value can be obtained for H_2, the skimming of 3:1 syngas (to make 1:1 syngas) is preferable to "partial" use of CO_2 import (i.e., skimming of 2:1 syngas) even when the CO_2 is available at "nil" cost.
- The "partial" use of CO_2 import (as implied in the skimming of 2:1 syngas) becomes preferable to the nil CO_2 import case (i.e., skimming 3:1 syngas) when the unit cost for the imported CO_2 does not exceed 2.5¢/lb and the skimmed coproduct H_2 has to be disposed of as fuel.

As emphasized before, the choice between various schemes entailing skimming of H_2 and/or import of CO_2, depends on the unit values for H_2 and CO_2 that may be relevant for a given situation. The data in Tables 4.31 through 4.35 and Figures 4.16 and 4.17 are offered for illustration and guidance.

Table 4.15

SYNGAS (H_2:CO RATIO = 3:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 RECYCLE

CAPITAL INVESTMENT

Plant Capacity: 97 x 10^9 scf/yr Syngas
at 0.90 Stream Factor
PEP Cost Index: 400

	Total	Natural Gas Steam Reforming	Carbon Dioxide Separation
Battery limits equipment, f.o.b.			
Columns	$ 1,531,400	$ —	$ 1,531,400
Vessels and tanks	2,206,700	331,600	1,875,100
Exchangers	8,128,700	3,463,100	4,665,600
Furnaces	22,192,000	22,192,000	—
Compressors	6,277,000	3,677,000	2,600,000
Miscellaneous equipment	200,000	200,000	—
Pumps	1,230,800	224,000	1,006,800
Total	$ 41,766,600	30,087,700	$11,678,900
Battery limits equipment installed	$ 81,812,000	$54,992,000	$26,820,000
Contingency, 20%	16,362,000	10,998,000	5,364,000
BATTERY LIMITS INVESTMENT	$ 98,174,000	$65,990,000	$32,184,000
Off-sites, installed			
Cooling tower	$ 5,311,000	—	5,311,000
Process water treatment	163,400	163,400	—
Utilities and storage	$ 5,474,000	$ 163,000	$ 5,311,000
General service facilities	17,457,000		
Waste treatment	4,364,000		
Total	$ 27,295,000		
Contingency, 20%	5,459,000		
OFF-SITES INVESTMENT	$ 32,755,000		
TOTAL FIXED CAPITAL	$130,929,000		

Table 4.16

SYNGAS (H_2:CO RATIO = 3:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 RECYCLE

PRODUCTION COSTS

Plant Capacity: 97 x 10^9 scf/yr Syngas
at 0.90 Stream Factor
PEP Cost Index: 400

			Total Costs	
	Basis or Unit Cost	Units/mscf	¢/mscf	Thousand $/yr
Labor				
Operating	4 men/shift, $17.50/man-hr	0.0004 man-hr	0.63	614
Maintenance	1.5%/yr of BL cost		1.51	1,473
Control laboratory	20% of operating labor		0.13	122
Total labor			2.27	2,209
Materials				
Natural gas feed	436¢/mscf	0.249 mscf	108.56	105,817
Natural gas fuel	436¢/mscf	0.151 mscf	65.84	64,170
Catalysts, adsorbent			0.47	458
Misc. chemicals util.			0.41	400
Maintenance	1.5%/yr of BL cost		1.51	1,473
Operating	10% of operating labor		0.06	62
Total materials			176.85	172,380
Utilities				
Cooling water	5.4¢/1,000 gal	218 gal	1.18	1,149
Process water	68¢/1,000 gal	6.31 gal	0.43	418
Electricity	3.6¢/kwh	0.996 kwh	3.59	3,495
Total utilities			5.20	5,062
TOTAL DIRECT OPERATING COST			184.32	179,651
Plant overhead	80% of total labor		1.81	1,767
Taxes and insurance	2%/yr of fixed capital		2.69	2,619
Plant cost			188.82	184,037
G&A, sales, research	4% of sales		10.00	9,747
Cash expenditures			198.82	193,784
Depreciation	10%/yr of fixed capital		13.43	13,093
TOTAL PRODUCTION COST			212.25	206,877
25%/yr pretax ROI			33.58	32,732
PRODUCT VALUE			245.83	239,609

Table 4.17

SYNGAS (H_2:CO RATIO = 2:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

CAPITAL INVESTMENT

Plant Capacity: 98 x 10^9 scf/yr Syngas
at 0.90 Stream Factor
PEP Cost Index: 400

	Total	Natural Gas Steam Reforming	Carbon Dioxide Separation
Battery limits equipment, f.o.b.			
Columns	$ 2,104,300	$ —	$ 2,104,300
Vessels and tanks	2,416,300	386,400	2,029,900
Exchangers	10,351,400	3,652,700	6,698,700
Furnaces	23,840,000	23,840,000	--
Compressors	8,270,100	4,190,100	4,080,000
Miscellaneous equipment	252,000	252,000	--
Pumps	1,429,300	224,000	1,205,300
Total	$ 48,663,400	$32,545,200	$16,118,200
Battery limits equipment installed	$ 98,156,000	$60,507,000	$37,649,000
Contingency, 20%	19,631,000	12,101,000	7,530,000
BATTERY LIMITS INVESTMENT	$117,787,000	$72,608,000	$45,179,000
Off-sites, installed			
Cooling tower	7,317,000	—	7,317,000
Process water treatment	163,400	163,400	—
Utilities and storage	$ 7,480,000	$ 163,000	$ 7,317,000
General service facilities	21,127,000		
Waste treatment	5,282,000		
Total	$ 33,889,000		
Contingency, 20%	6,778,000		
OFF-SITES INVESTMENT	$ 40,667,000		
TOTAL FIXED CAPITAL	$158,454,000		

Table 4.18

SYNGAS (H_2:CO RATIO = 2:1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS

Plant Capacity: 98 x 10^9 scf/yr Syngas
at 0.90 Stream Factor
PEP Cost Index: 400

			Total Costs	
	Basis or Unit Cost	Units/mscf	¢/mscf	Thousand $/yr
Labor				
Operating	4 men/shift, $17.50/man-hr	0.0004 man-hr	0.62	614
Maintenance	1.5%/yr of BL cost		1.79	1,767
Control laboratory	20% of operating labor		0.12	122
Total labor			2.53	2,503
Materials				
Natural gas feed	436¢/mscf	0.247 mscf	107.69	105,937
Natural gas fuel	436¢/mscf	0.178 mscf	77.61	76,343
Carbon dioxide	4.4¢/lb	8.86 lb	38.98	38,349
Catalysts, adsorbent			0.52	512
Misc. chemicals, util.			0.69	679
Maintenance	1.5%/yr of BL cost		1.80	1,767
Operating	10% of operating labor		0.06	62
Total materials			227.35	223,649
Utilities				
Cooling water	5.4¢/1,000 gal	313 gal	1.69	1,660
Process water	68¢/1,000 gal	6.25 gal	0.43	418
Electricity	3.6¢/kwh	1.18 kwh	4.26	4,194
Total utilities			6.38	6,272
TOTAL DIRECT OPERATING COST			236.26	232,424
Plant overhead	80% of total labor		2.04	2,002
Taxes and insurance	2%/yr of fixed capital		3.22	3,169
Plant cost			241.52	237,595
G&A, sales, research	4% of sales		12.00	11,804
Cash expenditures			253.52	249,399
Depreciation	10%/yr of fixed capital		16.11	15,845
TOTAL PRODUCTION COST			269.63	265,244
25%/yr pretax ROI			40.27	39,614
PRODUCT VALUE			309.90	304,858

Table 4.19

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS

CAPITAL INVESTMENT

Plant Capacity: 479 Million lb/yr
(217,000 Metric Tons/yr) Hydrogen, 100% Basis
at 0.90 Stream Factor
PEP Cost Index: 400

	Total	Natural Gas Steam Reforming	Carbon Dioxide Separation	CO Shift and Methanation Cost
Battery limits equipment, f.o.b.				
Columns	$ 7,474,700	$ —	$ 1,531,400	$5,943,300
Vessels and tanks	1,929,500	386,400	1,543,100	—
Exchangers	8,245,100	4,085,200	3,253,400	906,500
Furnaces	20,140,000	20,140,000	—	—
Compressors	3,061,200	3,061,200	—	—
Miscellaneous equipment	212,000	212,000	—	—
Pumps	873,900	224,000	649,900	—
Total	$ 41,936,400	$28,108,800	$ 6,977,800	$6,849,800
Battery limits equipment installed	$ 74,132,000	$51,757,000	$15,328,000	$7,047,000
Contingency, 20%	14,826,000	10,351,000	3,066,000	1,409,000
BATTERY LIMITS INVESTMENT	$ 88,958,000	$62,108,000	$18,394,000	$8,456,000
Off-sites, installed				
Cooling tower	4,773,400	1,712,400	2,675,700	385,300
Process water treatment	163,400	163,400	—	—
Steam generation	2,826,400	—	2,826,400	—
Utilities and storage	$ 7,763,000	$ 1,876,000	$ 5,502,000	$ 385,000
General service facilities	16,379,000			
Waste treatment	4,095,000			
Total	$ 28,237,000			
Contingency, 20%	5,647,000			
OFF-SITES INVESTMENT	$ 33,885,000			
TOTAL FIXED CAPITAL	$122,843,000			

Table 4.20

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS

PRODUCTION COSTS

Plant Capacity = 479 Million lb/yr
(217,000 Metric Tons/yr) Hydrogen, 100% Basis
at 0.90 Stream Factor
PEP Cost Index: 400

	Basis or Unit Cost	Units/lb	Total Costs ¢/lb	Total Costs Thousand $/yr
Labor				
Operating	4 men/shift, $17.50/man-hr	0.0001 man-hr	0.13	614
Maintenance	1.5%/yr of BL cost		0.28	1,335
Control laboratory	20% of operating labor		0.03	122
Total labor			0.44	2,071
Materials				
Natural gas feed	436¢/mscf	0.0504 mscf	21.97	105,345
Natural gas fuel	436¢/mscf	0.0264 mscf	11.51	55,181
Catalysts, adsorbent			0.35	1,678
Misc. chemicals, util.			0.10	479
Reformer steam	0.695¢/lb	10.32 lb	7.17	34,384
Maintenance	1.5%/yr of BL cost		0.28	1,335
Operating	10% of operating labor		0.01	62
Total materials			41.39	198,464
Utilities				
Cooling water	5.4¢/1,000 gal	38.3 gal	0.21	991
Steam	544¢/1,000 lb	2.55 lb	1.39	6,648
Process water	68¢/1,000 gal	1.28 gal	0.09	418
Electricity	3.6¢/kwh	0.159 kwh	0.57	2,740
Total utilities			2.26	10,797
TOTAL DIRECT OPERATING COST			44.09	211,332
Plant overhead	80% of total labor		0.35	1,657
Taxes and insurance	2%/yr of fixed capital		0.51	2,457
Plant cost			44.95	215,446
G&A, sales, research	4% of sales		1.80	8,629
Cash expenditures			46.75	224,075
Depreciation	10%/yr of fixed capital		2.56	12,284
TOTAL PRODUCTION COST			49.31	236,359
By-product credit				
HP steam export	0.775¢/lb	10.32 lb	-8.00	-38,342
NET PRODUCTION COST			41.31	198,017
25%/yr pretax ROI			6.41	30,711
PRODUCT VALUE			47.72	228,728

Table 4.21

METHANOL FROM NATURAL GAS BY ICI LP PROCESS (HIGH EFFICIENCY DESIGN)

CAPITAL INVESTMENT

Plant Capacity: 1,819 Million lb/yr
(825,000 Metric Tons/yr) Methanol
at 0.90 Stream Factor
PEP Cost Index: 400

	Total	Natural Gas Steam Reforming	Methanol Synthesis	Methanol Purification
Battery limits equipment, f.o.b.				
Reactors	$ 2,640,000	$ —	$ 2,640,000	$ —
Columns	6,878,300	2,751,900	234,900	3,891,500
Vessels and tanks	3,018,600	2,092,900	620,700	305,000
Exchangers	26,580,500	6,570,300	17,160,900	2,849,300
Furnaces	18,552,000	18,552,000	—	—
Compressors	11,032,200	2,928,200	8,104,000	—
Miscellaneous equipment	212,000	212,000	—	—
Pumps	1,087,300	942,200	—	145,100
Total	$ 70,000,900	$34,049,500	$28,760,500	$ 7,190,900
Battery limits equipment installed	$129,353,000	$60,636,000	$56,206,000	$12,511,000
Contingency, 20%	25,870,000	12,127,000	11,241,000	2,502,000
BATTERY LIMITS INVESTMENT	$155,223,000	$72,763,000	$67,447,000	$15,013,000
Off-sites, installed				
Cooling tower	5,921,000	105,700	4,440,800	1,374,500
Process water treatment	176,300	176,300	—	—
Steam generation	3,120,000	3,120,000	—	—
Tankage	6,669,000	—	—	6,669,000
Utilities and storage	$ 15,887,000	$ 3,402,000	$ 4,441,000	$8,044,000
General service facilities	29,048,000			
Waste treatment	3,060,000			
Total	$ 47,994,000			
Contingency, 20%	9,599,000			
OFF-SITES INVESTMENT	$ 57,593,000			
TOTAL FIXED CAPITAL	$212,817,000			

Table 4.22

METHANOL FROM NATURAL GAS BY ICI LP PROCESS (HIGH EFFICIENCY DESIGN)

PRODUCTION COSTS

Plant Capacity: 1,819 Million lb/yr
(825,000 Metric Tons/yr) Methanol
at 0.90 Stream Factor
PEP Cost Index: 400

	Basis or Unit Cost	Units/lb	Total Costs ¢/lb	Total Costs Thousand $/yr
Labor				
Operating	6 men/shift, $17.50/man-hr	0.0637 man-hr	0.05	921
Maintenance	1.5%/yr of BL cost		0.13	2,328
Control laboratory	20% of operating labor		0.01	183
Total labor			0.19	3,432
Materials				
Natural gas feed	436¢/mscf	0.0134 mscf	5.84	106,273
Natural gas fuel	436¢/mscf	0.00081 mscf	0.35	6,424
Active carbon	170¢/lb (374¢/kg)	0.00001 lb	—	31
Reforming catalyst	$2/lb ($4.41/kg)	0.00007 lb	0.01	255
Methanol catalyst	$4.40/lb ($9.70/kg)	0.00013 lb	0.06	1,040
Maintenance	1.5%/yr of BL cost		0.13	2,328
Operating	10% of operating labor		0.01	93
Total materials			6.40	116,444
Utilities				
Cooling water	5.4¢/1,000 gal (1.43¢/cu m)	13 gal	0.07	1,274
Steam	700¢/1,000 lb (1,543¢/ton)	0.004 lb	—	55
Process water	68¢/1,000 gal (18¢/cu m)	0.135 gal	0.01	167
Electricity	3.6¢/kwh	0.015 kwh	0.05	956
Total utilities			0.13	2,452
TOTAL DIRECT OPERATING COST			6.72	122,328
Plant overhead	80% of total labor		0.15	2,746
Taxes and insurance	2%/yr of fixed capital		0.23	4,256
Plant cost			7.10	129,330
G&A, sales, research	5% of sales		0.53	9,550
Cash expenditures			7.63	138,880
Depreciation	10%/yr of fixed capital		1.17	21,282
TOTAL PRODUCTION COST			8.80	160,162
By-product credit				
Higher alcohols	4.77¢/lb (10.5¢/kg)	0.00339 lb	-0.02	-294
NET PRODUCTION COST			8.78	159,868
25%/yr pretax ROI			2.92	53,204
PRODUCT VALUE			11.70	213,072

Table 4.23

CRUDE SYNGAS FROM STEAM REFORMING OF NATURAL GAS

CAPITAL INVESTMENT

Plant Capacity: 99 x 10^9 scf/yr Crude Syngas
at 0.90 Stream Factor
PEP Cost Index: 400

	Total
Battery limits equipment, f.o.b.	
Columns	$ 2,751,900
Vessels and tanks	2,092,900
Exchangers	6,570,300
Furnaces	18,552,000
Compressors	2,928,200
Miscellaneous equipment	212,000
Pumps	942,000
Total	$34,049,500
Battery limits equipment installed	$61,310,000
Contingency, 20%	12,262,000
BATTERY LIMITS INVESTMENT	$73,572,000
Off-sites, installed	
Cooling tower	388,600
Process water treatment	176,300
Utilities and storage	$ 565,000
General service facilities	12,375,000
Waste treatment	3,094,000
Total	$16,034,000
Contingency, 20%	3,207,000
OFF-SITES INVESTMENT	$19,241,000
TOTAL FIXED CAPITAL	$92,813,000

Table 4.24

CRUDE SYNGAS FROM STEAM REFORMING OF NATURAL GAS

PRODUCTION COSTS

Plant Capacity: 99 x 10^9 scf/yr Crude Syngas
at 0.90 Stream Factor
PEP Cost Index: 400

	Basis or Unit Cost	Units/mscf	Total Costs	
			¢/mscf	Thousand $/yr
Labor				
Operating	2 men/shift, $17.50/man-hr	0.0002 man-hr	0.31	307
Maintenance	1.5%/yr of BL cost		1.11	1,104
Control laboratory	20% of operating labor		0.06	61
Total labor			1.48	1,472
Materials				
Natural gas	436¢/mscf	0.3617 mscf	157.70	156,093
Activated carbon			0.01	14
Reforming catalyst			0.28	277
Steam (MP)	0.695¢/lb (1.53¢/kg)	18.31 lb	12.73	12,596
Miscellaneous	2.5¢/lb (5.51¢/kg)		2.50	2,474
Maintenance	1.5%/yr of BL cost		1.12	1,104
Operating	10% of operating labor		0.03	31
Total materials			174.37	172,589
Utilities				
Cooling water	5.4¢/1,000 gal (1.43¢/cu m)	4.16 gal	0.02	22
Process water	68¢/1,000 gal (18¢/cu m)	2.49 gal	0.17	167
Electricity	3.6¢/kwh	0.631 kwh	2.27	2,248
Total utilities			2.46	2,437
TOTAL DIRECT OPERATING COST			178.31	176,498
Plant overhead	80% of total labor		1.19	1,178
Taxes and insurance	2%/yr of fixed capital		1.88	1,856
Plant cost			181.38	179,532
G&A, sales, research	4% of sales		7.20	7,127
Cash expenditures			188.58	186,659
Depreciation	10%/yr of fixed capital		9.38	9,281
TOTAL PRODUCTION COST			197.96	195,940
By-product credit				
Steam export (HP)	0.775¢/lb (1.71¢/kg)	40.53 kg	-31.41	-31,090
NET PRODUCTION COST			166.55	164,850
25%/yr pretax ROI			23.44	23,203
PRODUCT VALUE			189.99	188,053

Table 4.25

CARBON DIOXIDE FROM FLUE GAS SCRUBBING WITH MEA SOLUTION (UCC AMINE GUARD)

MAJOR EQUIPMENT

Plant Capacity: 870 Million lb/yr
(395,000 Metric Tons/yr) CO_2
at 0.90 Stream Factor

Equipment Number	Name	Size (bhp)	Material of Construction	Remarks
	Compressors			
K-101	Flue gas compressor	12,014	Carbon steel	

Equipment Number	Name	Volume (gal)	Material of Construction	Remarks
	Pressure vessels			
V-101	Flue gas condensate	4,661	Carbon steel	
V-102	Stripper reflux drum	5,696	Carbon steel	

Equipment Number	Name	Height (ft)	Diameter (ft)	Material of Construction		Remarks
				Shell	Trays	
	Columns					
C-101	Absorber	65	21.4	Carbon steel	Carbon steel	25 sieve trays, 24 in. spacing.
C-102	Stripper	75	15.3	Carbon steel	Carbon steel	30 sieve trays, 24 in. spacing.

Equipment Number	Name	Size (sq ft)	Heat Load (MM Btu/hr)	Material of Construction		Remarks
				Shell	Tubes	
	Exchangers					
E-101	Flue gas coolers (10)	8,389 ea	12.95 ea	Carbon steel	Carbon steel	
E-102	Compressor after coolers (3)	8,596 ea	1.25 ea	Carbon steel	Carbon steel	
E-103	Interchangers (6)	8,907 ea	24.86 ea	Carbon steel	Carbon steel	
E-104	Stripper condensers (2)	5,696 ea	49.71 ea	Carbon steel	Carbon steel	
E-105	Stripper reboilers (3)	7,561 ea	79.75 ea	Carbon steel	Carbon steel	
E-106	Lean solution coolers (3)	7,664 ea	19.89 ea	Carbon steel	Carbon steel	
E-107	Absorber Cooler-I	9,839	33.14	Carbon steel	Carbon steel	
E-108	Absorber Cooler-II	8,804	29.00	Carbon steel	Carbon steel	
E-109	Absorber Cooler-III	8,804	29.00	Carbon steel	Carbon steel	

Equipment Number	Name	Volume (gal)	Material of Construction	Remarks
	Tanks			
T-101	Solvent holding tank	103,571	316 ss	

Pumps

100 Section - 4, including 2 operating, 2 spares, 163 operating bhp.

Table 4.26

CARBON DIOXIDE FROM FLUE GAS SCRUBBING WITH MEA SOLUTION
(UCC AMINE GUARD)

STREAM FLOWS

Plant Capacity: 870 Million lb/yr
(395 Metric Tons/yr) CO_2
at 0.90 Stream Factor

		Stream Flows (lb/hr)			
	Mol Wt	(1) Hot Flue Gas	(2) Condensate	(3) Cooled Flue Gas	(4) CO_2 Lean Gases
Methane	16	404	—	404	404
Carbon dioxide	44	122,610	40	122,570	12,220
Carbon monoxide	28	707	—	707	707
Ethane	30	44	—	44	44
C_3+	58	46	—	46	46
Nitrogen + inerts	28	662,966	—	662,966	662,966
Oxygen	32	25,440	—	25,660	25,440
Water	18	97,340	65,310	32,030	29,050
Monoethanol amine	61	—	—	—	—
Total		909,557	65,350	844,207	730,877

		Stream Flows (lb/hr)		
	Mol Wt	(5) Rich MEA Soln.	(6) Lean MEA Soln.	(7) CO_2 Stream
Methane	16	—	—	—
Carbon dioxide	44	149,300	38,950	110,350
Carbon monoxide	28	—	—	—
Ethane	30	—	—	—
C_3+	58	—	—	—
Nitrogen + inerts	28	—	—	—
Oxygen	32	—	—	—
Water	18	1,620,000	1,620,000	2,980
Monoethanol amine	61	560,000	540,00	—
Total		2,309,300	2,198,950	113,330

Table 4.27

CARBON DIOXIDE FROM FLUE GAS SCRUBBING WITH MEA SOLUTION (UCC AMINE GUARD)

CAPITAL INVESTMENT

Plant Capacity: 870 Million lb/yr
(395,000 Metric Tons/yr) CO_2
at 0.90 Stream
PEP Cost Index: 400

	Total
Battery limits equipment, f.o.b.	
Columns	$ 698,300
Vessels and tanks	1,526,300
Exchangers	3,004,600
Compressors	3,747,600
Pumps	67,400
Total	$ 9,044,200
Battery limits equipment installed	$25,085,000
Contingency, 20%	5,017,000
BATTERY LIMITS INVESTMENT	$30,102,000
Off-sites, installed	
Cooling tower	3,808,900
Steam generation	5,071,500
Utilities and storage	$ 8,880,000
General service facilities	6,793,000
Waste treatment	1,698,000
Total	$17,371,000
Contingency, 20%	3,474,000
OFF-SITES INVESTMENT	$20,846,000
TOTAL FIXED CAPITAL	$50,948,000

Table 4.28

CARBON DIOXIDE FROM FLUE GAS SCRUBBING WITH MEA SOLUTION (UCC AMINE GUARD)

PRODUCTION COSTS

Plant Capacity: 870 Million lb/yr
(395,000 Metric Tons/yr) CO_2
at 0.90 Stream Factor
PEP Cost Index: 400

			Total Costs		
	Basis or Unit Cost	Units/lb (units/1,000 kg)	¢/lb	¢/kg	Thousand $/yr
Labor					
Operating	2 men/shift, $17.50/man-hr		0.04	0.09	307
Maintenance	1.5%/yr of BL cost		0.05	0.11	452
Control laboratory	20% of operating labor		0.01	0.02	61
Total labor			0.10	0.22	820
Materials					
Solvent, inhibitors		1 lb (1 ton)	0.05	0.11	435
Maintenance	10%/yr of BL cost		0.05	0.11	452
Operating	10% of operating labor		—	—	31
Total materials			0.10	0.22	918
Utilities					
Cooling water	5.4¢/1,000 gal (1.43¢/cu m)	15.7 gal (131 cu m)	0.08	0.18	739
Steam	544¢/1,000 lb (1,199¢/ton)	2.36 lb (2.36 tons)	1.28	2.82	11,150
Electricity	3.6¢/kwh	0.091 kwh (202 kwh)	0.33	0.73	2,864
Total utilities			1.69	3.73	14,753
TOTAL DIRECT OPERATING COST			1.89	4.17	16,491
Plant overhead	80% of total labor		1.89	4.17	16,491
Taxes and insurance	2%/yr of fixed capital		0.12	0.26	1,019
Plant cost			2.09	4.61	18,166
G&A, sales, research	5% of sales		0.25	0.55	2,175
Cash expenditures			2.34	5.16	20,341
Depreciation	10%/yr of fixed capital		0.59	1.30	5,095
TOTAL PRODUCTION COST			2.93	6.46	25,436
25%/yr pretax ROI			1.46	3.22	12,737
PRODUCT VALUE			4.39	9.68	38,173

Table 4.29

SYNGAS (H_2:CO RATIO = 1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 10^{11} scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.242 mscf	105.51
Natural gas fuel	436¢/mscf	0.219 mscf	95.48
Carbon dioxide	4.4¢/lb	28.3 lb	124.52
Catalysts, adsorbent			0.84
Misc. chemicals, utilities			1.74
Gross raw materials			328.09
Utilities			
Cooling water	5.4¢/1,000 gal	737 gal	3.98
Steam	$5.44/1,000 lb	49.9 lb	27.15
Process water	68¢/1,000 gal	7.45 gal	0.51
Electricity	3.6¢/kwh	1.27 kwh	4.57
Total utilities			36.21

Table 4.29 (Concluded)

SYNGAS (H_2:CO RATIO = 1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 10^{11} scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	200.2
Off-sites	57.9
Total fixed capital	258.1
Production costs (¢/mscf)	
Raw materials	328.09
Utilities	36.21
Variable costs	364.30
Operating labor, 4/shift, $17.50/hr	0.61
Maintenance labor, 1.5%/yr of BL inv	3.00
Control lab labor, 20% of op labor	0.12
Labor costs	3.73
Maintenance materials, 1.5%/yr of BL inv	3.00
Operating supplies, 10% of op labor	0.06
TOTAL DIRECT COSTS	371.09
Plant overhead, 80% of labor costs	2.99
Taxes and insurance, 2%/yr of TFC	5.15
Depreciation, 10%/yr of TFC	25.76
Plant gate cost	404.99
G&A, sales, research	18.00
NET PRODUCTION COST	422.99
ROI before taxes, 25%/yr of TFC	64.40
PRODUCT VALUE	487.39

Table 4.30

SUMMARIZED COSTS FOR PRODUCTS FROM NATURAL GAS STEAM REFORMING

	Syngas, H_2:CO Ratio = 3	Syngas, H_2:CO Ratio = 2	Syngas, H_2:CO Ratio = 1	Hydrogen by Conventional Process*	Hydrogen with PSA System†	Methanol, ICI Low Pressure Process	Crude Syngas, Ex-methanol Reformer
Production scale (million scf/day)§	295	298	303	277 (480 million lb/yr)	277 (480 million lb/yr)	1,819 million lb/yr	300
Fixed capital ($ million)	131	158	258	123	126	213	92.8
Cost buildup	$/mscf	$/mscf	$/mscf	¢/lb	¢/lb	¢/lb	$/mscf
Natural gas feed	1.09	1.08	1.06	21.97	31.58	5.84	1.07
Natural gas fuel	0.66	0.78	0.95	11.51		0.35	0.51
Total natural gas cost	1.75	1.86	2.01	33.48	31.58	6.19	1.58
Labor and other variable costs‡	0.09	0.50	1.70	2.61	-5.15	0.51	-0.11
TOTAL DIRECT OPERATING COST	1.84	2.36	3.71	36.09	26.43	6.70	1.47
Fixed costs**	0.28	0.34	0.52	5.22	5.36	2.08	0.20
TOTAL PRODUCTION COST	2.12	2.70	4.23	41.31	31.79	8.78	1.67
25% ROI	0.34	0.40	0.64	6.41	6.58	2.92	0.23
PRODUCT VALUE	2.46	3.10	4.87	47.72	38.37	11.70	1.90

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*As described in text under Case C and illustrated by Figure 4.9.

†Where a pressure swing adsorption system replaces low temperature shift and CO_2 removal, as shown in Figure 4.16.

§The production scales for all cases, except H_2 with PSA system, corresponds to a fixed reformer natural gas feed rate that is equivalent to 2,500 metric tons/day of methanol (1,819 million lb/yr). Syngas rates are on a dry volumetric basis and both H_2 and MeOH rates are on a contained basis.

‡Includes by-product credits where applicable (e.g., in the PSA hydrogen and the crude syngas cases, the main by-product is steam).

**Includes overhead, taxes, insurance, G&A, research, sales, and depreciation.

Figure 4.15

SYNGAS COST AS A FUNCTION OF H_2:CO RATIO

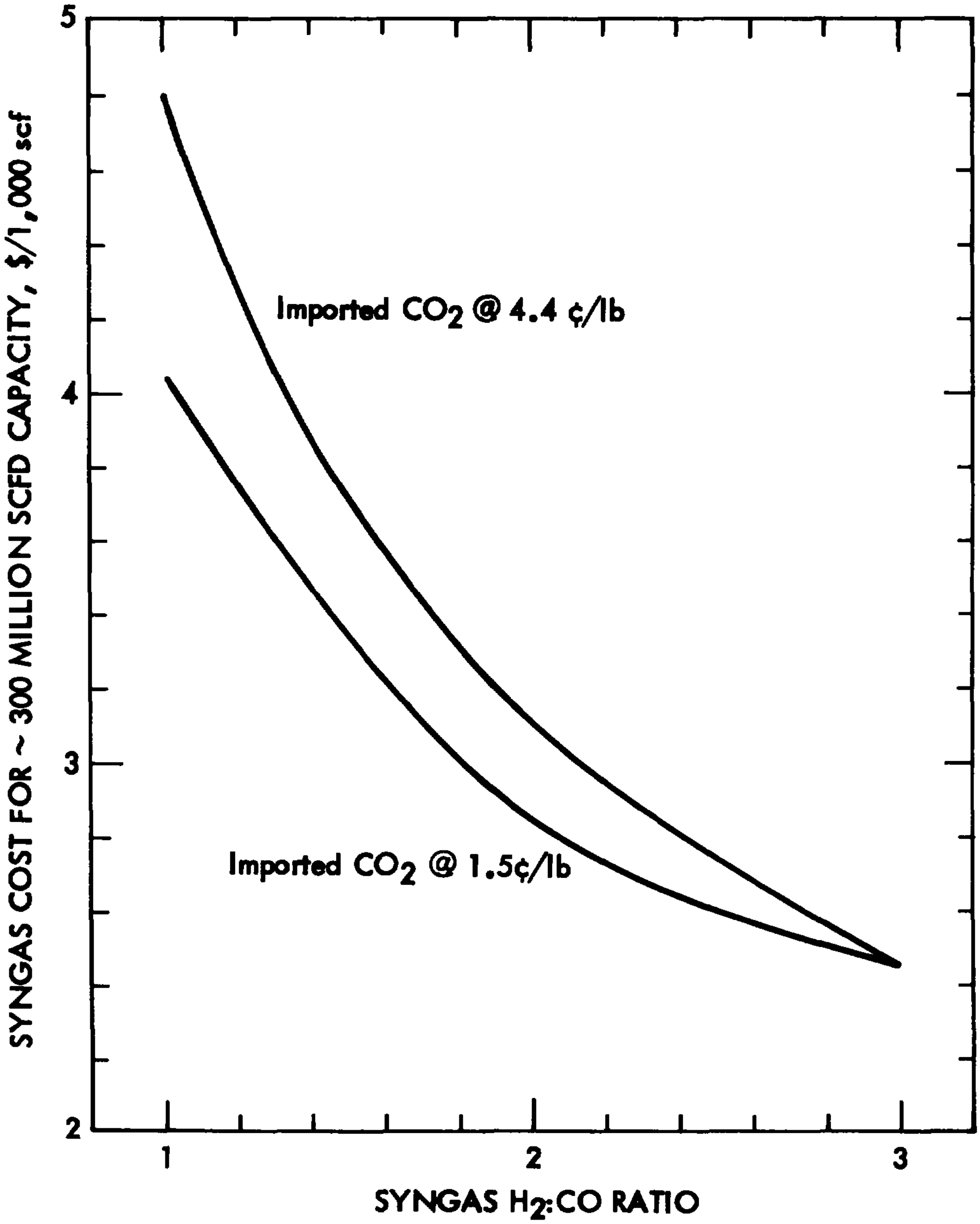


Table 4.31

ECONOMIC COMPARISON OF SKIMMING PROCESSES

Total Syngas Rate: 300 Million scfd
PEP Cost Index: 400

	PSA		Cryogenic		Cosorb®	Prism®	
Initial H_2:CO ratio	3	2	3	2	3	3	2
Syngas rate to skimming (million scfd)	111.6	178.6	99.8	154.3	97.1	300	300
Products (million scfd)							
Hydrogen rich product	71.44	98.44	72.48	99.90	72.52	76	104
Fuel	Nil	Nil	2.41	4.80	1.45	--	--
Syngas	228.56	201.56	225.11	195.3	226.03	224	196
H_2 purity of H_2 product (vol%)	99.999	99.999	98.5	98.5	98	97.9	96.8
Adjusted H_2:CO ratio in syngas	2	1	2	1	2	2	1
Fixed capital ($ million)	26.71	46.95	11.85	16.69	19.43	11.81	18.83
Energy requirements							
Electricity (kwh/hr)	5,760	11,520	14,640	24,110	8,420	8,400	11,800
Steam (1,000 lb/hr)	--	--	--	--	74.7	--	--
Fuel (million Btu/hr)	--	--	--	--	--	3.6	5.1
Cost buildup ($1,000/yr)							
Utilities	1,642	3,285	4,174	6,874	6,010	2,514	3,533
Materials	--	--	--	--	257	--	--
Capital related	10,684	18,780	4,977	7,010	8,161	4,724	7,532
Total	12,326	22,065	9,151	13,884	14,428	7,238	11,065
Unit cost (¢/mscf fed to skimming)	33.34	37.44	27.79	27.27	45.02	7.31	11.18
Unit cost (¢/mscf of adjusted syngas)	16.34	33.17	12.31	21.54	19.34	9.79	17.37

Notes: (1) Unit costs of electricity and steam taken at 3.6¢/kwh and $6.1/1,000 lb respectively. Fuel, as in previous cases, is taken at $4.17/million Btu.

(2) Raw materials cost for Cosorb® is for toluene replacement, taken at $1.40/gallon.

(3) Capital related charges are 40% for PSA and Prism® separators and 42% for cryogenic and Cosorb® processes; the lower charges reflect less maintenance costs.

(4) The quoted H_2 rates in the Prism® case refer to the permeate stream, which contains 2-3% carbon oxides. A methanation stage was included to make the H_2 acceptable as chemical grade. The final H_2 purity is for the methanated product expressed on a dry basis.

(5) The costs shown above are independent of the effects of by-product values, i.e., they represent the costs of carrying out the skimming operation when all streams are assigned identical values. The effect of by-product valuation is discussed later.

Table 4.32

SYNGAS (H_2:CO RATIO = 2) FROM THE SKIMMING OF 3:1 SYNGAS; PRISM® SEPARATORS

PRODUCTION COSTS FOR 73.9 x 10^9 scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.334 mscf	145.62
Natural gas fuel	436¢/mscf	0.202 mscf	88.07
Catalyst, misc. chem/util.			1.18
Gross raw materials			234.87
By-products			
Hydrogen	50¢/lb	-1.65 lb	-82.50
Utilities			
Cooling water	5.4¢/1,000 gal	292 gal	1.58
Process water	68¢/1,000 gal	8.45 gal	0.57
Electricity	3.6¢/kwh	2.23 kwh	8.04
Natural gas	$4.17/mm Btu	386 Btu	0.16
Total utilities			10.35

Table 4.32 (Concluded)

SYNGAS (H_2:CO RATIO = 2) FROM THE SKIMMING OF 3:1 SYNGAS; PRISM® SEPARATORS

PRODUCTION COSTS FOR 73.9 x 10^9 scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	110.0
Off-sites	32.8
Total fixed capital	142.8
Production costs (¢/mscf)	
Raw materials	234.87
By-products	-82.50
Utilities	10.35
Variable costs	162.72
Operating labor, 4/shift, $17.50/hr	0.83
Maintenance labor, 1.5%/yr of BL inv	2.23
Control lab labor, 20% of op labor	0.17
Labor costs	3.23
Maintenance materials, 1.5%/yr of BL inv	2.23
Operating supplies, 10% of op labor	0.08
TOTAL DIRECT COSTS	168.26
Plant overhead, 80% of labor costs	2.58
Taxes and insurance, 2%/yr of TFC	3.86
Depreciation, 10%/yr of TFC	19.32
Plant gate cost	194.02
G&A, sales, research	13.00
NET PRODUCTION COST	207.02
ROI before taxes, 25%/yr of TFC	48.30
PRODUCT VALUE	255.32

Table 4.33

SYNGAS (H_2:CO RATIO = 1) FROM THE SKIMMING OF 3:1 SYNGAS; PRISM® SEPARATORS

PRODUCTION COSTS FOR 47.5 x 10^9 scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.5187 mscf	226.15
Natural gas fuel	436¢/mscf	0.3146 mscf	137.17
Catalyst, misc. chem/util.			1.83
Gross raw materials			365.15
By-products			
Hydrogen	50¢/lb	-5.01 lb	-250.5
Utilities			
Cooling water	5.4¢/1,000 gal	454 gal	2.45
Process water	68¢/1,000 gal	13.1 gal	0.89
Electricity	3.6¢/kwh	3.54 kwh	12.76
Natural gas	$4.17/mm Btu	1,235 Btu	0.51
Total utilities			16.61

Table 4.33 (Concluded)

SYNGAS (H_2:CO RATIO = 1) FROM THE SKIMMING OF 3:1 SYNGAS; PRISM® SEPARATORS

PRODUCTION COSTS FOR 47.5 x 10^9 scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	124.9
Off-sites	32.8
Total fixed capital	157.7
Production costs (¢/mscf)	
Raw materials	365.15
By-product	-250.50
Utilities	16.61
Variable costs	131.26
Operating labor, 4/shift, $17.50/hr	1.29
Maintenance labor, 1.5%/yr of BL inv	3.94
Control lab labor, 20% of op labor	0.26
Labor costs	5.49
Maintenance materials, 1.5%/yr of BL inv	3.94
Operating supplies, 10% of op labor	0.13
TOTAL DIRECT COSTS	140.82
Plant overhead, 80% of labor costs	4.39
Taxes and insurance, 2%/yr of TFC	6.64
Depreciation, 10%/yr of TFC	33.19
Plant gate cost	185.04
G&A, sales, research	20.00
NET PRODUCTION COST	205.04
ROI before taxes, 25%/yr of TFC	82.97
PRODUCT VALUE	288.01

Table 4.34

SYNGAS (H_2:CO RATIO = 1) FROM THE SKIMMING OF 2:1 SYNGAS; PRISM® SEPARATORS

PRODUCTION COSTS FOR 63.7 x 10^9 scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.3839 mscf	167.38
Natural gas fuel	436¢/mscf	0.2767 mscf	120.64
Carbon dioxide	4.4¢/lb	13.77 lb	60.59
Catalyst, misc. chem/util.			1.88
Gross raw materials			350.49
By-products			
Hydrogen	50¢/lb	-2.48 lb	-124.00
Utilities			
Cooling water	5.4¢/1,000 gal	486 gal	2.62
Process water	68¢/1,000 gal	9.72 gal	0.66
Electricity	3.6¢/kwh	3.3 kwh	11.88
Natural gas	$4.17/mm Btu	634 Btu	0.26
Total utilities			15.42

Table 4.34 (Concluded)

SYNGAS (H_2:CO RATIO = 1) FROM THE SKIMMING OF 2:1 SYNGAS; PRISM® SEPARATORS

PRODUCTION COSTS FOR 63.7 x 10^9 scf/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	136.6
Off-sites	40.7
Total fixed capital	177.3
Production costs (¢/mscf)	
Raw materials	350.49
By-products	-124.00
Utilities	15.42
Variable costs	241.91
Operating labor, 4/shift, $17.50/hr	0.96
Maintenance labor, 1.5%/yr of BL inv	3.22
Control lab labor, 20% of op labor	0.19
Labor costs	4.37
Maintenance materials, 1.5%/yr of BL inv	3.22
Operating supplies, 10% of op labor	0.10
TOTAL DIRECT COSTS	249.60
Plant overhead, 80% of labor costs	3.50
Taxes and insurance, 2%/yr of TFC	5.57
Depreciation, 10%/yr of TFC	27.84
Plant gate cost	286.51
G&A, sales, research	19.00
NET PRODUCTION COST	305.51
ROI before taxes, 25%/yr of TFC	69.59
PRODUCT VALUE	375.10

Table 4.35

COSTS FOR H_2:CO RATIO ADJUSTMENT BY CO_2 IMPORT AND/OR SKIMMING SURPLUS H_2

	Case 1 - Syngas H_2:CO Ratio = 2		Case 2 - Syngas H_2:CO Ratio = 1		
	CO_2 Imported for Reformer Feed; No Skimming.	Primary Syngas with H_2:CO Ratio = 3; Produced by Total CO_2 Recycle; Surplus H_2 Skimmed in Monsanto's Prism® Separators.	CO_2 Imported for Reformer Feed; No Skimming.	Primary Syngas with H_2:CO Ratio = 3; Surplus H_2 Skimmed by Prism® Separators.	Primary Syngas with H_2:CO_2 Ratio = 2 Achieved by CO_2 Import; Surplus H_2 Skimmed by Prism® Separators.
Product output (million scfd)	Syngas (H_2:CO ratio = 2) : 300	Syngas (H_2:CO ratio = 2) 224 97.8 vol% H_2 product 76 Total 300	Syngas (H_2:CO ratio = 1) : 300	Syngas (H_2:CO ratio = 1) 144 97.3 vol% H_2 product 156 Total 300	Syngas (H_2:CO ratio = 1) 193 96.8 vol% H_2 product 107 Total 300
Total fixed capital ($ million)	158.5 (Table 4.17)	142.8 (Table 4.32)	258.1 (Table 4.29)	157.7 (Table 4.33)	177.3 (Table 4.34)
Equation for cost of syngas product ($/mscf)	2.71 + 8.86 CO_2 CO_2 = unit cost in $/lb	3.38 - 1.65 H_2 H_2 = unit cost in $/lb	3.63 + 28.3 CO_2	5.385 - 5.01 H_2	4.385 + 13.77 CO_2 - 2.48 H_2
Calculated cost ($/mscf) assuming:					
(a) Cheap CO_2 (1.5¢/lb)	2.84	—	4.05	—	—
(b) Flue gas scrubbed CO_2 (4.4¢/lb)	3.10	—	4.87	—	—
(c) Coproduct H_2 at chemical value (50¢/lb)	—	2.55	—	2.88	—
(d) Coproduct H_2 at fuel value (24¢/lb)	—	2.98	—	4.18	—
(e) Cheap CO_2 + chemical value H_2	—	—	—	—	3.35
(f) Cheap CO_2 + fuel value H_2	—	—	—	—	4.00
(g) Scrubbed CO_2 + chemical value H_2	—	—	—	—	3.75
(h) Scrubbed CO_2 + fuel value H_2	—	—	—	—	4.40

Note: For e-h above, CO_2 and H_2 unit values as in a-d.

Figure 4.16

COSTS FOR ADJUSTING SYNGAS H_2:CO RATIO

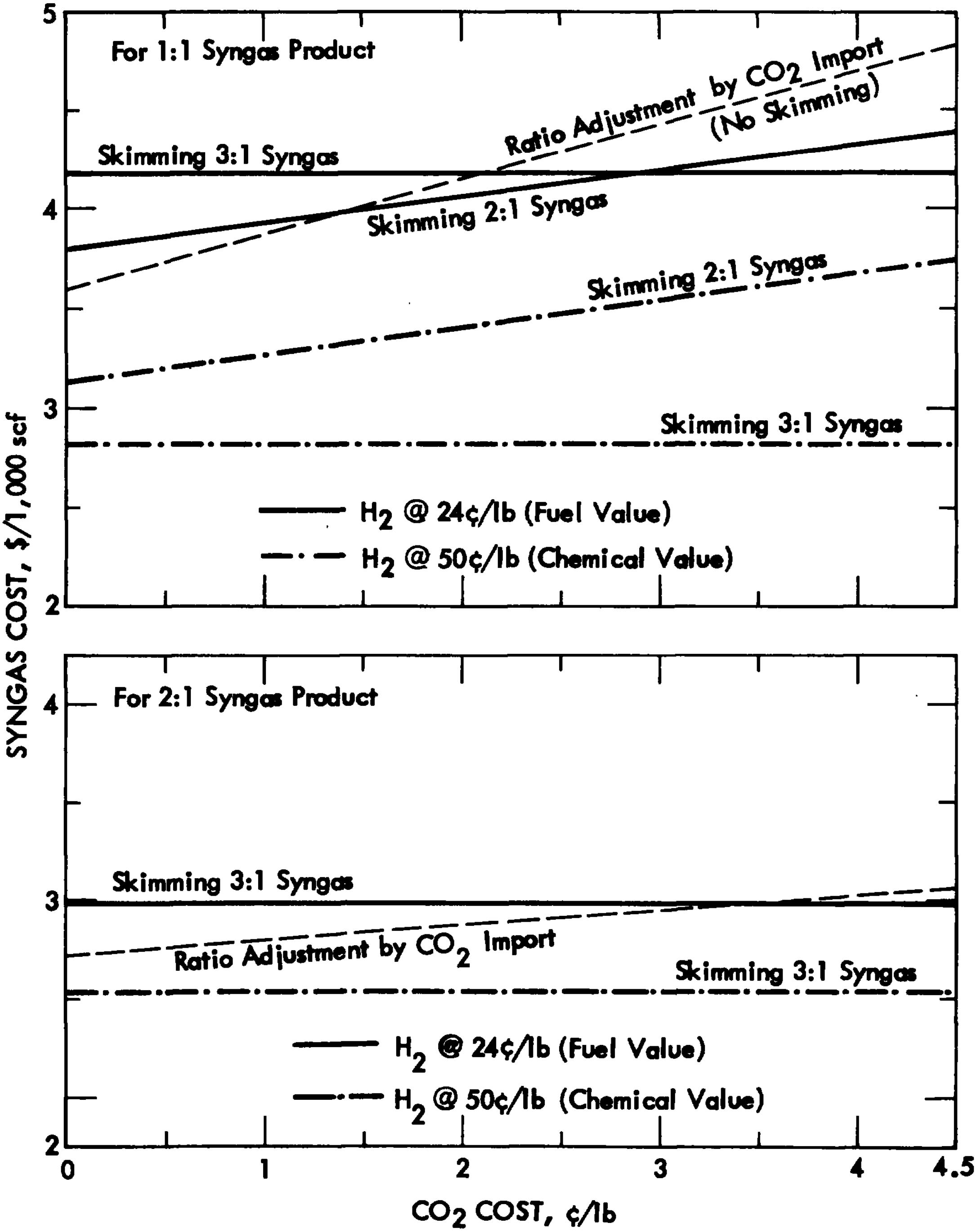
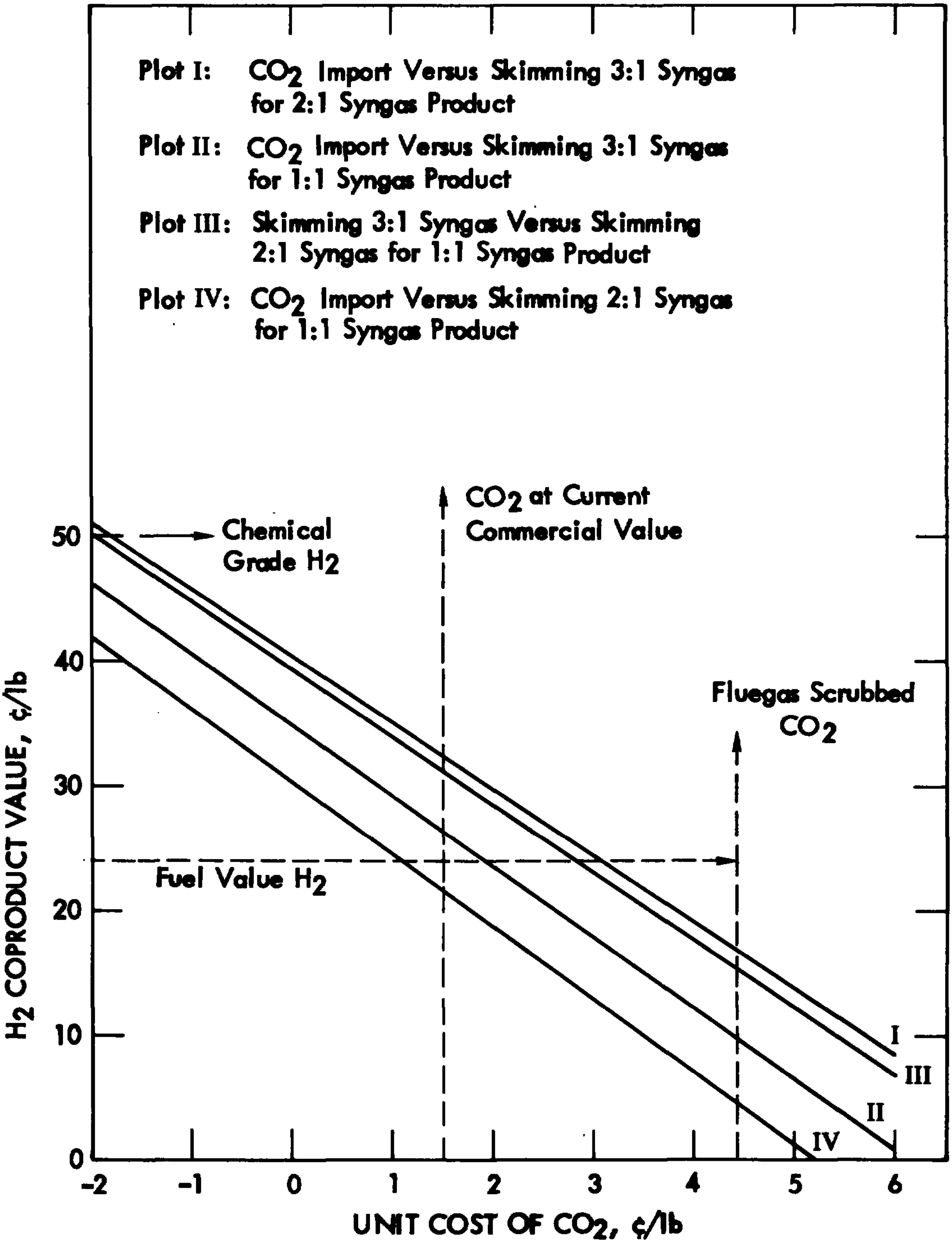


Figure 4.17

CO_2 IMPORT COMPARED WITH H_2 SKIMMING
(Showing CO_2/H_2 Breakeven Values)



Costs of Syngas Compression

In most applications of syngas the reaction stage is operated at pressures much higher than those at which syngas is obtained from a natural steam reforming system. In the syngas Cases A and B (H_2:CO ratios of 3:1 and 2:1), the syngas pressure is 240 psia. The cost of compressing syngas was examined as a function of output rate and final compression pressure. The ranges considered were as follows:

Output rates	30-300 million scfd
Final pressures	480-1200 psia

The essential results are presented in Figures 4.18 through 4.20. Figure 4.18 is a plot of the brake-horsepower requirement as a function of final pressure. It will be seen that the power requirements for Case B (H_2:CO ratio = 2) are slightly greater than for Case A (H_2:CO ratio = 3) owing to the higher gas density. Figure 4.19 shows the fixed capital cost requirements as a function of the syngas output rate. The capital costs represented are for the 2:1 H_2:CO ratio and we found that, within the accuracy of our estimates, these are also applicable for the 3:1 ratio syngas. For compressor drives both electric motors and steam turbines were examined. The latter were assumed to be of the noncondensing type with steam conditions as for the high pressure (at inlet) and medium pressure (at exit) grades defined earlier. As shown in Figure 4.19, we did not examine steam turbine drives below an output rate of 75 million scfd. At this rate the brake horsepower of the individual turbines is down to about 5,000 which was assumed to be an approximate cut-off point at which electric motors became more economic.

Figure 4.20 illustrates the total costs of compression in cents/ 1,000 scf as a function of the final compression pressure for an output rate of 300 million scfd. The results for both the steam turbine and electric motor drives are presented. At the values assumed for the steam and electricity (3.6¢/kwh), steam drives are more economic.

However, from the range of the overall costs for compression depicted in Figure 4.20 (5-13¢/1,000 scf, depending on the final pressure), we see that these constitute a relatively small contribution to the overall cost of syngas. The computations on which Figure 4.20 is based are summarized in Table 4.36.

Figure 4.18

BRAKE HORSEPOWER REQUIREMENT AS A FUNCTION OF SYNGAS COMPRESSION PRESSURE

(300 Million scfd Capacity)

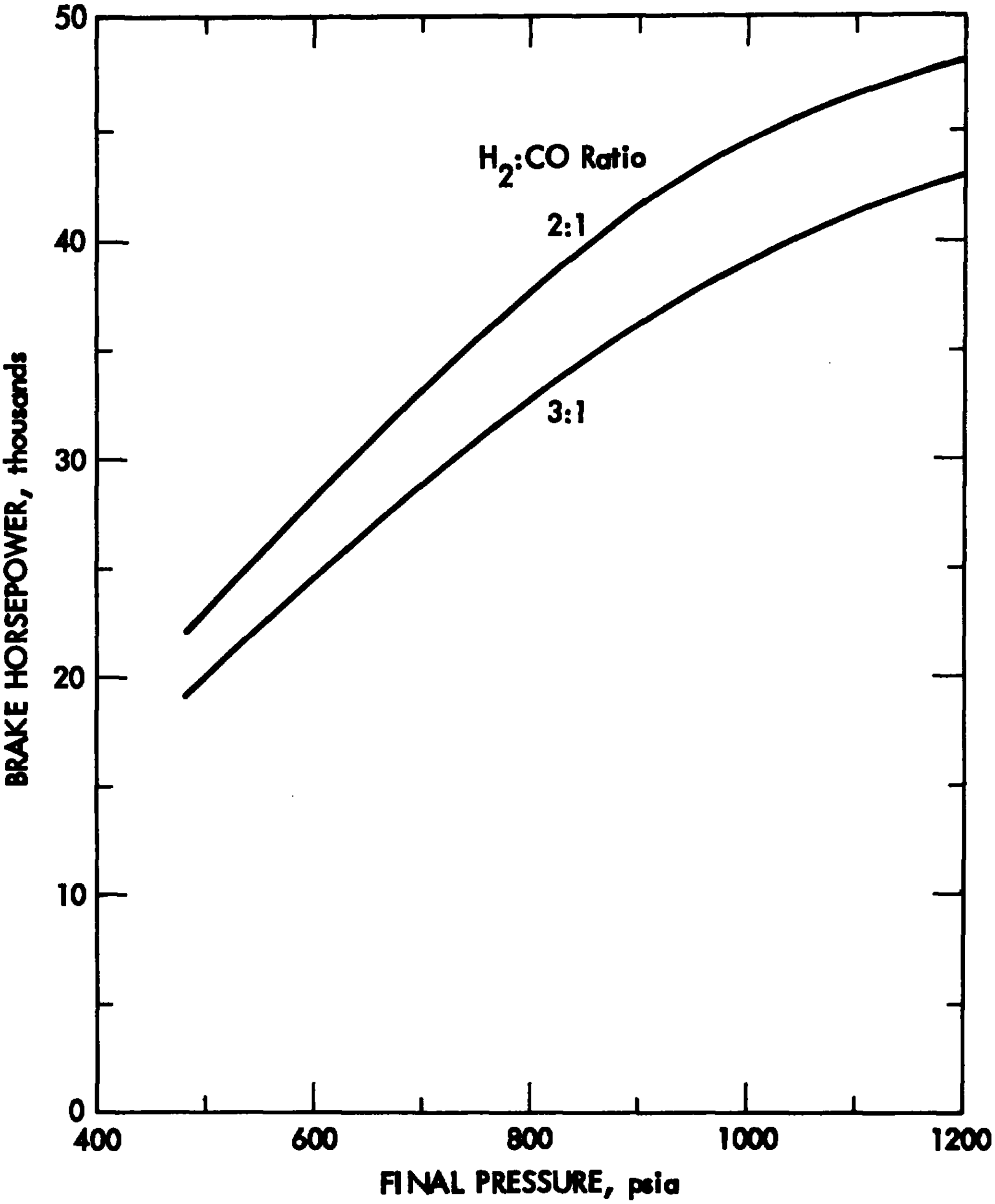


Figure 4.19

SYNGAS COMPRESSION CAPITAL AS A FUNCTION OF FINAL PRESSURE AND SCALE OF OPERATION

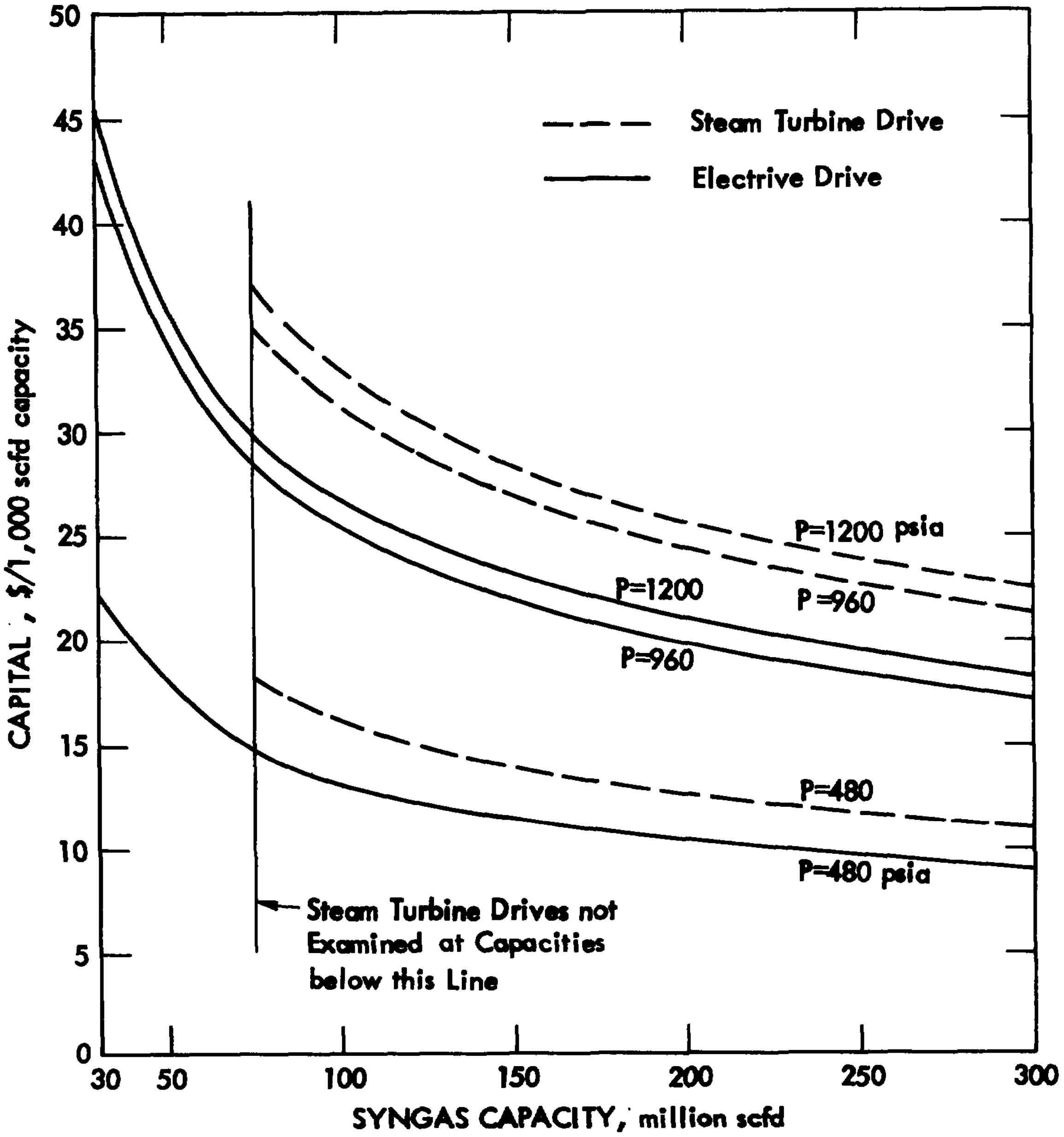
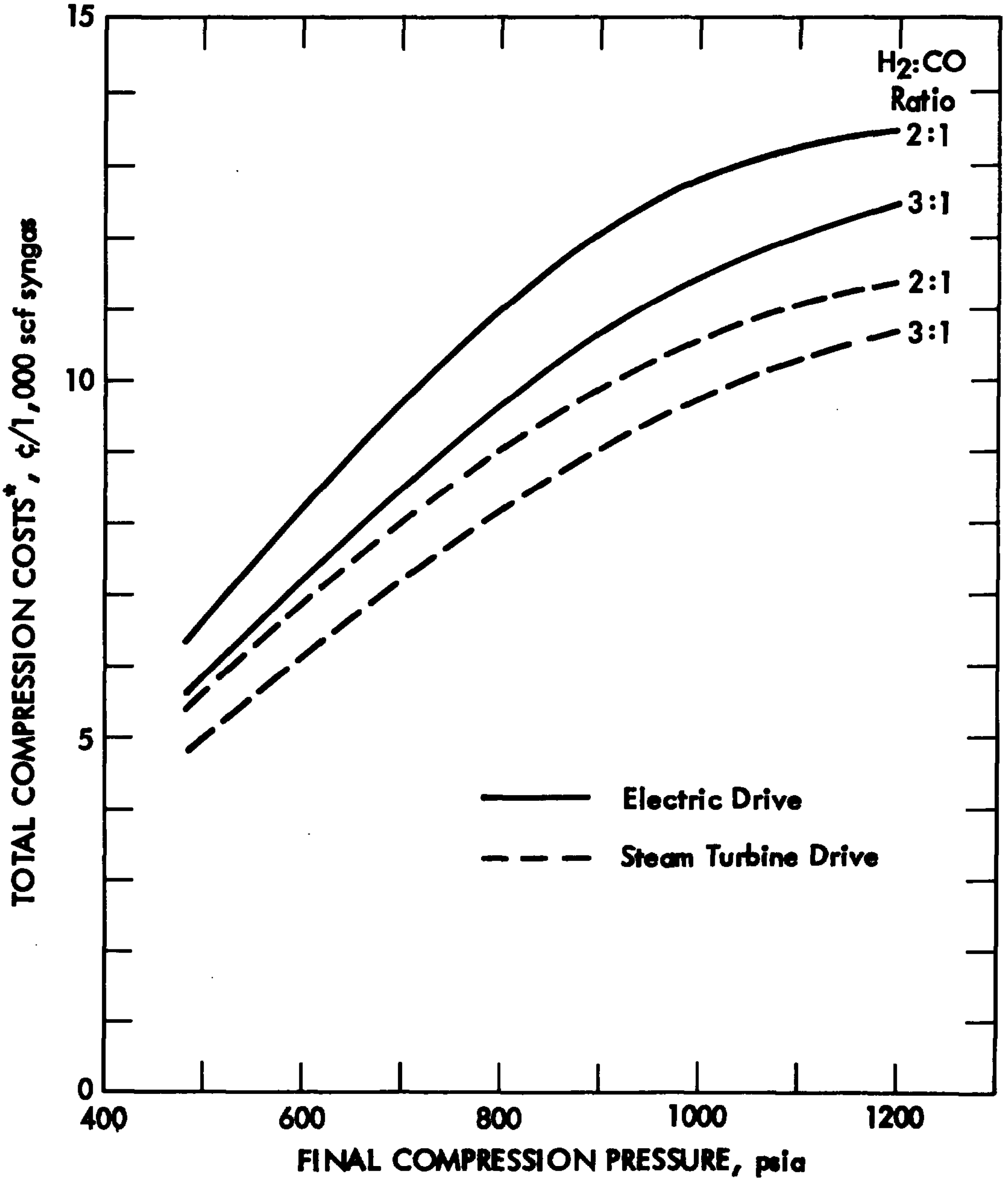


Figure 4.20

SYNGAS COMPRESSION COSTS AS A FUNCTION OF PRESSURE
(300 Million scf/Day Capacity)



* Includes 25% ROI.

Table 4.36

SYNGAS COMPRESSION COSTS

Scale: 300 Million scfd, Initial Pressure 240 psia,
at Stream Factor 0.90
PEP Cost Index: 400

	H_2:CO Ratio = 3					
Final pressure (psia)	480		960		1200	
	Electric Drive	Steam Drive	Electric Drive	Steam Drive	Electric Drive	Steam Drive
Fixed capital ($ thousand)	2,575	3,080	4,985	5,995	5,420	6,550
Total brake-horsepower	19,000	19,000	38,000	38,000	43,000	43,000
Cost buildup (¢/mscf syngas)						
Steam[*]	—	3.54	—	7.07	—	8.00
Electricity[†]	4.54	—	9.07	—	10.27	—
Other[§]	1.04	1.24	2.01	2.42	2.18	2.65
Total	5.58	4.78	11.08	9.49	12.45	10.65

	H_2:CO Ratio = 2					
Final pressure (psia)	480		960		1200	
	Electric Drive	Steam Drive	Electric Drive	Steam Drive	Electric Drive	Steam Drive
Fixed capital ($ thousand)	2,690	3,260	5,145	6,290	5,520	6,610
Total brake-horsepower	22,000	22,000	44,000	44,000	47,000	47,000
Cost buildup (¢/mscf syngas)						
Steam[*]	—	4.09	—	8.19	—	8.74
Electricity[†]	5.25	—	10.50	—	11.22	—
Other[§]	1.08	1.32	2.08	2.54	2.23	2.67
Total	6.33	5.41	12.58	10.73	13.45	11.41

---

[*] It is assumed that HP steam at 900 psia and 900°F is used at turbine inlet, exhausting at 350 psia; total enthalpy fall is 120 Btu/lb. Theoretical steam rate is 28.45 lb/kwh. For an estimated 73% turbine efficiency "actual steam rate" is 38.97 lb/kwh. As detailed earlier, the "differential" steam cost is $0.8/1,000 lb.

[†] Assumes a unit cost of 3.6¢/kwh and electrical efficiency of 90%.

[§] Mainly capital related charges which are taken at a "notional" 40% per annum of the fixed capital investment (including depreciation and 25% ROI).

Effect of Scale of Operation

The scale of operation for the base cases was fixed in a region which is considered close to the limit of a single-train facility. This corresponds to about 300 million scfd of syngas and in the hydrogen and methanol cases to 480 and 1,820 million lb/yr respectively. The latter figure is equivalent to the 2,500 metric tons methanol/day, mentioned earlier as the reference point.

For higher capacities multi-trains become necessary and we estimate that the scale exponent would be roughly 0.9. For operation below the base capacities, an averaged exponent of 0.75 is considered appropriate for extrapolations down by a factor of 0.4-0.5. To investigate the relationship of capital cost and capacity at lower capacities, we used some data available to SRI for smaller syngas and hydrogen plants. The results are presented in Figures 4.21 and 4.22. The former shows scale exponent as a function of capacity in the mode of a continuous curve. Figure 4.22 shows capital costs as a function of capacity, where the capital costs were calculated for selected points on the basis of averaged exponents. The scale exponents for lower capacities decrease to about 0.55 at a methanol equivalent of 150 metric tons/day. It should be noted that the data used in Figures 4.21 and 4.22 include the effect of plant size on the design philosophy. For smaller plants, a reduction in energy efficiency is usually acceptable owing to a disporportionate increase in the capital costs for matching or approaching the higher efficiencies of larger plants. Also, there are other design features which alter as transition is made to lower scales of operation. For instance, in compression systems the steam turbine drives are more economical for high horsepower machines. For smaller plants calling for lower horsepower drives, electric motors are preferred—their lower capital cost compensates for the higher unit energy costs.

To illustrate the effect of the scale of operation on the production economics for syngas, hydrogen, and methanol, we examined a few selected cases as detailed in Table 4.37. As shown in the table, due allowance was made for reduction in energy efficiencies and for possible changes in the design basis. The capital and production costs for these cases are presented in Tables 4.38 through 4.47. Some applications to which the lower scales of operation might be relevant are indicated in Table 4.37.

Figure 4.21

SCALE EXPONENT AS A FUNCTION OF CAPACITY

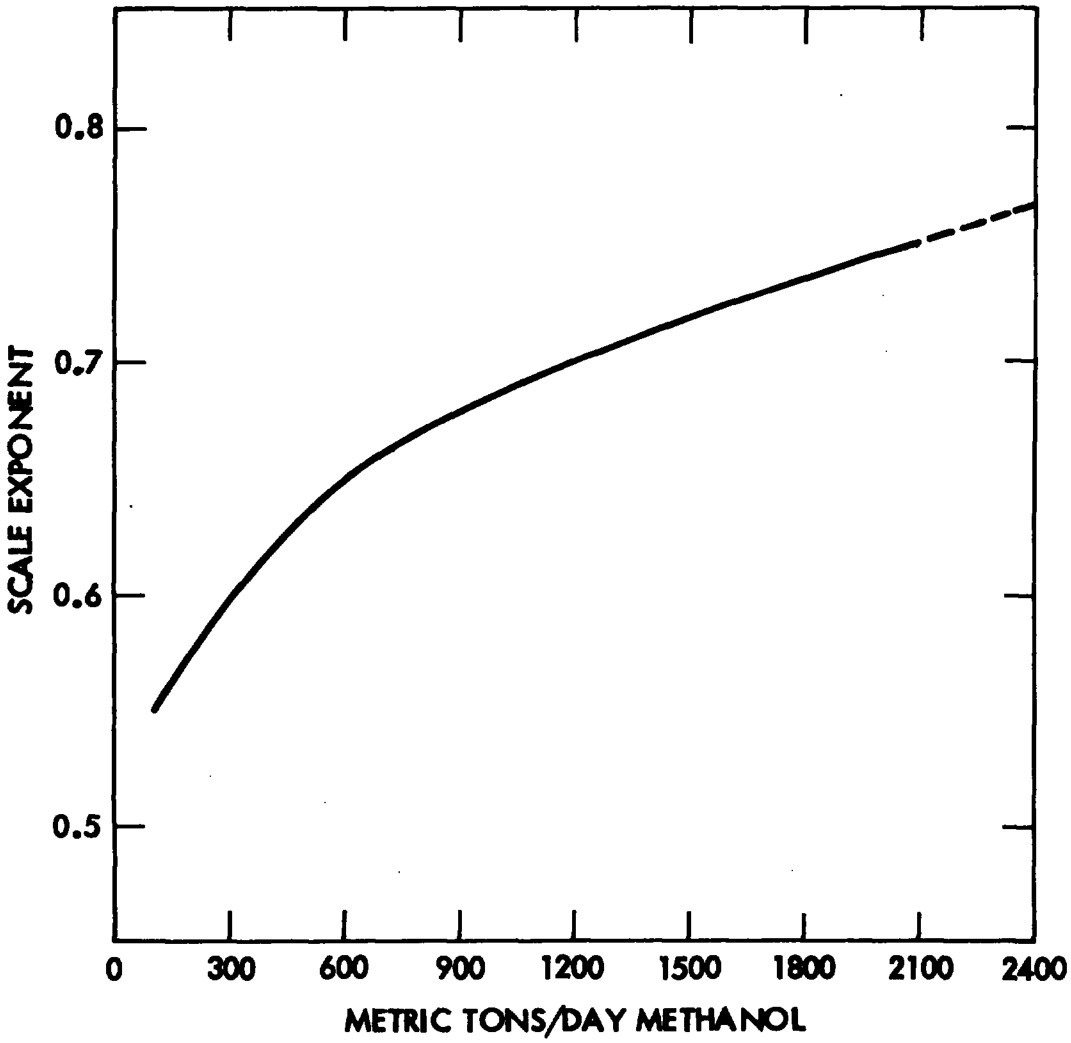


Figure 4.22

CAPITAL COST AS A FUNCTION OF CAPACITY

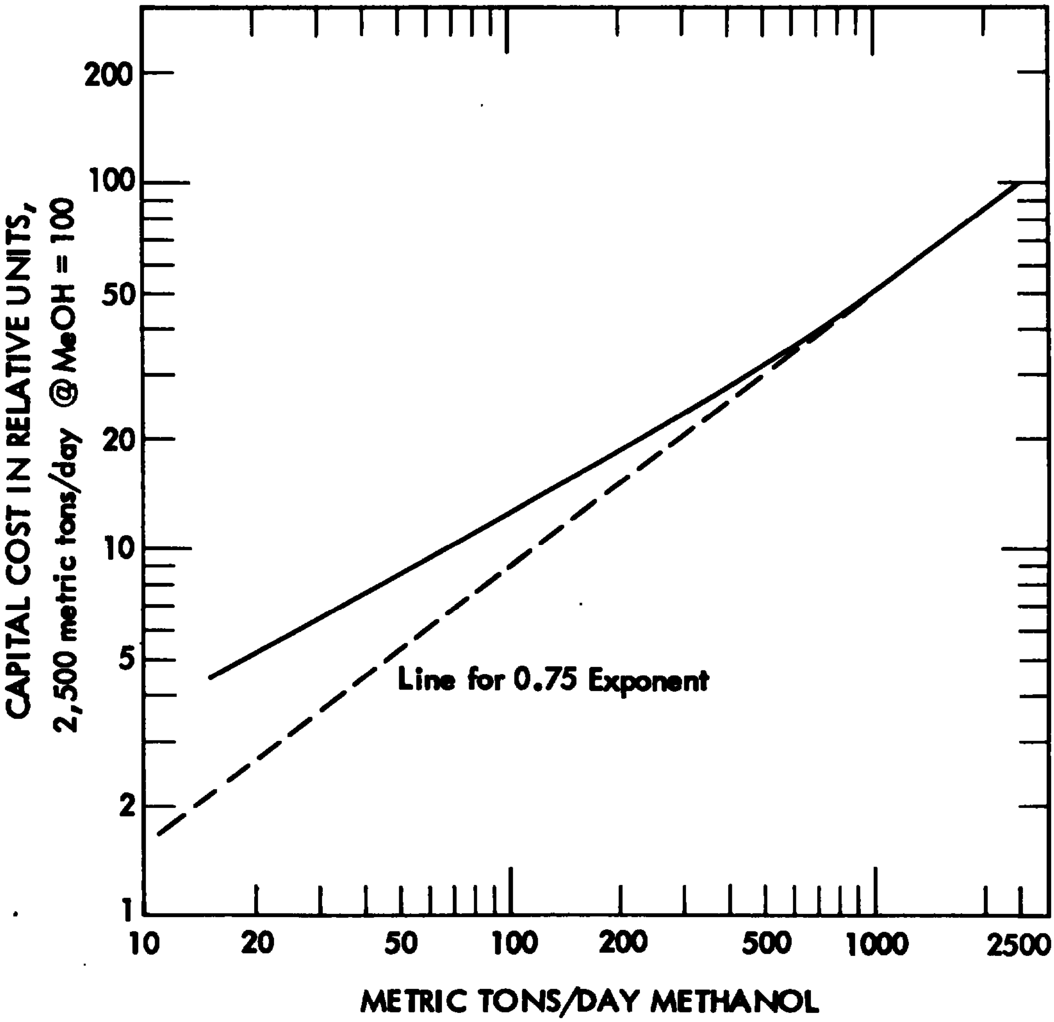


Table 4.37

CASES EXAMINED TO ILLUSTRATE EFFECT OF PLANT CAPACITY ON PRODUCTION ECONOMICS

<table>
<tr><th>Product</th><th>Base Scale Used in Syngas Study</th><th>Reduced Scales Examined</th></tr>
<tr><td>Methanol</td><td>2,500 metric tpd</td><td>1,000 Metric tpd
500
250</td></tr>
<tr><td colspan="3">For the base capacity the reformer furnace efficiency assumed was 85%. At 500 metric tpd and 250 metric tpd the efficiencies drop to 80% and 75% respectively; also, for the latter capacity electric drives are used for compression and there are no power recovery turbines.</td></tr>
<tr><td>Hydrogen</td><td>480 million lb/yr (equivalent to 2,500 metric tpd methanol)</td><td>200 million lb/yr
100
50</td></tr>
<tr><td colspan="3">Thermal efficiency drop is as for methanol case on an "equivalent capacity basis." Upper range of capacity is similar to typical sized plants for refinery hydrocracking; lower range is close to units for miscellaneous chemical hydrogenations.</td></tr>
<tr><td>Syngas with H_2:CO ratio = 2</td><td>300 million scfd (equivalent to 2,500 metric tpd methanol)</td><td>100 million scfd
50</td></tr>
<tr><td colspan="3">Again thermal efficiency drop is as for the methanol case. Below 50 million scfd, CO_2 feed compressors are driven by electric motors.</td></tr>
<tr><td>Syngas with H_2:CO ratio = 1</td><td>As above</td><td>20 million scfd</td></tr>
<tr><td colspan="3">Upper end of scale examined would be appropriate for synthesis of chemical products such as monoethylene glycol. Lowest scale (viz, 20 million scfd) would be for a typical sized oxo unit, e.g., for 2-ethyl hexanol. Syngas with H_2:CO ratio = 1 for this case is examined for both options, i.e., CO_2 addition and skimming of syngas with H_2/CO ratio = 2.</td></tr>
</table>

Table 4.38

SYNGAS (H_2:CO RATIO = 2) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 33 x 10^9 scf/yr
(Equivalent to 100 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.247 mscf	107.69
Natural gas fuel	436¢/mscf	0.178 mscf	77.61
Carbon dioxide	4.4¢/lb	8.86 lb	38.98
Catalysts, adsorbent			0.52
Misc. chemicals, utilities			0.69
Gross raw materials			225.49
Utilities			
Cooling water	5.4¢/1,000 gal	313 gal	1.69
Process water	68¢/1,000 gal	6.25 gal	0.42
Electricity	3.6¢/kwh	1.18 kwh	4.25
Total utilities			6.36

Table 4.38 (Concluded)

SYNGAS (H_2:CO RATIO = 2) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 33 x 10^9 scf/yr
(Equivalent to 100 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	54.8
Off-sites	19.0
Total fixed capital	73.8
Production costs (¢/mscf)	
Raw materials	225.49
Utilities	6.36
Variable costs	231.85
Operating labor, 4/shift, $17.50/hr	1.86
Maintenance labor, 2%/yr of BL inv	3.32
Control lab labor, 20% of op labor	0.37
Labor costs	5.55
Maintenance materials, 1.5%/yr of BL inv	2.49
Operating suppliers, 10% of op labor	0.19
TOTAL DIRECT COSTS	240.08
Plant overhead, 80% of labor costs	4.44
Taxes and insurance, 2%/yr of TFC	4.47
Depreciation, 10%/yr of TFC	22.36
Plant gate cost	271.35
G&A, sales, research	14.00
NET PRODUCTION COST	285.35
ROI before taxes, 25%/yr of TFC	55.91
PRODUCT VALUE	341.26

Table 4.39

SYNGAS (H_2:CO RATIO = 2) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 16.5 x 10^9 scf/yr
(Equivalent to 50 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs

	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.247 mscf	107.69
Natural gas fuel	426¢/mscf	0.189 mscf	82.40
Carbon dioxide	4.4¢/lb	8.86 lb	38.98
Catalysts, adsorbent			0.52
Misc. chemicals, utilities			0.69
Gross raw materials			230.28
Utilities			
Cooling water	5.4¢/1,000 gal	313 gal	1.69
Process water	68¢/1,000 gal	6.25 gal	0.42
Electricity	3.6¢/kwh	1.18 kwh	4.25
Total utilities			6.36

Table 4.39 (Concluded)

SYNGAS (H_2:CO RATIO = 2) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 16.5 x 10^9 scf/yr
(Equivalent to 50 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	34.9
Off-sites	12.1
Total fixed capital	47.0
Production costs (¢/mscf)	
Raw materials	230.28
Utilities	6.36
Variable costs	236.64
Operating labor, 4/shift, $17.50/hr	3.72
Maintenance labor, 2%/yr of BL inv	4.23
Control lab labor, 20% of op labor	0.74
Labor costs	8.69
Maintenance materials, 1.5%/yr of BL inv	3.17
Operating supplies, 10% of op labor	0.37
TOTAL DIRECT COSTS	248.87
Plant overhead, 80% of labor costs	6.95
Taxes and insurance, 2%/yr of TFC	5.70
Depreciation, 10%/yr of TFC	28.48
Plant gate cost	290.00
G&A, sales, research	16.00
NET PRODUCTION COST	306.00
ROI before taxes, 25%/yr of TFC	71.21
PRODUCT VALUE	377.21

Table 4.40

SYNGAS (H_2:CO RATIO = 1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 6.7 x 10^9 scf/yr
(Equivalent to 20 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.242 mscf	105.51
Natural gas fuel	436¢/mscf	0.248 mscf	108.13
Carbon dioxide	4.4¢/lb	28.3 lb	124.52
Catalysts, adsorbent			0.84
Misc. chemicals, utilities			1.74
Reformer steam	0.695 ¢/lb	49.72 lb	34.56
Gross raw materials			375.30
By-products			
HP steam	0.775¢/lb	-60.62 lb	-46.98
Utilities			
Cooling water	5.4¢/1,000 gal	737 gal	3.98
Steam	$5.44/1,000 lb	49.9 lb	27.15
Process water	68¢/1,000 gal	7.45 gal	0.51
Electricity	3.6¢/kwh	5.54 kwh	19.94
Total utilities			51.58

Table 4.40 (Concluded)

SYNGAS (H_2:CO RATIO = 1) FROM STEAM REFORMING OF NATURAL GAS, WITH CO_2 IMPORT

PRODUCTION COSTS FOR 6.7 x 10^9 scf/yr
(Equivalent to 20 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	31.0
Off-sites	9.0
Total fixed capital	40.0
Production costs (¢/mscf)	
Raw materials	375.30
By-products	-46.98
Utilities	51.58
Variable costs	379.90
Operating labor, 4/shift, $17.50/hr	9.19
Maintenance labor, 3%/yr of BL inv	13.94
Control lab labor, 20% of op labor	1.84
Labor costs	24.97
Maintenance materials, 2% of BL inv	9.30
Operating supplies, 10% of op labor	0.92
TOTAL DIRECT COSTS	415.09
Plant overhead, 80% of labor costs	19.98
Taxes and insurance, 2%/yr of TFC	11.99
Depreciation, 10%/yr of TFC	59.97
Plant gate cost	507.03
G&A, sales, research	25.00
NET PRODUCTION COST	532.03
ROI before taxes, 25%/yr of TFC	149.93
PRODUCT VALUE	681.92

Table 4.41

SYNGAS (H_2:CO RATIO = 1) FROM SKIMMING OF SYNGAS OF 2:1 RATIO

PRODUCTION COSTS FOR 6.7 x 10^9 scf/yr
(Equivalent to 20 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs

	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Natural gas feed	436¢/mscf	0.384 mscf	167.42
Natural gas fuel	436¢/mscf	0.314 mscf	136.90
Carbon dioxide	4.4¢/lb	13.8 lb	60.72
Catalysts, adsorbent			0.80
Misc. chemicals, utilities			1.07
Reformer steam	0.695¢/lb	78.52 lb	54.57
Gross raw materials			421.48
By-products			
HP steam	0.775¢/lb	-78.52 lb	-60.85
Hydrogen	50¢/lb	-2.48 lb	-124.0
Total by-products			-184.85
Utilities			
Cooling water	5.4¢/1,000 gal	486 gal	2.62
Process water	68¢/1,000 gal	9.72 gal	0.66
Electricity	3.6¢/kwh	4.37 kwh	15.73
Total utilities			19.01

Table 4.41 (Concluded)

SYNGAS (H_2:CO RATIO = 1) FROM SKIMMING OF SYNGAS OF 2:1 RATIO

PRODUCTION COSTS FOR 6.7 x 10^9 scf/yr
(Equivalent to 20 x 10^6 scfd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Investment ($ million)	
Battery limits	27.8
Off-sites	8.6
Total fixed capital	36.4
Production costs (¢/mscf)	
Raw materials	421.48
By-products	-184.85
Utilities	19.01
Variable costs	255.64
Operating labor, 4/shift, $17.50/hr	9.19
Maintenance labor, 3%/yr of BL inv	12.50
Control lab labor, 20% of op labor	1.84
Labor costs	23.53
Maintenance materials, 2% of BL inv	8.34
Operating supplies, 10% of op labor	0.92
TOTAL DIRECT COSTS	288.43
Plant overhead, 80% of labor costs	18.83
Taxes and insurance, 2%/yr of TFC	10.91
Depreciation, 10%/yr of TFC	54.57
Plant gate cost	372.74
G&A, sales, research	25.00
NET PRODUCTION COST	397.74
ROI before taxes, 25%/yr of TFC	136.43
PRODUCT VALUE	534.17

Table 4.42

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS (CONVENTIONAL)

PRODUCTION COSTS FOR 200 Million lb/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Natural gas feed	436¢/mscf	0.0504 mscf	21.97
Natural gas fuel	436¢/mscf	0.0264 mscf	11.51
Catalysts, adsorbent			0.35
Misc. chemicals, utilities			0.10
Reformer steam	0.695¢/lb	10.32 lb	7.17
Gross raw materials			41.10
By-products			
HP steam	0.775¢/lb	-10.32 lb	-8.00
Total by-products			-8.00
Utilities			
Cooling water	5.4¢/1,000 gal	38 gal	0.21
Steam	$5.44/1,000 lb	2.55 lb	1.39
Process water	68¢/1,000 gal	1.28 gal	0.09
Electricity	3.6¢/kwh	0.159 kwh	0.57
Total utilities			2.26

Table 4.42 (Concluded)

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS (CONVENTIONAL)

PRODUCTION COSTS FOR 200 Million lb/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)	200
Investment ($ million)	
Battery limits	48.2
Off-sites	18.4
Total fixed capital	66.6
Production costs (¢/lb)	
Raw materials	41.10
By-products	-8.00
Utilities	2.26
Variable costs	35.36
Operating labor, 4/shift, $17.50/hr	0.31
Maintenance labor, 2%/yr of BL inv	0.48
Control lab labor, 20% of op labor	0.06
Labor costs	0.85
Maintenance materials, 1.5% of BL inv	0.36
Operating supplies, 10% of Op labor	0.03
TOTAL DIRECT COSTS	36.60
Plant overhead, 80% of labor costs	0.68
Taxes and insurance, 2%/yr of TFC	0.67
Depreciation, 10%/yr of TFC	3.33
Plant gate cost	41.28
G&A, sales, research	2.00
NET PRODUCTION COST	43.28
ROI before taxes, 25%/yr of TFC	8.32
PRODUCT VALUE	51.60

Table 4.43

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS (CONVENTIONAL)

PRODUCTION COSTS FOR 100 Million lb/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Natural gas feed	436¢/mscf	0.0504 mscf	21.97
Natural gas fuel	436¢/mscf	0.0281 mscf	12.25
Catalysts, adsorbent			0.35
Misc. chemicals, utilities			0.10
Reformer steam	0.695¢/lb	10.32 lb	7.17
Gross raw materials			41.84
By-products			
HP steam	0.775¢/lb	-10.32 lb	-8.00
Total by-products			-8.00
Utilities			
Cooling water	5.4¢/1,000 gal	38 gal	0.21
Steam	$5.44/1,000 lb	2.55 lb	1.39
Process water	68¢/1,000 gal	1.28 gal	0.09
Electricity	3.6¢/kwh	0.159 kwh	0.57
Total utilities			2.26

Table 4.43 (Concluded)

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS (CONVENTIONAL)

PRODUCTION COSTS FOR 100 Million lb/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)	100
Investment ($ million)	
Battery limits	30.7
Off-sites	11.7
Total fixed capital	42.4
Production costs (¢/lb)	
Raw materials	41.84
By-products	-8.00
Utilities	2.26
Variable costs	36.10
Operating labor, 4/shift, $17.50/hr	0.61
Maintenance labor, 2%/yr of BL inv	0.61
Control lab labor, 20% of op labor	0.12
Labor costs	1.34
Maintenance materials, 1.5% of BL inv	0.46
Operating supplies, 10% of Op labor	0.06
TOTAL DIRECT COSTS	37.96
Plant overhead, 80% of labor costs	1.08
Taxes and insurance, 2%/yr of TFC	0.85
Depreciation, 10%/yr of TFC	4.24
Plant gate cost	44.13
G&A, sales, research	3.00
NET PRODUCTION COST	47.13
ROI before taxes, 25%/yr of TFC	10.60
PRODUCT VALUE	57.73

Table 4.44

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS (CONVENTIONAL)

PRODUCTION COSTS FOR 50 Million lb/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Natural gas feed	436¢/mscf	0.0504 mscf	21.97
Natural gas fuel	436¢/mscf	0.03 mscf	13.08
Catalysts, adsorbent			0.35
Misc. chemicals, utilities			0.10
Reformer steam	0.695¢/lb	10.32 lb	7.17
Gross raw materials			42.67
By-products			
HP steam	0.775¢/lb	-10.32 lb	-8.00
Total by-products			-8.00
Utilities			
Cooling water	5.4¢/1,000 gal	38 gal	0.21
Steam	$5.44/1,000 lb	2.55 lb	1.39
Process water	68¢/1,000 gal	1.28 gal	0.09
Electricity	3.6¢/kwh	0.159 kwh	0.57
Total utilities			2.26

Table 4.44 (Concluded)

HYDROGEN (97 vol%, 220 psia) FROM STEAM REFORMING OF NATURAL GAS (CONVENTIONAL)

PRODUCTION COSTS FOR 50 Million lb/yr

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)	50
Investment ($ million)	
Battery limits	20.3
Off-sites	7.7
Total fixed capital	28.0
Production costs (¢/lb)	
Raw materials	42.67
By-products	-8.00
Utilities	2.26
Variable costs	36.93
Operating labor, 4/shift, $17.50/hr	1.23
Maintenance labor, 2%/yr of BL inv	0.81
Control lab labor, 20% of op labor	0.25
Labor costs	2.29
Maintenance materials, 1.5% of BL inv	0.61
Operating supplies, 10% of op labor	0.12
TOTAL DIRECT COSTS	39.95
Plant overhead, 80% of labor costs	1.83
Taxes and insurance, 2%/yr of TFC	1.12
Depreciation, 10%/yr of TFC	5.60
Plant gate cost	48.50
G&A, sales, research	3.50
NET PRODUCTION COST	52.00
ROI before taxes, 25%/yr of TFC	14.00
PRODUCT VALUE	66.00

Table 4.45

METHANOL FROM NATURAL GAS BY THE ICI PROCESS

PRODUCTION COSTS FOR 728 Million lb/yr
(Equivalent to 1,000 Metric tpd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Natural gas feed	436¢/mscf	0.0134 mscf	5.84
Natural gas fuel	436¢/mscf	0.0008 mscf	0.35
Active carbon	$1.70/lb	0.00001 lb	--
Reforming catalyst	$2.00/lb	0.00007 lb	0.01
Methanol catalyst	$4.40/lb	0.00013 lb	0.06
Gross raw materials			6.26
Utilities			
Cooling water	5.4¢/1,000 gal	13 gal	0.07
Process water	68¢/1,000 gal	0.135 gal	0.01
Electricity	3.6¢/kwh	0.015 kwh	0.05
Total utilities			0.13

Table 4.45 (Concluded)

METHANOL FROM NATURAL GAS BY THE ICI PROCESS

PRODUCTION COSTS FOR 728 Million lb/yr
(Equivalent to 1,000 Metric tpd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)	728
Investment ($ million)	
Battery limits	78.1
Off-sites	29.0
Total fixed capital	107.1
Production costs (¢/lb)	
Raw materials	6.26
Utilities	0.13
Variable costs	6.39
Operating labor, 6/shift, $17.50/hr	0.13
Maintenance labor, 2%/yr of BL inv	0.21
Control lab labor, 20% of op labor	0.03
Labor costs	0.37
Maintenance materials, 1.5% of BL inv	0.16
Operating supplies, 10% of op labor	0.01
TOTAL DIRECT COSTS	6.93
Plant overhead, 80% of labor costs	0.29
Taxes and insurance, 2%/yr of TFC	0.29
Depreciation, 10%/yr of TFC	1.47
Plant gate cost	8.98
G&A, sales, research	0.60
NET PRODUCTION COST	9.58
ROI before taxes, 25%/yr of TFC	3.68
PRODUCT VALUE	13.26

Table 4.46

METHANOL FROM NATURAL GAS BY THE ICI PROCESS

PRODUCTION COSTS FOR 364 Million lb/yr
(Equivalent to 500 Metric tpd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Natural gas feed	436¢/mscf	0.0134 mscf	5.84
Natural gas fuel	436¢/mscf	0.0012 mscf	0.52
Active carbon	$1.70/lb	0.00001 lb	--
Reforming catalyst	$2.00/lb	0.00007 lb	0.01
Methanol catalyst	$4.40/lb	0.00013 lb	0.06
Gross raw materials			6.43
Utilities			
Cooling water	5.4¢/1,000 gal	13 gal	0.07
Process water	68¢/1,000 gal	0.135 gal	0.01
Electricity	3.6¢/kwh	0.015 kwh	0.05
Total utilities			0.13

Table 4.46 (Concluded)

METHANOL FROM NATURAL GAS BY THE ICI PROCESS

PRODUCTION COSTS FOR 364 Million lb/yr
(Equivalent to 500 Metric tpd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)	364
Investment ($ million)	
Battery limits	48.1
Off-sites	17.8
Total fixed capital	65.9
Production costs (¢/lb)	
Raw materials	6.43
Utilities	0.13
Variable costs	6.56
Operating labor, 6/shift, $17.50/hr	0.25
Maintenance labor, 2%/yr of BL inv	0.26
Control lab labor, 20% of op labor	0.05
Labor costs	0.56
Maintenance materials, 1.5% of BL inv	0.20
Operating supplies, 10% of op labor	0.03
TOTAL DIRECT COSTS	7.35
Plant overhead, 80% of labor costs	0.45
Taxes and insurance, 2%/yr of TFC	0.36
Depreciation, 10%/yr of TFC	1.81
Plant gate cost	9.97
G&A, sales, research	0.80
NET PRODUCTION COST	10.77
ROI before taxes, 25%/yr of TFC	4.53
PRODUCT VALUE	15.30

Table 4.47

METHANOL FROM NATURAL GAS BY THE ICI PROCESS

PRODUCTION COSTS FOR 182 Million lb/yr
(Equivalent to 250 Metric tpd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable Costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Natural gas feed	436¢/mscf	0.0134 mscf	5.84
Natural gas fuel	436¢/mscf	0.0017 mscf	0.74
Active carbon	$1.70/lb	0.00001 lb	--
Reforming catalyst	$2.00/lb	0.00007 lb	0.01
Methanol catalyst	$4.40/lb	0.00013 lb	0.06
Reformer steam	0.695¢/lb	0.997 lb	0.69
Gross raw materials			7.34
By-products			
HP steam	0.775¢/lb	-2.21 lb	-1.71
Total by-products			-1.71
Utilities			
Cooling water	5.4¢/1,000 gal	13 gal	0.07
Process water	68¢/1,000 gal	0.135 gal	0.01
Electricity	3.6¢/kwh	0.285 kwh	1.03
Total utilities			1.11

Table 4.47 (Concluded)

METHANOL FROM NATURAL GAS BY THE ICI PROCESS

PRODUCTION COSTS FOR 182 Million lb/yr
(Equivalent to 250 Metric tpd)

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)	182
Investment ($ million)	
Battery limits	30.7
Off-sites	11.3
Total fixed capital	42.0
Production costs (¢/lb)	
Raw materials	7.34
By-products	-1.71
Utilities	1.11
Variable costs	6.74
Operating labor, 6/shift, $17.50/hr	0.51
Maintenance labor, 2%/yr of BL inv	0.34
Control lab labor, 20% of op labor	0.10
Labor costs	0.95
Maintenance materials, 1.5% of BL inv	0.25
Operating supplies, 10% of op labor	0.05
TOTAL DIRECT COSTS	7.99
Plant overhead, 80% of labor costs	0.76
Taxes and insurance, 2%/yr of TFC	0.46
Depreciation, 10%/yr of TFC	2.31
Plant gate cost	11.52
G&A, sales, research	1.00
NET PRODUCTION COST	12.52
ROI before taxes, 25%/yr of TFC	5.77
PRODUCT VALUE	18.29

5 SYNGASES AND HYDROGEN BY THE PARTIAL OXIDATION OF VACUUM RESIDUE

In the conversion of hydrocarbons to syngas the use of steam reforming is restricted to those having carbon numbers up to the naphtha range (i.e., up to C_9 max.) and to sulfur free feedstocks. The catalysts used in steam reforming cannot tolerate sulfur and exhibit an increased tendency to coke with heavier feedstocks. Gasification by a noncatalytic partial oxidation process was developed mainly to utilize the "bottom of the barrel," which often has high sulfur and metal contents. This process has been used to produce syngas mixtures for large applications such as ammonia, methanol, and hydrogen and also smaller uses such as oxo chemicals, acetic acid and carbon monoxide. The economics of partial oxidation relative to those of steam reforming depend largely on feedstock costs and the price of oxygen. Partial oxidation is more capital intensive, even when an air separation unit is not included (and the oxygen is purchased) and can only be justified when suitable feedstocks (usually sour and heavy residues) are available at an attractive price relative to the price of natural gas. In some exceptional situations partial oxidation has also been applied to natural gas and naphtha. This is when a lower H_2:CO ratio is required than is possible with steam reforming and CO_2 gas is not economically available to produce the desired H_2:CO ratio by the steam reforming process.

The cost of oxygen is important in the economics of partial oxidation and the inclusion of an air separation unit is justified only at the larger capacities. The precise capacity for which captive oxygen generation becomes economically attractive depends on the local situation. From data published by EPRI and Air Products Inc. (472199, 483000) on oxygen prices and economics, we estimate that the oxygen consumption must be at least 1,000 short tons/day (equivalent roughly to 85 million scfd syngas or 1,100 short tons/day of methanol by the partial oxidation of vacuum residue) to justify the inclusion of air separation as opposed to purchasing oxygen across the fence.

Brief Description of Cases Examined

We have examined the economics of partial oxidation of a high sulfur vacuum residue. The composition and characteristics of the feedstock are given in Table 5.1. We used a concept basically similar to that described in PEP Report 110, Synthesis Gas Production, issued in January 1977. The main process steps consist of a Texaco partial oxidation stage (including indirect cooling for heat recovery, and soot recovery and recycle) and Rectisol®-based stages for the selective separation of (H_2S + COS) and CO_2. A Claus system is included for sulfur recovery and is used in conjunction with a SCOT® (Shell Claus Off-Gas Treating) unit to reduce sulfur emissions in the tail gas from the Claus system. For the base case we set the H_2:CO ratio at 2:1, which is similar to that of the syngas feed to a methanol plant. A high temperature CO shift system was used to effect the H_2:CO ratio adjustment. The other cases examined are syngas with an H_2:CO ratio of 1:1, and chemical grade hydrogen. The schematic diagram in Figure 5.1 illustrates the three modules.

Table 5.1

SOME CHARACTERISTICS OF
ASSUMED VACUUM RESIDUE FEEDSTOCK

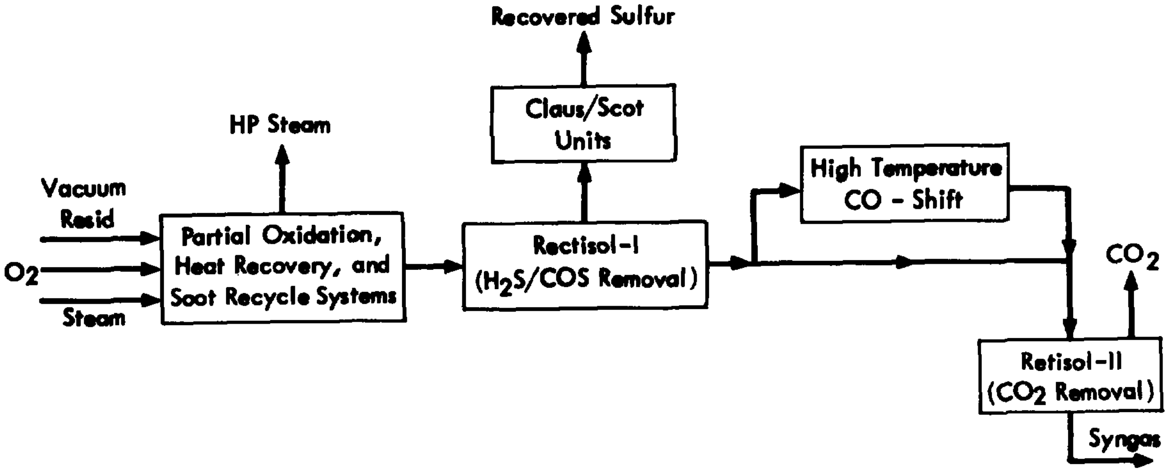
Composition (wt%)	
Carbon	83.80
Hydrogen	9.65
Nitrogen	0.31
Sulfur	6.20
Ash	0.04
Total	100.00

Higher heating value = 17,344 Btu/lb

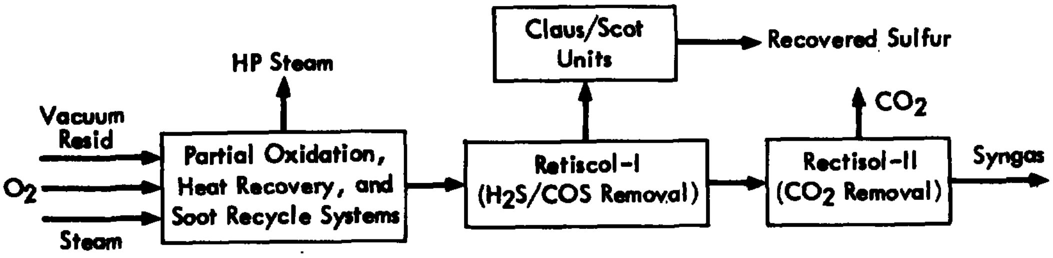
°API = 4.3

Figure 5.1

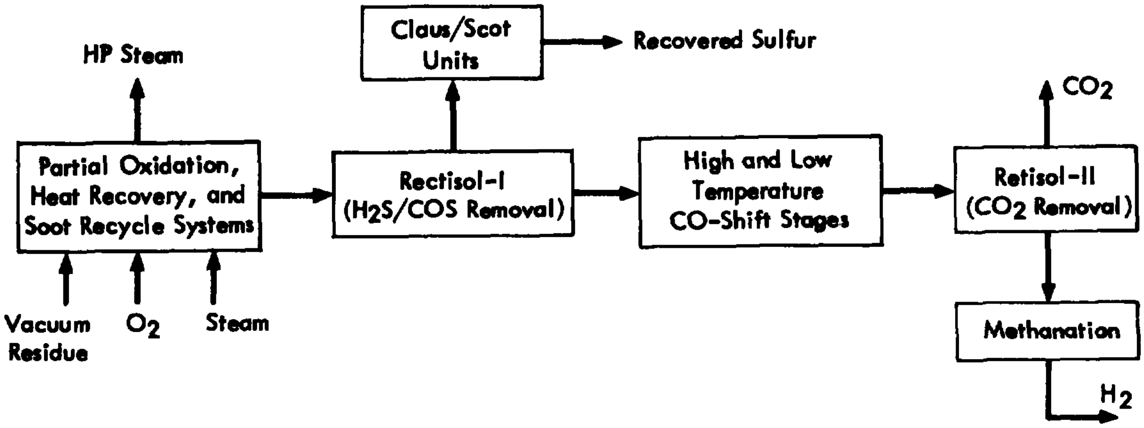
SCHEMATIC DIAGRAM SHOWING PROCESS STAGES
FOR PARTIAL OXIDATION CASES EXAMINED



Schematic Arrangement for Syngas with H2/CO Ratio = 2



Schematic Arrangement for Syngas with H2/CO Ratio=1



Schematic Arrangement for Hydrogen Production

For the base 2:1 case we interposed the CO shift system between two acid gas removal stages, Rectisol®-I and Rectisol®-II (see Figures 5.1 and 5.3). The first of these selectively removes (H_2S + COS) along with some CO_2 as Claus feed. Rectisol®-II removes the balance of the CO_2 to 100 ppm in the syngas. The reason for putting sulfur acid gas removal before the CO shift is to make the Rectisol®-I separation easier. The presence of large amounts of CO_2 in the syngas renders the selective acid gas separation more difficult (415023).

As shown in Figure 5.1 the arrangement for the H_2 case is similar to that for the base case, with the difference that a low temperature shift and methanation stages are added. The former reduces the CO level to 0.4 vol% and the latter methanates oxides of carbon to <10 ppm to give a hydrogen product of about 98 vol% (dry basis) purity.

For syngas with an H_2:CO ratio of 1:1 we dispensed with a shift system. The necesssary adjustment in the ratio is made by increasing the steam fed to the partial oxidation reactor. This is in accord with published conclusions (393232) that "moderate" (10 to 15%) adjustments in the H_2:CO ratio are more economically made by increasing the steam feed. (Under the standard partial oxidation conditions used for the 2:1 syngas and H_2 cases, the H_2:CO ratio obtained with the vacuum residue, of composition as detailed in Table 5.2, is ~0.864.)

As with the natural gas steam reforming cases covered in Section 4, we took the scale of operation at 100 billion scf/yr (roughly equivalent to 300 million scfd, 330 operating days/yr). As in the case of H_2 product, the syngas purity is about 98 vol% (CO + H_2, dry basis). The key parameters for the three cases are shown in Table 5.2.

The economics of the three cases cited were examined on the basis of information available to SRI on the capital costs of the individual plant sections. This information was supplemented by calculations on mass and energy balances. The evaluation is therefore not as detailed as a traditional PEP estimate. We believe, however, that the capital costs are reasonably accurate and relate consistently with the other capital costs presented in this report.

Table 5.2

KEY PARAMETERS FOR PARTIAL OXIDATION CASES EXAMINED

Plant Capacity: 300 x 10^6 scfd Product

	Syngas With H_2:CO Ratio = 2	Syngas With H_2:CO Ratio = 1	Hydrogen Product
Partial oxidation reactor			
Temperature (°F)	2650	2700	2650
Pressure (psia)	1200	1200	1200
Oxidation product composition (vol%, dry)			
CO	49.91	45.70	As for syngas with H_2:CO ratio = 2
H_2	43.09	45.70	
CO_2	4.95	6.54	
CH_4	0.30	0.28	
A + N_2	0.22	0.23	
H_2S	1.45	1.47	
COS	0.08	0.08	
Vacuum residue usage (lb/mscf)	22.1	22.5	4.32 lb/lb H_2
Oxygen/residue ratio (lb/lb)	1.07	1.15	1.07
Feed steam/residue ratio (lb/lb)	0.407	0.70	0.407
HP steam balances*			
Produced in heat recovery (lb/hr)	849,600	934,000	849,600
Used (lb/hr)			
Air separation	520,000	561,000	520,000
Partial oxidation feed	112,340	194,000	112,340
CO shift	190,500	—	760,000
Rectisol® and others	154,000	130,000	195,000
Total	976,240	885,000	1,587,340
Balance	-127,400	+49,000	-738,360

---

*Figures quoted are illustrative only. Balances shown are for HP steam alone. Other grades of steam (MP and LP) are also produced from the exhaust of some turbines. These grades of steam are totally utilized elsewhere in the process.

Chemistry

The partial oxidation reaction which is carried out at elevated temperatures (2000–2700°F) may be represented by the following overall reaction:

$$C_nH_mS_r + \frac{n}{2} O_2 \longrightarrow nCO + \left(\frac{m}{2} - r\right) H_2 + rH_2S \qquad (5.1)$$

The reaction is highly exothermic and becomes increasingly so with higher molecular weight hydrocarbons and polynuclear hydrocarbons, owing to the greater energy of formation of CO from C–C bonds compared with that from C–H bonds.

In addition to reaction 5.1 there is some CO_2 formation, resulting primarily from:

$$CO + 1/2\ O_2 \longrightarrow CO_2 \qquad (5.2)$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad (5.3)$$

Both these reactions are also exothermic. The equilibrium for reaction 5.3 determines the proportion of carbon that is converted to CO_2 and hence the H_2:CO ratio. The bulk of the hydrocarbons is consumed by the oxidation reaction 5.1 but a small proportion reacts endothermically with steam as follows:

$$C_nH_m + nH_2O \rightleftharpoons n\ CO + \left(n + \frac{m}{2}\right) H_2 \qquad (5.4)$$

Total sulfur from the feedstock appears as hydrogen sulfide (H_2S) and carbonyl sulfide (COS), the ratio being determined by the equilibrium of the "sulfur shift" reaction.

$$H_2 + COS \rightleftharpoons H_2S + CO \qquad (5.5)$$

Methane and carbon (soot) are the only other compounds present in more than trace amounts. It has been reported that the yield of carbon is an empirical function of feed oxygen/oil ratio and that this yield is only slightly affected by other process variables (472133). The level of methane, the only surviving hydrocarbon in the product gas, is determined by the equilibrium of the reaction:

$$CO + 3H_2 \rightleftharpoons CH_4 + H_2O \qquad (5.6)$$

However, in practice the methane level varies inversely with temperature, which in turn depends on both the oxygen/oil and steam/oil ratios (472133). It is therefore possible to independently control both the carbon and methane levels by these two feed ratios. Thus, once the methane and soot levels have been fixed, the remaining gas composition is readily calculated from material balances and the equilibrium relationships, primarily for reactions 5.3 and 5.5. In current industrial practice it is normal to keep the soot level to about 3-4% and methane at less than 1%.

Nitrogen and argon in the product gas follow from their presence in the oxygen stream and the fixed nitrogen in the feedstock. A small fraction of the nitrogen appears in the product gas in trace amounts as ammonia and hydrogen cyanide. Under conditions used in partial oxidation reactors the oxygen is completely consumed.

Characterization of Partial Oxidation Reactor Performance

The performance of the gasifier (the partial oxidation reactor) has been characterized (472133) by two parameters: "cold gas efficiency" (CGE) and "specific oxygen consumption" (SOC), defined as follows:

$$\text{CGE} = \frac{\text{Higher heating vaue of } (CO + H_2) \text{ produced}}{\text{Higher heating value of feedstock consumed}}$$

$$\text{SOC} = \frac{\text{Normal cubic meters of pure } O_2 \text{ used}}{\text{Thousand normal cubic meters of } (CO + H_2) \text{ produced}}$$

CGE is not a thermodynamic efficiency but merely a statement of yield and lies in the range of 82 to 85% for most liquid and gaseous feedstocks. When the heat recovered (in the steam produced) is included, the overall efficiency is usually 92 to 94%.

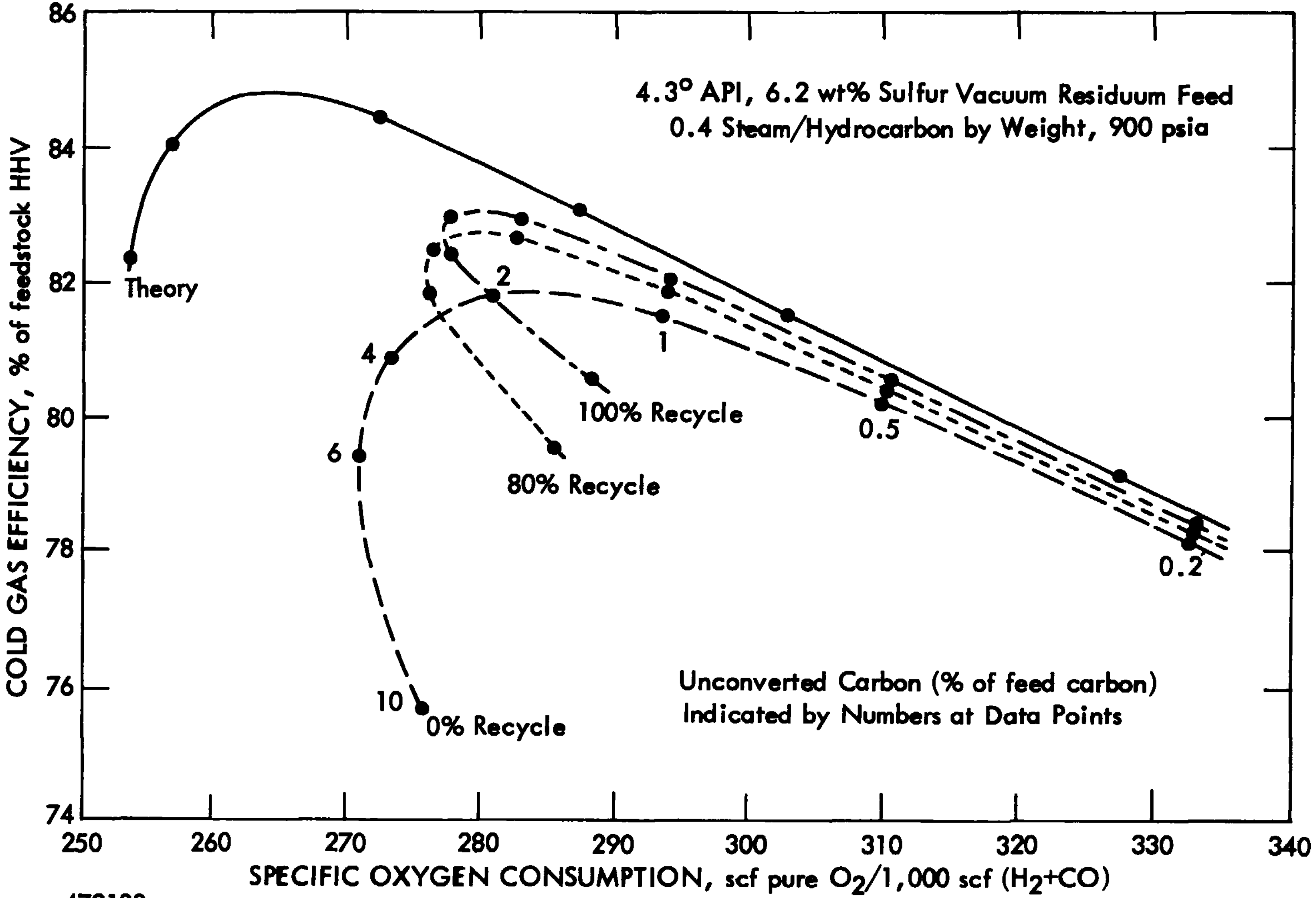
Figure 5.2 is a graphical representation of the dependence of CGE on SOC for the vacuum residue feedstock assumed in our study. The "theoretical" curve shows the performance when carbon (soot) formation is zero and methane formation corresponds to the thermodynamic equilibrium. The CGE's shown include an allowance for normal heat losses. At the right of the maxima for CGE, the efficiency decreases because of more complete combustion, and toward the left the fall off in efficiency is due to increased methane production (caused by the drop in reactor temperatures in this direction). Curves for the real situation where soot formation does occur are also shown in Figure 5.2 for zero, 80%, and 100% levels of soot recycle. The levels of unconverted carbon are indicated by numbers at the data points. Again, toward the right of the maxima, in the fuel-lean region, more complete combustion leads to a decrease in CGE with increased SOC. To the left (in the fuel-rich region) CGE decreases because of increasing soot and methane formation. At very low feed oxygen/oil ratios, the SOC increases again, as this is the ratio of oxygen to product rather than to feed.

Since both oxygen and feedstock consumptions represent key raw materials costs, the optimum point is usually slightly displaced from the peak CGE. When soot is not recycled, the optimum oxygen/feedstock ratio is on the fuel-rich side of the maxima. With soot recycle to extinction, assumed in our study, the CGE obtainable is higher than without recycle but in this case the optimum oxygen/feedstock ratio

Figure 5.2

PARTIAL OXIDATION REACTOR PERFORMANCE

Effects of Feed Oxygen/Oil Ratio and Soot Recycle



Source: 472133.

shifts to the fuel-lean side of the maxima, because of the capital and operating costs for recycling the carbon.

The other parameters which determine partial oxidation reactor performance are the steam/oil ratio and the operating pressure. Increasing the steam/oil ratio leads to enhanced H_2:CO ratios (as discussed for our case with H_2:CO ratio of 1:1) but lead to a higher SOC and a lower CGE (see Table 5.2). Increased pressures result in greater methane production and this implies a lower CGE for any given SOC. Usually this effect is small compared with the other advantages; greater output per gasifier, lower compression power (when syngas is required at higher pressures), more efficient steam generation, and reduced costs for separation of acid gas.

Brief Review of Processes

Partial Oxidation Stage

As discussed before, the noncatalytic partial oxidation of hydrocarbons has several advantages over the catalyzed steam reforming process for the production of syngas. It can use a wider range of feedstocks from methane to sour, heavy residues, and it can be operated at much higher pressures, and thus reduces the need for subsequent compression.

The main commercial processes available are those developed by Shell and Texaco (393232, 472177, 472133, 472186). The installed worldwide capacity is divided about equally between the two technologies. Single-train capacities of ~100 million scfd are now claimed to be practical for both processes. However, with the Texaco process, which is usually operated at a higher pressure (up to 1200 psia in proven commercial plants) than the Shell process (~850 psia), single-train capacities greater than 100 million scfd should be feasible. The principal differences between the Texaco and Shell processes are in their burner designs and the soot recovery/recycle systems.

In the Texaco process, partial combustion is carried out in a vertical combustion chamber having no internals other than a refractory lining. A sophisticated control system ensures that oxygen/oil and steam/oil ratios are maintained within narrow limits. The hydrocarbon-steam mixture and oxygen are fed separately to the burner through annular passages and the combustion occurs away from the nozzle tip to prevent its deterioration. In the Shell design the reactor is, again, a vertical pressure vessel with a refractory lining. The steam is premixed with oxygen and intimately contacted with the atomized hydrocarbon in the fuel injection region of the reactor. The oxidant enters the reactor as a rotating vortex around the hydrocarbon vortex spray in the combustion zone. The atomized hydrocarbon is heated and vaporized by the back radiation from the flame front and the reactor walls.

In the cooling of the reactor effluent, Texaco offers both a "direct quench" (using water) and an indirect waste heat boiler. Texaco recommends the former (as an effective way of providing the necessary dilution steam) when all the product gas is fed to the CO-shift system as required for hydrogen and ammonia plants. In this system the water quench can be operated either inside the reactor or in a vessel adjacent to the reactor. The soot is removed from the bottom of the vessel in admixture with water and discharged to the soot-extraction system. The Texaco waste heat boiler or syngas cooler is essentially a heat exchanger in which high pressure steam is generated. No details are available for the design of the cooler used in the Texaco process. Shell offers an indirect cooling system which generates high pressure steam; and the design consists of helical coils (through which the hot gas flows) mounted in the exchanger shell. The use of helical tubes and sufficiently high gas velocities minimizes the severity of soot deposition.

The Texaco soot recovery consists of water scrubbing. This is followed by contacting the water slurry with naphtha, which preferentially wets the carbon particles, thus transferring them to the naphtha hydrocarbon phase. The soot-naphtha mixture is decanted from water and mixed with a portion of the feedstock oil and fed to a stripper. The naphtha is recovered overhead for recycle and the soot-oil mixture can be recycled to the oxidation reactor or burnt in conventional oil burners. One variant of the Shell system for carbon recovery and recycle, called the Shell Closed Carbon Recovery System (SCCRS), is essentially similar to the Texaco system and uses the sequence of water scrubbing, naphtha extraction, fresh feedstock introduction, and fractionation, to recovery naphtha for recycle. In addition to this system Shell also offers a variant which it calls the Shell Pelletizing System (SPS). This system is less capital intensive than SCCRS and is usually applied when the soot is not recycled to the oxidation reactor. It can only be used when a suitable pelletizing oil is available and the partial oxidation feedstock has a viscosity low enough to permit pumping at 200°F. In SPS the water/carbon slurry is contacted with a low viscosity oil (<300 cs at 200°F) in a pelletizer. The oil preferentially wets the soot particles and forms pellets that can be screened from the water. The pellets can then either be mixed with the feedstock oil and recycled to the reactor, or used separately as a fuel in a coal-fired boiler. The pellets can also be mixed in a separate oil for use in an oil burning furnace.

Acid Gas Removal System

For the particular feedstock (vacuum residue) chosen in our examination of the partial oxidation process, the requirements that must be fulfilled by a gas separation process are: selective separation of H_2S + COS for feed to a Claus unit and reduction of sulfur to <1 ppm and reduction of CO_2 to about 100 ppm. Possible candidate processes are Rectisol® (licensed by Lurgi and Linde) and Selexol® (Norton Chemical Process Products), Adip® (Shell), Catacarb® (Eickmeyer) and Giammarco Vetrocoke® (Giammarco). Among these Rectisol® and Selexol® are physical solvent processes and the others employ "chemical solvents" (i.e., solvents which remove acid gas by reversible chemical reactions). A brief comparison of the main features of these processes has been presented in Section 4 (see Table 4.5). At the higher pressures used in partial oxidation (compared with steam reforming) physical solvent processes can be economically applied and are generally preferred to "chemical solvent" processes because of their lower energy usage in the regeneration step (e.g., ~6000 Btu/lb-mol for Rectisol® compared with >30,000 Btu/lb-mol for chemical solvent processes). We chose Rectisol® primarily because of our greater knowledge of the process from earlier SRI studies of partial oxidation and coal gasification. An economic comparison between Rectisol® and Selexol® is outside the scope of this study.

Sulfur Recovery

The Claus process for sulfur recovery makes use of the following reaction:

$$2H_2S + SO_2 \rightleftharpoons 3S + 2H_2O$$

The conventional Claus plant uses a burner system to provide the appropriate amount of SO_2 by burning H_2S with air or O_2. The sulfur recovery achieved by the process is about 95%. To minimize sulfur emissions, the tail gas from the Claus plant can be fed to a SCOT® unit, where most of this sulfur is recovered for recycle to the Claus plant and tail gas sulfur emissions are reduced to less than 250 ppm.

Process Description

A vacuum residue based partial oxidation process for the production of syngas (with an H_2:CO ratio = 2) is shown in Figure 5.3. As indicated earlier, the diagram represents an SRI concept formulated from published information (415023, 472133, 472186, 472187). No detailed equipment design was carried out and capital investment costs were derived from information available to SRI. However, we calculated the essential materials and energy balances. The key mass flows for the flow sheet in Figure 5.3 are presented in Table 5.3.

The vacuum residue is kept in a mobile, pumpable condition by a steam callandria in the storage tank. It is preheated to about 500°F and mixed with high pressure steam which comes from the waste heat recovery boiler. The steam conditions are to 1250 psia and 800°F. Two centrifugal pumps in series (comprising several stages) raise the vacuum residue to this pressure. The steam/oil mixture is introduced into the partial oxidation reactor together with O_2. The O_2 produced in the air separation plant is to about 97 vol% pure.

The partial oxidation reaction takes place at 2600-2700°F and the exit pressure is to 1200 psia. The reactor effluent is cooled to 600°F in a specially designed waste-heat boiler which generates high pressure steam of the quality indicated before. Further heat is recovered and utilized in heating the demineralized water. The gas leaving the heat recovery equipment contains the carbon formed in the reactor along with any ash that results from inorganic compound in the feedstock.

The unconverted carbon in the cooled raw gas is removed by water washing. The extract water is then contacted with naphtha and the mixture is transferred to a decanter. The soot is transferred preferentially to the naphtha phase. The soot-naphtha slurry is mixed with fresh vacuum residue feedstock and fractionated in a column to recover the naphtha overhead, which is recycled. The residual oil/soot slurry is recycled to the partial oxidation reactor. The water phase from the decanter is stripped to recover traces of naphtha, and a major proportion of the water is recycled to the soot scrubber. The ash from the feedstock builds up to a steady state concentration in the oxidizer-feed and leaves the system with the purge water as soluble salts and finely divided particulate matter.

The gases leaving the soot recovery system are processed in an acid gas removal system which, as described before, consists of two stages with an interposed CO shift reactor. The first acid gas removal system (Rectisol®-I) recovers the H_2S + COS along with some CO_2, all of which is fed to the Claus unit. The second, Rectisol-II, removes the balance of the CO_2 from the gas. The raw gas leaving the soot scrubber at 100°F is saturated with water. It is mixed with methanol to prevent icing and is then cooled in an economizer and a refrigerated heat exchanger to about -60°F and scrubbed countercurrently with methanol (which contains some CO_2, as it is taken from a downstream stripping stage). In this unit (the desulfurization absorber) the sulfur content of the scrubbed gases is reduced to <1 ppm. The acid gas rich solvent from this absorber is stripped in the H_2S/COS regenerator. The lean solvent goes to the CO_2 regeneration unit.

The sulfur-free gases from the desulfurization absorber are (after heat exchange) split into two streams. One of these (~40%) goes through a high temperature CO shift reactor and the other (~60%) bypasses. The reactant stream is mixed with HP steam and enters the shift reactor at 435°F. The reactor consists of two separate catalyst beds and an intermediate heat exchange callandria to maintain control of the exit temperature at ~465°F. The heat recovered from the reactor and from the cooling of the reactor product are absorbed in boiler feedwater. The shift reactor is operated at 95% CO conversion and a steam/gas ratio of 0.78 mol/mol to give the desired final H_2:CO ratio of 2:1.

The reactor effluent and the bypassing stream are processed in an CO_2 absorber/CO_2 stripper system (Rectisol®-II) which operates on the same principles as the desulfurizer Rectisol®-I arrangement. As shown in Figure 5.3 there is considerable integration of the two systems with regard to the solvent flow. This is designed to optimize the systems for minimum energy usage.

Figure 5.3

SYNGAS (H_2:CO RATIO = 1) BY PARTIAL OXIDATION OF VACUUM RESIDUE

PARTIAL OXIDATION/SOOT RECYCLE SECTIONS

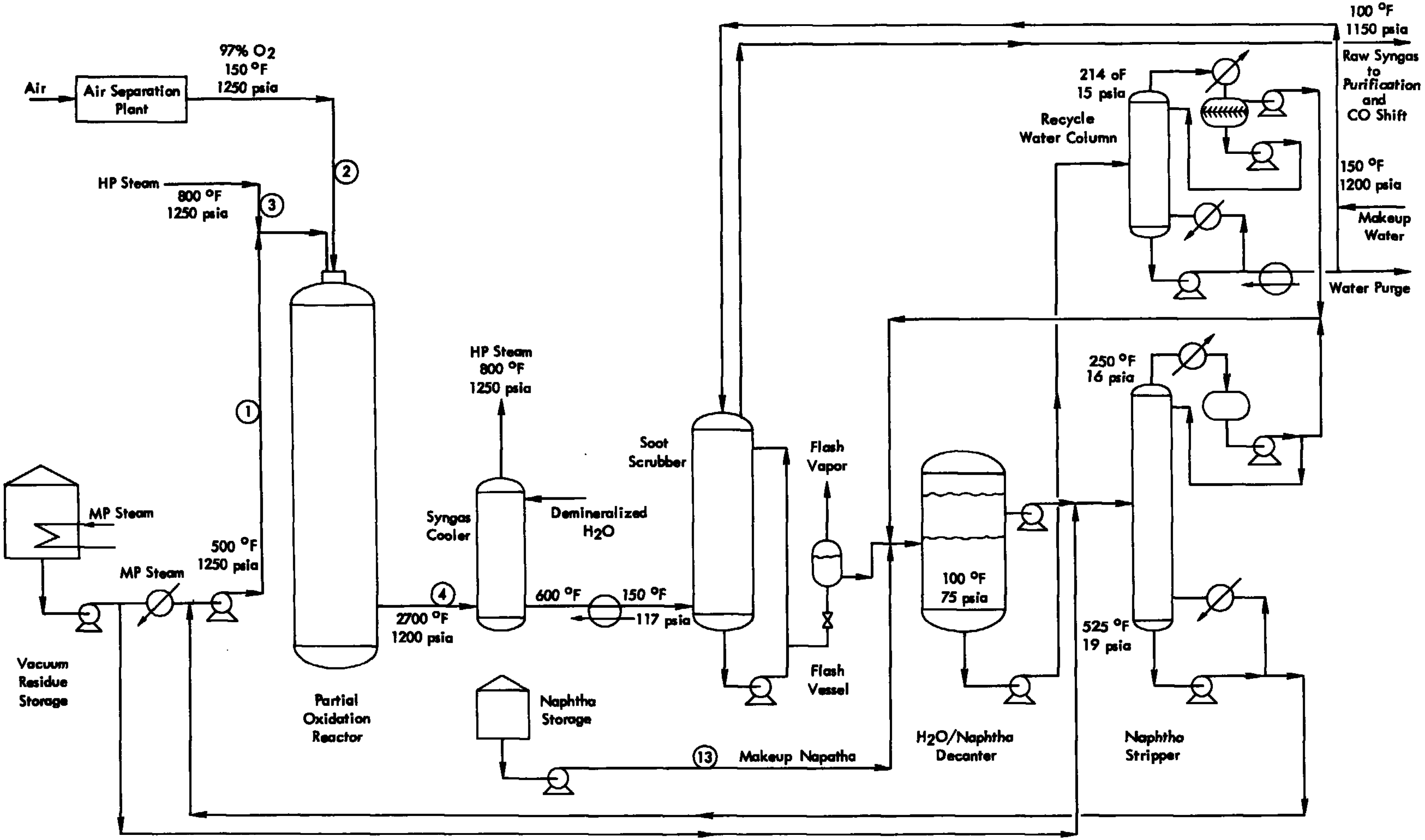


Figure 5.3 (Concluded)

SYNGAS (H_2:CO RATIO = 1) BY PARTIAL OXIDATION OF VACUUM RESIDUE
ACID GAS REMOVAL AND CO SHIFT SECTIONS

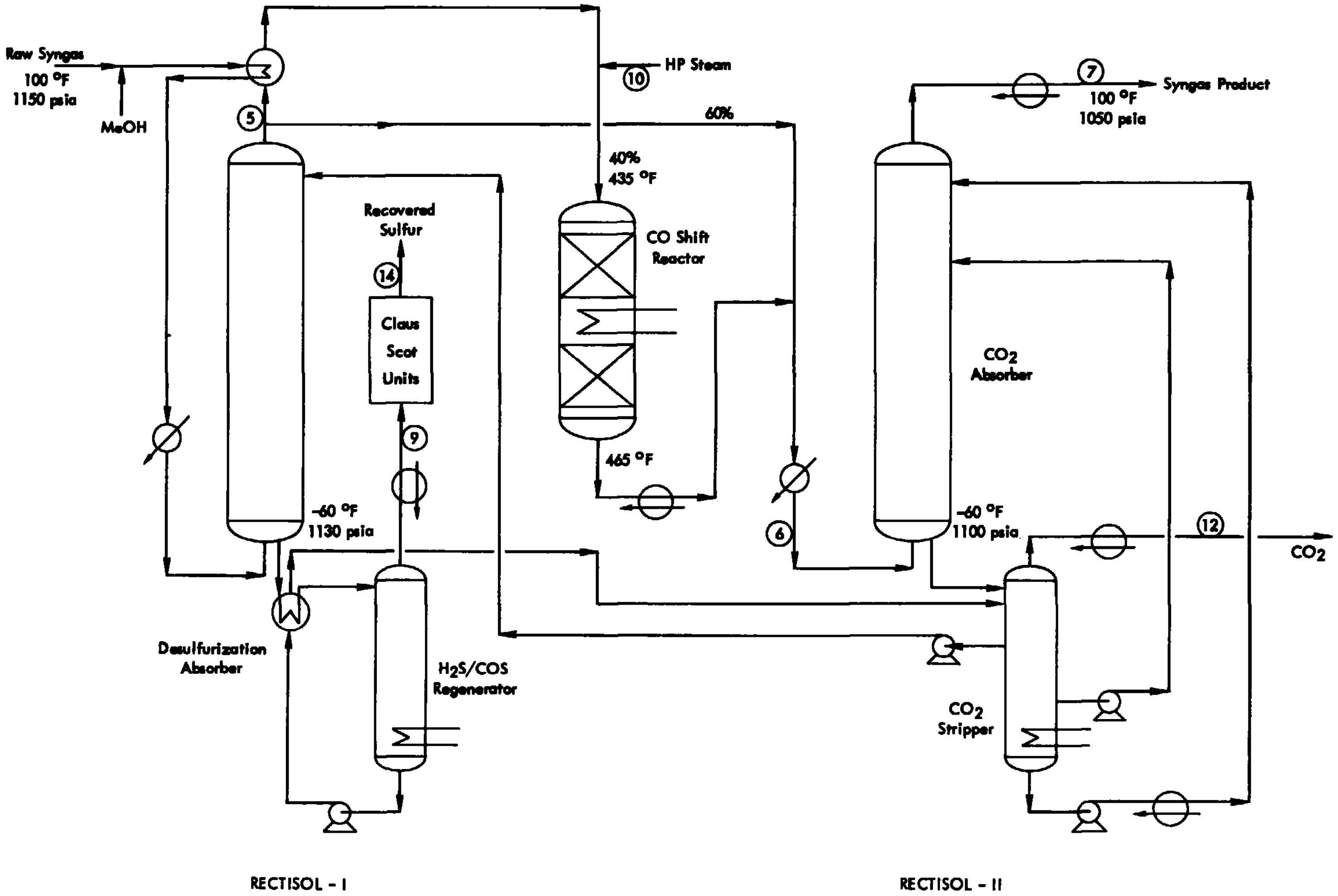


Table 5.3

SYNGAS (H_2:CO RATIO = 2:1) BY PARTIAL OXIDATION OF VACUUM RESIDUE

STREAM FLOWS

Plant Capacity: 300 x 10^6 scfd Syngas

		Stream Flows (lb/hr)						
Component	Mol Wt	(1) Vacuum Residue*	(2) Oxygen	(3) Oxidizer Steam	(4) Oxidation Product	(5) Desulfurized Product	(6) Rectisol-I Feed	(7) Syngas Product
Carbon monoxide	28	—	—	—	488,203	488,203	303,235	303,235
Hydrogen	2	26,667	—	—	30,109	30,109	43,319	43,319
Carbon dioxide	44	—	—	—	76,087	40,563	331,228	145
Methane	16	—	—	—	1,676	1,676	1,676	1,676
Nitrogen	28	858	4,032	—	4,890	4,890	4,890	4,890
Argon	40	—	6,985	—	6,985	6,985	6,985	6,985
Hydrogen sulfide	34	—	—	—	17,244	—	tr	—
COS	60	—	—	—	1,674	—	tr	—
Water	18	—	—	112,343	68,534	—	tr	tr
Carbon	12	231,578	—	—	—	—	—	—
Oxygen	32	—	295,848	—	tr	—	—	—
Sulfur	32	17,128	—	—	—	—	—	—
Ash	—	110	—	—	110	—	—	—
Naphtha makeup[†]	—	—	—	—	—	—	—	—
Total		276,341	306,865	112,343	695,512	572,426	691,333	360,250

		Stream Flows (lb/hr)						
Component	Mol Wt	(8) Pre-Rectisol-I Condensate	(9) Claus Feed	(10) CO Shift Steam	(11) Pre-Rectisol-II Condensate	(12) Desorbed CO_2	(13) Naphtha Makeup	(14) Recovered Sulfur
Carbon monoxide	28	—	tr	—	—	tr	—	—
Hydrogen	2	—	tr	—	—	tr	—	—
Carbon dioxide	44	—	35,524	—	—	331,083	—	—
Methane	16	—	tr	—	—	tr	—	—
Nitrogen	28	—	tr	—	—	tr	—	—
Argon	40	—	tr	—	—	tr	—	—
Hydrogen sulfide	34	—	17,244	—	—	—	—	—
COS	60	—	1,674	—	—	—	—	—
Water	18	112,343	—	190,440	190,400	—	—	—
Carbon	12	—	—	—	—	—	—	—
Oxygen	32	—	—	—	—	—	—	—
Sulfur	32	—	—	—	—	—	—	16,443
Ash	—	—	—	—	—	—	—	—
Naphtha makeup[†]	—	—	—	—	—	—	2,375	—
Total		112,343	54,442	190,440	190,400	331,083	2,375	16,443

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*Figures show elemental C, H, S, and N in vacuum residue.

[†] Used in soot recovery and recycle.

Cost Estimates

The production cost estimates for the three cases examined are presented in Tables 5.4 through 5.6. The unit cost for the vacuum residue feedstock (as characterized in Table 5.1) was taken at $20.6/bbl (equivalent to 5.65¢/lb). This is an SRI estimate of typical U.S. transfer prices for a high sulfur vacuum residue in mid-1981. Feedstock costs constitute the major element, with capital-related charges being close behind in importance. As shown in Table 5.2 for the base case (H_2:CO ratio = 2) and the hydrogen case there is a net HP steam deficit. For the case with H_2:CO ratio = 1 there is a net HP steam surplus. For the present we have used the same unit value for this steam ($7.75/1,000 lb) as discussed in Section 4. The key cost numbers for the three cases are summarized as follows:

	Syngas With H_2:CO Ratio = 2	Syngas With H_2:CO Ratio = 1	98 Vol% Hydrogen
Scale of operation			
10^9 sccf/yr	100	100	100
lb/yr	—	—	506
Capital invesment including air separation ($ million)			
Battery limits	243.0	232.0	273.0
Off-sites	85.0	74.0	95.0
Total fixed capital	328.0	306.0	368.0
Cost buildup ($/1,000 scf for syngas, ¢/lb for H_2:			
Variable costs	131.7	122.1	33.5
Product value (inc. 25% ROI)	278.0	259.9	65.2

As shown we used a scale of operation corresponding to 100 billion scf/yr (roughly equivalent to 300 million scfd, 330 operating days/yr, the same as we assumed for the basic cases in the steam reforming of natural gas. The nonavailability of data for a large range of scales of operation prevented us from analyzing of the effects of plant capacity on costs in the same detail that we have done for natural gas steam reforming. However, we judge that a scale exponent of 0.90 would be appropriate for higher capacities and 0.80 for lower capacities down to 100 million scfd.

Table 5.4

SYNGAS (H_2:CO RATIO = 2:1) BY PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Vacuum residue	5.65¢/lb	22.1 lb	124.87
Misc. chem, utilities	—	—	0.50
Gross raw materials			125.37
By-product			
Sulfur	4.54¢/lb	-1.3 lb	-5.90
Utilities			
Cooling water	5.4¢/1,000 gal	115 gal	0.62
Steam	$7.75/1,000 lb	10.3 lb	7.98
Process water	68¢/1,000 lb	8.1 gal	0.55
Electricity	3.6¢/kwh	0.85 kwh	3.06
Total utilities			12.21

Table 5.4 (Concluded)

SYNGAS (H_2:CO RATIO = 2:1) BY PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (10^9 scf/yr)*	50		100†		200
Investment ($ million)					
Battery limits	139.6		243.0		453.5
Off-sites	48.8		85.0		158.6
Total fixed capital	188.4		328.0		612.1
Scaling exponents		0.80		0.90	
Production costs (¢/mscf)					
Raw materials	125.37		125.37		125.37
By-products	-5.90		-5.90		-5.90
Utilities	12.21		12.21		12.21
Variable costs	131.68		131.68		131.68
Operating labor, 8/shift§, $17.50/hr	2.45		1.23		0.61
Maintenance labor, 1.5%/yr of BL inv	4.19		3.64		3.40
Control lab labor, 20% of op labor	0.49		0.25		0.12
Labor costs	7.13		5.12		4.13
Maintenance materials, 1.5%/yr of BL inv	4.19		3.64		3.40
Operating supplies, 10% of op labor	0.25		0.12		0.06
TOTAL DIRECT COSTS	143.25		140.56		139.27
Plant overhead, 80% of labor costs	5.70		4.09		3.31
Taxes and insurance, 2%/yr of TFC	7.54		6.56		6.12
Depreciation, 10%/yr of TFC	37.68		32.80		30.60
Plant gate cost	194.17		184.01		179.30
G&A, sales, research	12.00		12.00		12.00
NET PRODUCTION COST	206.17		196.01		191.30
ROI before taxes, 25%/yr of TFC	94.20		82.00		76.51
PRODUCT VALUE	300.37		278.01		267.81

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*Of syngas (H_2:CO ratio = 2).

†Base case.

§For base case; may be different for other capacities.

Table 5.5

SYNGAS (H_2:CO RATIO = 1:1) BY PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs	Unit Cost	Consumption/mscf	¢/mscf
Raw materials			
Vacuum residue	5.65¢/lb	22.5 lb	127.13
Misc. chem, utilities	—	—	0.45
Gross raw materials			127.58
By-product			
Sulfur	4.54¢/lb	-1.33 lb	-6.04
Utilities			
Cooling water	5.4¢/1,000 gal	96 gal	0.52
Steam	$7.75/1,000 lb	-3.9 lb	-3.01
Process water	68¢/1,000 lb	8.9 gal	0.61
Electricity	3.6¢/kwh	0.68 kwh	2.45
Total utilities			0.57

Table 5.5 (Concluded)

SYNGAS (H_2:CO RATIO = 1:1) BY PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (10^9 scf/yr)*	50	100†	200
Investment ($ million)			
Battery limits	133.2	232.0	432.9
Off-sites	42.6	74.0	138.1
Total fixed capital	175.8	306.0	571.0
Scaling exponents		0.80	0.90
Production costs (¢/mscf)			
Raw materials	127.58	127.58	127.58
By-products	-6.04	-6.04	-6.04
Utilities	0.57	0.57	0.57
Variable costs	122.11	122.11	122.11
Operating labor, 8/shift§, $17.50/hr	2.45	1.23	0.61
Maintenance labor, 1.5%/yr of BL inv	4.00	3.48	3.25
Control lab labor, 20% of op labor	0.49	0.25	0.12
Labor costs	6.94	4.96	3.98
Maintenance materials, 1.5%/yr of BL inv	4.00	3.48	3.25
Operating supplies, 10% of op labor	0.25	0.12	0.06
TOTAL DIRECT COSTS	133.30	130.67	129.40
Plant overhead, 80% of labor costs	5.55	3.96	3.19
Taxes and insurance, 2%/yr of TFC	7.03	6.12	5.71
Depreciation, 10%/yr of TFC	35.15	30.60	28.55
Plant gate cost	181.03	171.35	166.85
G&A, sales, research	12.00	12.00	12.00
NET PRODUCTION COST	193.03	183.35	178.85
ROI before taxes, 25%/yr of TFC	87.90	76.50	71.38
PRODUCT VALUE	280.93	259.85	250.23

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*Of syn gas (H_2:CO ratio = 1).

†Base case.

§For base case; may be different for other capacities.

Table 5.6

HYDROGEN (98%) BY PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs

	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Vacuum residue	5.65¢/lb	4.32 lb	24.41
Misc. chem, utilities	--	--	0.15
Gross raw materials			24.56
By-product			
Sulfur	4.54¢/lb	-0.257 lb	-1.17
Utilities			
Cooling water	5.4¢/1,000 gal	32 gal	0.17
Steam	$7.75/1,000 gal	11.6 lb	8.99
Process water	68¢/1,000 gal	1.6 gal	0.11
Electricity	3.6¢/kwh	0.235 kwh	0.85
Total utilities			10.12

Table 5.6 (Concluded)

HYDROGEN (98%) BY PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)[*]	253		506[†]		1,012
Investment ($ million)					
Battery limits	156.8		273.0		509.4
Off-sites	54.6		95.0		177.3
Total fixed capital	211.4		368.0		686.7
Scaling exponents		0.80		0.90	
Production costs (¢/mscf)					
Raw materials	24.56		24.56		24.56
By-products	-1.17		-1.17		-1.17
Utilities	10.12		10.12		10.12
Variable costs	33.51		33.51		33.51
Operating labor, 8/shift[§], $17.50/hr	0.48		0.24		0.12
Maintenance labor, 1.5%/yr of BL inv	0.93		0.81		0.76
Control lab labor, 20% of op labor	0.10		0.05		0.02
Labor costs	1.51		1.10		0.90
Maintenance materials, 1.5%/yr of BL inv	0.93		0.81		0.76
Operating supplies, 10% of op labor	0.05		0.02		0.01
TOTAL DIRECT COSTS	36.00		35.44		35.18
Plant overhead, 80% of labor costs	1.12		0.88		0.72
Taxes and insurance, 2%/yr of TFC	1.67		1.45		1.36
Depreciation, 10%/yr of TFC	8.36		7.27		6.79
Plant gate cost	47.24		45.04		44.05
G&A, sales, research	2.00		2.00		2.00
NET PRODUCTION COST	49.24		47.04		46.05
ROI before taxes, 25%/yr of TFC	20.90		18.19		16.97
PRODUCT VALUE	70.14		65.23		63.02

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[*] Of hydrogen.

[†] Base case.

[§] For base case; may be different for other capacities.

6 COAL GASIFICATION

This section presents screening level economics for gasification of coal. The context for the analyses is the production of bulk chemicals from coal; cost data are presented for the large scale production of syngases, hydrogen, carbon monoxide, and methanol. Some general background on gasification is included.

The investment estimates presented here are derived primarily from data published in a study (472120) by Fluor Inc. for the Electric Power Research Institute (EPRI).* The scheme evaluated by Fluor was for gasifying an Illinois No. 6 bituminous coal in Texaco gasifiers, with the Rectisol® process being used for acid gas removal, and ICI technology being used for synthesizing methanol. This section examines the key features and costs associated with such a scheme, and its modification to produce syngas (of various H_2/CO ratios), hydrogen, and methanol over a range of scales of production (See Figure 6.1 and Table 6.1). The separation of CO from a coal derived syngas is covered in Section 7. A more detailed technical and economic evaluation of both Texaco and Winkler gasification technologies was done as part of a subsequent study and is presented in PEP Report 154, Coal Gasification.

The data presented below form the basis for the modular costs for coal based processes incorporated into the computerized model described in Appendix B.

Please note that in the present section all capacities and costs are per unit of (CO + H_2) for syngas, and on the basis of the pure product content for methanol and hydrogen.

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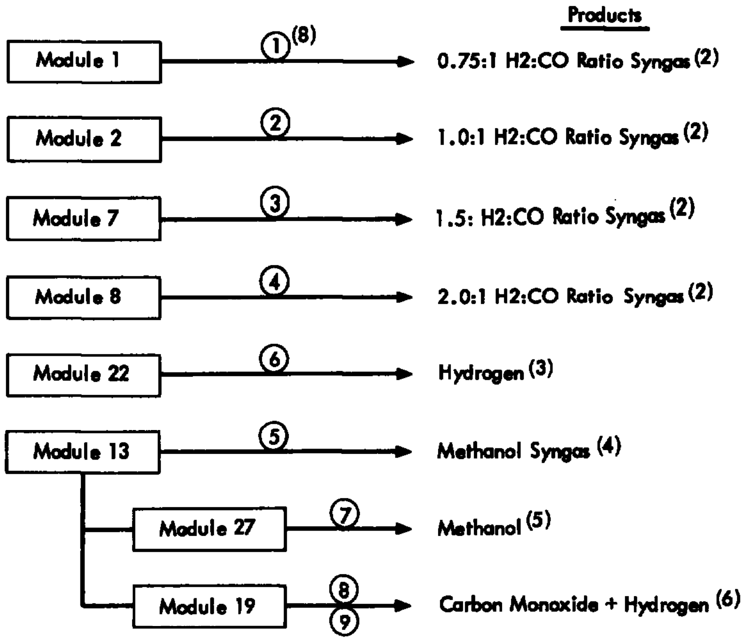
*Continuing evaluation of gasification designs and discussions with industry lead us to believe that these costs are likely to be optimistic. In the computerized data base (see Section 2) we have therefore allowed for a more conservative design which increases the syngas investment estimates by about 25%.

Figure 6.1

COAL GASIFICATION MODULES (1)



Process units contained in the above modules and the range of capacities covered are as follows:

Module 1	Module 2,7,8,13	Module 22	Module 27	Module 19
Coal Preparation Air Separation Coal Gasification (7) COS Hydrolysis Acid Gas Removal Sulfur Recovery	Coal Preparation Air Separation Coal Gasification (7) Shift Conversion COS Hydrolysis Acid Gas Removal Sulfur Recovery	Coal Preparation Air Separation Coal Gasification (7) High and Low Temperature Shift Acid Gas Removal Sulfur Recovery Methanation	Methanol Synthesis Methanol Purification	Separation of CO and H_2 by COSORB
50-1600 million scfd (Contained CO+H2)	50-1600 million scfd (Contained CO+H2)	50-1560 million scfd Hydrogen	600-20,000 metric tons/day Methanol	3-25 million scfd Carbon Monoxide

(1) Module numbers refer to those in the SYNCOST computer program.

(2) The syngas is delivered at 770 psig and 86 °F. Compositions are shown in Table 6.1.

(3) The hydrogen is delivered at 650 psig and 120 °F.

(4) Methano syngas here has an H_2/CO ratio of 2.26:1 and contains 3% of CO_2.

(5) The methanol purity is 99 wt %.

(6) See Section 7.

(7) Texaco gasifier with waste heat boiler, 915 psig, using Illinois No. 6 coal. Base case sized for 10,000 *metric tons/day methanol equivalent. Raw gas composition shown in Table 6.1 as stream 10.*

(8) Stream numbers in Table 6.1.

Table 6.1

PRODUCT COMPOSITIONS AND FLOW RATES*

		(1) 0.75:1 Syngas Product		(2) 1.0:1 Syngas Product		(3) 1.5:1 Syngas Product		(4) 2.0:1 Syngas Product		(5) Methanol Syngas	
	Mol Wt	lb-mols/hr	Mol%	lb-mols/hr	Mol%	lb-mols/hr	Mol%	lb-mols/hr	Mol%	lb-mols/hr	Mol%
Hydrogen	2	37,703	42.0	44,095	49.1	52,984	58.9	58,940	65.4	61,303	65.9
Carbon monoxide	28	50,400	56.1	44,092	49.0	35,322	39.2	29,446	32.7	27,111	29.1
Carbon dioxide	44	9	100 ppm	9	100 ppm	3	100 ppm	9	100 ppm	2,872	3.1
Methane	16	360	0.4	360	0.4	360	0.4	360	0.4	359	0.4
Oxygen	32	tr	—	tr	—	tr	—	tr	—	tr	—
Nitrogen	28	743	0.8	743	0.8	743	0.8	743	0.8	744	0.8
Argon	40	621	0.7	621	0.7	621	0.7	621	0.7	621	0.7
Hydrogen sulfide	34	tr	—	tr	—	tr	—	tr	—	tr	—
Carbonyl sulfide	60	tr	—	tr	—	tr	—	tr	—	tr	—
Ammonia	17										
Methanol	32	2	25 ppm	2	25 ppm	2	25 ppm	2	25 ppm	2	25 ppm
Light ends	46	—	—	—	—	—	—	—	—	—	—
Higher alcohols	46	—	—	—	—	—	—	—	—	—	—
Coal (maf)	—	—	—	—	—	—	—	—	—	—	—
Ash	—	—	—	—	—	—	—	—	—	—	—
Water (steam)	18	—	—	—	—	—	—	—	—	—	—
Total		89,838	100.0	89,922	100.0	90,041	100.0	90,122	100.0	93,015	100.0
Million scfd of CO + H_2		802.4		803.2		804.3		805.0		805.3	
Temp (°F)		86		86		86		86		86	
Press (psig)		770		770		770		770		770	

		(6) Hydrogen Product		(7) Methanol		(8) Carbon Monoxide		(9) Hydrogen Coproduct		(10) Clean Raw Gas	
	Mol Wt	lb-mols/hr	Mol%	lb-mols/hr	Mol%	lb-mols/hr	Mol%	lb-mols/hr	Mol%	lb-mols/hr	Mol%
Hydrogen	2	21,438	96.2	—	—	1.59	0.23	1,528.1	93.0	37,784	20.6
Carbon monoxide	28	—	<10 ppm	—	—	676.41	99.75	0.8	0.05	51,189	27.9
Carbon dioxide	44	—	<10 ppm	50	—	0.07	0.01	71.6	4.3	19,459	10.6
Methane	16	297	1.3	—	—	0.01	1,500 ppm	9.0	0.55	383	0.2
Oxygen	32	—	—	—	—	—	—	—	—	tr	—
Nitrogen	28	186	0.8	—	—	0.04	0.01	34.0	2.1	759	0.4
Argon	40	155	0.7	—	—	—	—	—	—	633	0.3
Hydrogen sulfide	34	—	—	—	—	—	—	—	—	1,244	0.7
Carbonyl sulfide	60	—	—	—	—	—	—	—	—	83	—
Ammonia	17	—	—	—	—	—	—	—	—	tr	—
Methanol	32	—	—	918,750	99.1	—	—	—	—	—	—
Light ends	46	—	—	600	0.1	—	—	—	—	—	—
Higher alcohols	46	—	—	700	0.1	—	—	—	—	—	—
Coal (maf)	—	—	—	—	—	—	—	—	—	—	—
Ash	—	—	—	—	—	—	—	—	—	—	—
Water (steam)	18	221	1.0	6,900	0.7	tr	<1 ppm	—	—	72,109	39.3
Total		22,297	100.0	927,000	100.0	678.12	100.0	1,643.5	100.0	183,643	100.0
Million scfd of CO + H_2		195		—		—		—		810	
Temp (°F)		120		110		—		—		400	
Press (psig)		700		Atm		—		—		880	

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*Except for streams 6, 8, and 9 the base case gasification capacity corresponds to 10,000 metric tons/day methanol equivalent.

Historic Development

Fuel gas has been manufactured from coal now for close to two centuries. The first coal-gas company, which distributed its product for lighting, was chartered in London in 1812. The first U.S. company was chartered in Baltimore in 1816.

In the early days coal gas (used as town gas) was produced entirely by destructive distillation of the coal. Subsequently this was supplemented with water gas (formed by alternately blowing air and steam through a coke bed), and producer gas (made by blowing a mixture of air and steam continuously through a bed of coke or coal). Variations of this basic technology continued to be developed for the production of both fuel (town gas) and chemical feedstock (syngas). Together with the advent of tonnage oxygen plants, these developments culminated in commercial operation of what are now often called the first generation large scale coal gasification processes, namely:

- The Winkler fluidized bed (1927)
- The Lurgi "fixed bed" (1936)
- The Koppers-Totzek (K-T) entrained flow gasifier (1952).

The year noted is that in which the first commercial plant was built. Except for the Lurgi, these gasifiers operate at close to atmospheric pressure.

With the advent of cheap oil and natural gas, interest in coal gasification technology generally flagged in the mid 1950s. A notable exception was the continued development of the Lurgi technology in South Africa for indirect liquid fuel production by Fischer-Tropsch processes. The Soviet Union as well appears to have continued with the development of its own versions of the Lurgi and Winkler gasifiers. Koppers-Totzek gasifiers also continued to be built right through to the 1970s. These were primarily for ammonia production in areas such as India and Turkey, where indigenous oil and gas are in short supply.

Parallel with this, the early 1950s saw the development of both catalytic steam reforming and partial oxidation processes for the production of fuel and syngas from various hydrocarbon feedstocks. Steam reforming of natural gas or naphtha typically turned out to be by far the most economic process for syngas production. However, in part because of its ability to use almost any gaseous or liquid hydrocarbon as a feedstock, partial oxidation remained attractive in certain circumstances for large scale production of syngas or hydrogen. Montecatini, Shell, and Texaco all developed partial oxidation processes on a commercial scale. The partial oxidation reactors are, of course, entrained flow gasifiers.

The Montecatini process, which operated at atmospheric pressure, was eventually abandoned. The Shell and Texaco processes operated at elevated pressures (originally up to some 30 atm). Shell, with its European bent, had initially focused on the gasification of residual hydrocarbons. Texaco started its developments in the United States with natural gas as feedstock, and worked on a prototype coal gasification process as early as the 1950s. When interest in coal was suddenly revived in the mid 1970s, Texaco therefore had a running start for extending its well established partial oxidation technology to coal gasification. In competition, Shell and Krupp-Koppers joined forces in 1974 to pool their respective know-how with Shell and Koppers-Totzek technologies, and to develop a high-pressure entrained flow gasification process for coal. More recently this association has been terminated and each company is continuing development on its own.

Meanwhile, the British Gas Corporation (BGC) was developing a higher efficiency slagging version of the Lurgi process, and Rheinbraun in West Germany was working on a pressurized version of the Winkler process called, somewhat misleadingly, the High Temperature Winkler.

The above four developments have become generally known as the second generation coal gasification processes. All are being piloted at a substantial scale, as shown below:

	Metric Tons/Day Coal
High Temperature Winkler	24
BGC/Lurgi Slagger	350
Shell/Koppers	150
Texaco	150

Demonstration on a commercial scale is expected by the middle of this decade for the Texaco and HT Winkler processes.

In addition, more than thirty other gasifiers are estimated to be at various stages of development. These include "allothermal" designs, in which the heat is supplied from external sources rather than from partial combustion of the feed as in the traditional "autothermal" designs. A number are aimed at directly producing substitute natural gas (SNG) rather than syngas. The majority of these developments were commenced in the 1970s and, as a group, they are sometimes called third-generation gasifiers. As regards technological sophistication or potential economic attractiveness though, they are generally comparable with the second generation processes noted above, rather than being superior. Their development, however, is generally less advanced. One system which appears to have excellent potential for syngas generation is the Saarberg/Otto slag-bath (472141), an entrained flow gasifier in many ways similar to the Shell/Koppers gasifier.

Technical Background

General Considerations

The traditional gasification of coal combines devolatilization and partial oxidation. In simple terms it may be represented by:

$$\text{Coal} + O_2 + H_2O \longrightarrow H_2 + CO + CO_2 + CH_4 + \text{ash} \qquad (1)$$

In high temperature cocurrent gasifiers methane is further almost entirely reformed to H_2 and CO. In countercurrent gasifiers substantial amounts of methane and other volatiles are released directly by devolatilization into the product stream.

Cocurrent entrained flow gasifiers are in principle very similar to the partial oxidation reactors used to produce syngas and hydrogen from miscellaneous hydrocarbon feedstocks. However, as compared with using gaseous or liquid feedstocks, use of coal obviously presents special problems. Large flows of abrasive and corrosive solids must be handled under extreme conditions. The design of safe and efficient pressure feeders has proved to be particularly intractable.

In addition, because the makeup of coal is complex and highly variable, different coals behave very differently both in the way they handle physically and in the way they react chemically. Even coal from a given geological formation may vary considerably.

The ratios of H_2, CO, CO_2, and CH_4 in a gasifier product vary only slightly with the type of coal, but are highly dependent on the type of gasification system. The amounts of oxygen and steam required vary both with the type of coal and the process. Some illustrative data on raw gas compositions are shown in Table 6.2. Comparisons with partial oxidation reactors using feedstocks other than coal are shown in Table 6.3.

When making syngas for chemical use, low H_2/CO ratios (less than 2) are typically required, and it is also of advantage to minimize the residual methane in the product (each mol of methane represents the loss of three mols of syngas). These facts tend to favor an entrained flow gasifier for production of syngas for chemical use. However, because certain types of gasifiers are inherently more suitable for certain coals, the optimal choice of a gasifier is rarely clear cut. For commercial systems, demonstrated operability may of course prove to be the dominating factor.

Variability of Coal

The main properties of coal that influence selection and design of gasifier systems are:

- Caking tendencies when heated
- Mineral (ash) content, fusion temperature, and corrosivity

- Moisture content
- Reactivity
- Volatiles content
- Hetero atom content (S, N, and O)
- Heating value.

In the context of gasification, coals are often classified into two broad groups:

- Bituminous coals
- Subbituminous coals and lignites.

Bituminous coals tend to cake and agglomerate on heating. Compared with subbituminous coals, they are of "higher rank" and usually have a higher heating value and a lower oxygen content. They are lower in moisture and less reactive (i.e., they gasify more slowly). Illinois No. 6, an "Eastern" coal often used for comparison is a typical bituminous coal.

Subbituminous coals, lignites, and brown coals are noncaking. They are progressively younger and more reactive than bituminous coals, and have higher inherent moisture levels and lower heating values. Their higher oxygen content is of particular advantage in gasification in that it reduces external oxygen requirements. This is in contrast to coal liquefaction processes, where oxygen is detrimental because it consumes hydrogen to produce water.

In the United States, coals are often loosely referred to as "Eastern" or "Western." Eastern coals normally are bituminous, while in the West, subbituminous coals predominate, but this identification should not be taken for granted. Some illustrative compositions for North American coals are shown in Table 6.4.

Table 6.2

TYPICAL SYNGAS COMPOSITIONS FROM VARIOUS GASIFIERS

	Texaco	Shell/Koppers	Shell/Koppers	Saarberg/Otto	Koppers-Totzek	Winkler
Type	Entrained flow	Entrained flow	Entrained flow	Entrained flow	Entrained flow	Fluidized bed
Ash handling	Slagging	Slagging	Slagging	Slagging	Slagging	Dry ash
Coal type	Bituminous	Bituminous	Subbitum.	Subbitum.	Subbitum.	Subbitum.
Raw gas composition (vol%, dry basis)						
Hydrogen	33.8	32.1	33.4	31.0	31.6	33.8
Carbon monoxide	45.8	65.0	64.5	58.0	58.5	45.8
Carbon dioxide	17.6	0.8	1.3	10.0	8.0	15.1
Methane	0.3	—	—	0.5	—	3.9
Nitrogen and argon	1.3	0.7	0.5	0.2	1.2	1.4
H_2S + COS	1.2	1.4	0.3	0.3	0.7	
	100.0	100.0	100.0	100.0	100.0	100.0
H_2/CO ratio	0.74	0.49	0.52	0.53	0.54	0.74
Reference	472120	58166	58166	472141	58215	472150

	High Temp. Winkler	U-Gas	Lurgi	Lurgi	BGC/Lurgi
Type	Fluidized bed	Fluidized bed	Fixed bed	Fixed bed	Fixed bed
Ash handling	Dry ash	Agglomerating	Dry ash	Dry ash	Slagging
Coal type	Lignite	Bituminous	Bituminous	Subbitum.	Bituminous
Raw gas composition (vol%, dry basis)					
Hydrogen	35.3	42.9	38.8	39.1	28.9
Carbon monoxide	51.8	22.8	17.9	18.9	54.9
Carbon dioxide	8.9	29.8	30.8	29.7	3.4
Methane	3.2	3.7	9.4	11.9	7.9
Nitrogen and argon	0.7	0.6	2.4	0.3	4.4
H_2S + COS	0.1	0.2	0.7	0.1	0.5
	100.0	100.0	100.0	100.0	100.0
H_2/CO ratio	0.68	1.43	2.17	2.07	0.53
Reference	472147	B-1515	472149	472142	472149

Table 6.3

PARTIAL OXIDATION COMPARISONS

	Natural Gas	Vacuum Residue	Illinois No. 6 Coal	Illinois No. 6 Coal
Process	Texaco	Texaco	Shell/Koppers	Texaco
Feedstock comp (wt%, dry)				
Carbon	73.4	83.7	68.2	69.7
Hydrogen	22.7	9.7	4.8	4.9
Oxygen	0.8	—	9.5	8.9
Nitrogen	3.1	0.3	1.1	1.5
Sulfur	—	6.2	3.7	3.5
Ash	—	0.1	12.7	11.5
	100.0	100.0	100.0	100.0
C/H wt ratio	3.2	8.7	14.2	14.2
HHV Btu/lb (dry)	22,630	17,340	12,380	12,670
Slurry solids (wt%)	na	na	na	60
Oxygen required scf/mscf (CO + H_2)	276	283	278	413
Steam/oxygen (lb/lb)	minimal	0.38	0.09	0.69*
Typical yield of CO + H_2 mscf/metric ton dry feed	130	100	70	60
Raw gas composition (vol%, dry)				
Hydrogen	61.1	43.1	32.1	33.8
Carbon monoxide	35.0	49.9	65.0	45.8
Carbon dioxide	2.6	5.0	0.8	17.6
Methane	0.3	0.3	—	0.3
Nitrogen and argon	1.0	0.2	0.7	1.3
H_2S + COS	—	1.5	1.4	1.2
	100.0	100.0	100.0	100.0
H_2/CO mol ratio	1.75	0.86	0.49	0.74
Reference	(472152)	(472148)	(58166)	(472120)

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*Water in slurry.

na = not applicable.

Table 6.4

TYPICAL COAL COMPOSITIONS AND HIGHER HEATING VALUES

	Illinois No. 6	Powder River Subbituminous	Texas Lignite
Ultimate analysis (wt%)			
Carbon	62.1	49.5	40.8
Hydrogen	4.3	3.6	3.4
Oxygen	7.9	13.3	11.1
Nitrogen	1.3	0.7	0.7
Sulfur	3.2	0.3	0.9
Ash	10.2	5.5	11.4
Moisture	11.0	27.1	31.7
Total	100.0	100.0	100.0
Higher heating value (Btu/lb)			
As received	11,280	8,260	7,050
Moisture-free (mf)	12,670	11,330	10,320
Moisture- and ash-free (maf)	14,310	12,260	12,390

Temperature Constraints

The characteristics of a gasifier are to a large extent related to its temperature profile. Gasification temperatures have a pervasive effect on:

- Handling of the ash
- The reaction kinetics and equilibria
- Materials of construction
- Efficiency of the process.

The interrelation of these factors can lead to severe design constraints. For example, gasifiers are often classified with respect to the mode of ash handling, e.g.,

- Dry ash—operated well below ash fusion temperature
- Agglomerating ash—operated at temperatures approaching the ash melting point so that ash particles will soften and stick together.
- Slagging ash—operated with a molten slag.

Coal ash fusion temperatures are typically about 2100°F (1150°C), but may vary over a wide range, 2000-2800°F (1100-1500°C). The ash fusion temperature (or more specifically the initial deformation temperature) therefore is a key factor in gasifier design and in matching a coal to a gasifier.

At temperatures below 1800°F (1000°C) high coal conversion becomes increasingly difficult to achieve. Also, as discussed in Section 4, methane formation starts to become appreciable at lower temperatures. Dry ash gasifiers thus tend to operate at lower carbon conversion and produce significant amounts of methane.

In slagging gasifiers of the entrained flow type the maximum temperatures typically are 2400 to 2700°F (1300 to 1500°C). High coal conversion is therefore readily achieved. However, heat recovery in the erosive, corrosive, and potentially highly fouling environment becomes critical for good thermal efficiency.

Gasification Pressure

The economics of gasification systems operated at elevated pressures (15 atm plus) normally are much more favorable than those for systems operated close to atmospheric pressure. For chemical syntheses, the syngas is almost invariably needed at elevated pressures (see Section 3) and the costs of compression can represent a fairly severe penalty. For example, compression of syngas from 1 atm to 70 atm requires about 20% of the energy contained in the gas, while compression from 35 atm to 70 atm requires less than 4%.

Also, increased throughputs per unit volume of gasification and downstream equipment reduce capital requirements. A major reduction in plot and equipment sizes is that associated with removing ash entrained in the raw product gas. Low pressure processes typically require large numbers of cyclones followed by wash towers and electrostatic precipitators for final clean-up, together with a large surge gas holder.

These items take up a very large portion of the process area. Pressurized processes, in contrast, are able to remove ash to the same level with, for example, much smaller and cheaper venturi scrubbers.

There are, obviously, also disadvantages to operating at pressure. Oxygen is expensive to compress, and some of the gasification reactions show an adverse pressure dependence. Methane formation tends to increase with pressure, which is a minus for syngas production. Increasing pressure also makes feeding of the coal into the reactor more difficult. The most common of the dry feed systems, the lock hopper system, has been operated successfully only at pressures less than 40 atm. For pressures higher than this, the only currently proven method is to feed a coal slurry, which entails additional penalties (see below).

The optimum pressure is likely to differ for each application. Reference 472041 suggests that the optimum pressure is likely to be between 15 and 35 atm, and closer to the upper level for syngas applications. References 472043 and 472113 detail a trade-off study to identify the optimum gasification pressure for ammonia production by Texaco gasification. The study indicated that in this instance the optimum may be closer to 75 atm but that the cost-versus-pressure curve is relatively flat around the optimum.

Flow Characteristics

The primary classification of gasifiers is typically according to their flow characteristics. The three major types are:

- Fixed bed
- Fluidized bed
- Entrained flow.

As it turns out, the three commercial first generation gasifiers, the Lurgi, the Winkler, and the Koppers-Totzek, each represent one of these types respectively. The Winkler process was, in fact, one of the first commercial applications of the fluidized bed concept. The fixed and fluid bed reactors have, of course, found wide application in the petrochemical industry for reactions employing heterogeneous catalysts. A difference in coal gasification is that the solid bed itself comprises one of the prime reactants.

Schematic illustrations of the reactor types are shown in Figure 6.2, together with the temperature profiles typically encountered in some real versions of these gasifier types. Some of the general characteristics are compared in the Table 6.5. The references noted in the table typically give a description of the process and the developer's status report on developments. For excellent capsule descriptions and critiques of most of these processes, see Shires (472146). Some salient features of the main gasifier types are highlighted in the following pages.

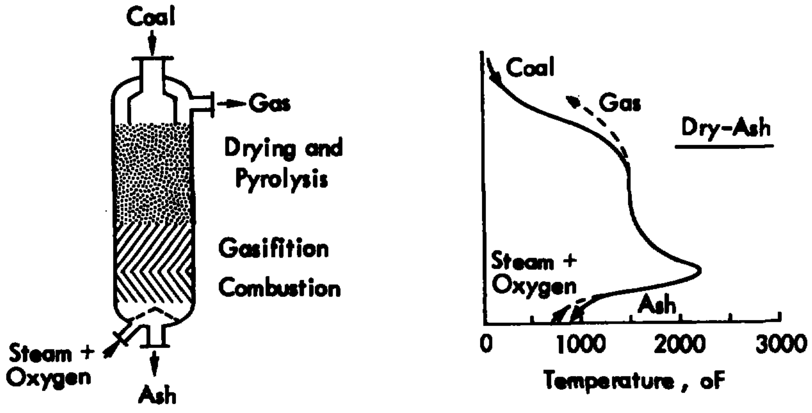
Table 6.5

GASIFIER CHARACTERISTICS

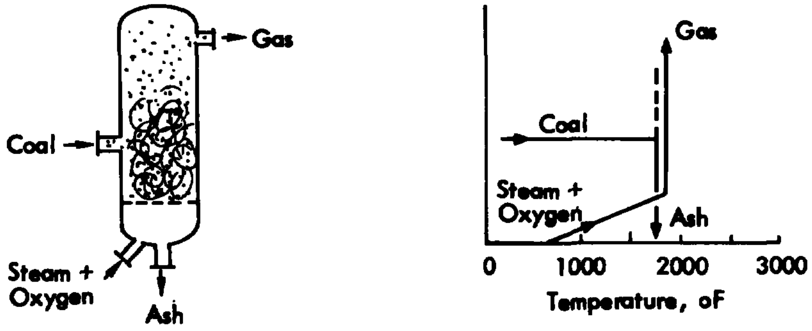
	Fixed Bed	Fluid Bed	Entrained Flow
Flow and mixing patterns	Countercurrent, plug flow of solids	Countercurrent, well-mixed solid phase	Cocurrent
Coal feed	Lumps, no fines	Crushed, some fines	Powder
Coal residence time	Hours	Minutes	Seconds
Capacity	Low	Medium	High
Methane in product	High	Moderate	Low
Ash handling	Dry ash or slagging	Dry or agglomerating ash	Slagging ash
Examples	Lurgi (472093, 472149, 472147)	Winkler (472147, 472150)	Koppers-Totzek (58215, 472147)
	BGC/Lurgi (472149)	HT Winkler (472149, 472147)	Texaco (472149, 472147)
		Westinghouse (472123, 472149)	Shell-Koppers (472149, 58166)
		U-Gas (472149, 472147)	Saarberg-Otto (472149, 472141)

Figure 6.2

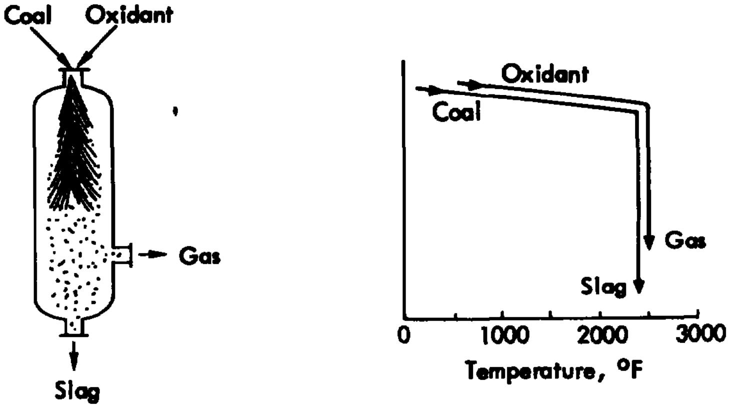
MAIN GASIFIER TYPES AND ILLUSTRATIVE TEMPERATURE PROFILES



FIXED BED GASIFIER



FLUIDIZED BED GASIFIER



ENTRAINED FLOW GASIFIER

Recently Shell and Krupp-Koppers terminated their associations and each company is continuing development on its own. The Shell technology will be known as the Shell Coal Gasification Process (SCGP).

Fixed Bed

In "fixed" bed gasifiers, there is no mixing of the solid phase but the whole bed moves slowly downward. In all the types developed to date, steam and oxygen are injected at the bottom and flow countercurrently to coal fed at the top. The coal thus passes successively through zones where the principal reactions are in turn drying, devolatilization, gasification, and combustion (see further below for details of specific reactions). Successive zones operate at increasingly higher temperatures. Depending on the amount of steam fed, the gasifier can be operated in either a dry ash mode (e.g., the commercial Lurgi) or a slagging ash mode (e.g., the developmental BGC/Lurgi). With coals of low reactivity the dry ash fixed bed pays a penalty in that very large amounts of steam are needed for temperature moderation. This also results in a high H_2/CO ratio in the product gas (see subsection on stoichiometric constraints).

Another constraint on the fixed bed operation is that it does not readily accept coal fines in any appreciable quantity. Since modern mining methods produce as much as 40-50% fines this can be a serious disadvantage; also handling of caking coals is problematic in fixed beds.

An inherent feature of the countercurrent mode of operation is the in-situ heat exchange between feed and product. This improves thermal efficiency of the process but the devolatilization associated with it gives a product containing substantial levels of methane and tars. The need to process or reinject the tars is normally a detriment. For high-volatile, high-moisture lignites, condensation of the tars within the bed itself may also cause problems. Methane production on the other hand is highly desirable if the gas is to be used as a fuel or for conversion to SNG, but usually represents an economic penalty if the end use of the gas is a chemical synthesis in which methane is inert.

The ideal application of fixed bed types would thus be for fuel gas production at a site where coal fines can also be used (e.g., for boiler fuel). Subbituminous coals are likely to be optimal for the dry ash type, while a slagging type also economically processes coals of lower reactivity. However, because its prime example, the Lurgi dry ash process, is currently the only high pressure gasification process which has been well proven on a commercial scale, its application in less than ideal circumstances may nevertheless make sense.

Fluidized Bed

In a fluidized bed gasifier, crushed and sized coal is introduced together with steam and oxygen into a fluidized bed of char. The bed is highly back mixed and the coal undergoes drying, devolatilization, gasification, and combustion at an essentially uniform temperature. The temperature level in the bed is maintained below the fusion temperature of the ash (i.e., typically below 1800°F). The fluidized bed is therefore inherently a "low temperature" gasifier with a limited residence time. High conversions of carbon (greater than 90%) are difficult to achieve. It is thus best suited for highly reactive coals such as the lignites.

Even in the HT Winkler process being developed by Rheinbraun, operating temperature remains relatively low (ca 1100°C), and the development is still keyed to gasifying lignite--the somewhat higher temperatures are achieved by adding limestone to raise the softening point of the ash.

Other developments of the fluid bed concept, i.e., the U-Gas process and Westinghouse process, aim at increasing carbon conversion by increasing residence time of the ash. These are operated at slightly higher temperatures and depend on rather intricate hydrodynamic design to soften, agglomerate, and separate the ash.

An attractive feature of the fluidized bed is that the large inventory of carbon in the bed provides operational stability and ease of control. The penalty of low carbon conversions is also in part compensated by easier materials selection for the lower temperatures. Hence, for lignites, which are inherently attractive gasification feedstocks but present problems in some other types of gasifiers, a second generation fluid bed gasifier could be an optimal selection.

Entrained Flow

The entrained flow gasifiers are characterized by a flame-like high temperature reaction. The residence times of the coal are of the order of seconds, flow velocities are high, and the product contains entrained molten ash.

The coal is entrained as a dilute suspension in the flowing gas and the mechanics of the process are thus well suited to handling coal fines. Caking coals present no special problems. The least ideal coals are those with high ash fusion temperatures. These may require unacceptably high operating temperatures, or use of fluxing agents.

The high temperature operation destroys the tars and volatiles, and the methane content of the product is very low. A very "clean" syngas can thus be produced from a wide range of coals.

There are naturally problems associated with the fairly extreme conditions of operation. The molten slag is both corrosive and erosive and attacks the refractory lining. Developing refractories with adequate life (e.g., longer than 6 months) has been a key problem.

For good thermal efficiency, the heat in the raw gas needs to be recovered at as high a temperature as possible. This heat recovery has to be done in conjunction with cooling, solidification, and removal of the slag from the gas streams. Quenching of the raw gas with either cold gas or water to solidify the slag before heat recovery is the simplest option, but by lowering the temperature of the steam generated, it lowers the thermal efficiency of the process. Use of radiant heat boilers instead of a quench for initial cooling of the gas and slag is much more efficient, but substantially increases the complexity and the cost of the gasifier. Both types of systems are under active development, but the detailed arrangements are generally kept proprietary.

Because the entrained flow gasifier has a very low coal holdup, accurate metering and control of the coal and oxidant feeds is critical for safe operation. Development of systems for feeding dry coal powder into the reactor under pressure has been one of the least tractable aspects of entrained flow gasifier development. To date, satisfactory operation and control of dry feeding appears to have been achieved only with large and rather complex lock-hopper systems. The alternative of feeding the coal as a water slurry (as in the Texaco process) is much more attractive from an operability standpoint, but typically entails some penalty in terms of thermal efficiency (see below). For lignites, which typically have an intrinsically high moisture content, the economics of slurry feeding may be particularly adverse.

In general, because the entrained flow gasifiers can readily gasify a wide variety of coals to produce a syngas that is without tars, is low in methane, and has a low H_2/CO ratio, they are inherently well suited for the production of feedstocks for chemical syntheses.

Stoichiometric Considerations

As Wei (472145) points out, "Despite a bewildering variety of coal gasification systems and the complexity of reactions that take place in them, the gaseous product distributions are severely constrained by reaction stoichiometry and thermal balance considerations." Even a brief examination of some of these constraints is thus revealing. It is fairly readily seen, for example, that operation with low H_2/CO ratios in the product favors thermal efficiency, or that the yield of syngas (H_2/CO) is determined by coal composition and oxygen consumption, but does not directly depend on the amount of steam fed.

We take a brief look at some simplified heat and mass balance constraints below. For a detailed analysis, see Shinnar (472041). For a method of manually calculating the complete heat and mass balances around a gasifier, see the early work of Edmister et al. (472121). Computer simulations of various gasifiers have also been developed (see, for example, reference 472012), but the details of these models are generally kept proprietary.

Considering only the carbon in the coal, equation (1) above is generally taken to represent the net result of the principal reactions shown below (472041). The heats of reaction are shown in kcal/g-mol at 650°K (710°F), a negative sign indicating an exothermic reaction. (To obtain values of ΔH in Btu/lb-mol, multiply by 1,800.)

Coal combustion:

$$C + 1/2\ O_2 \longrightarrow CO \qquad \Delta H = -26.4 \qquad (2)$$

$$C + O_2 \longrightarrow CO_2 \qquad \Delta H = -94.1 \qquad (3)$$

Coal gasification:

$$C + H_2O \rightleftharpoons CO + H_2 \qquad \Delta H = +32.2 \qquad (4)$$

$$C + CO_2 \rightleftharpoons 2CO \qquad \Delta H = +41.4 \qquad (5)$$

$$C + 2H_2 \rightleftharpoons CH_4 \qquad \Delta H = -20.2 \qquad (6)$$

Gas combustions:

$$H_2 + 1/2\ O_2 \longrightarrow H_2O(g) \qquad \Delta H = -58.6 \qquad (7)$$

$$CO + 1/2\ O_2 \longrightarrow CO_2 \qquad \Delta H = -67.8 \qquad (8)$$

Gas reactions:

$$CO + H_2O \rightleftharpoons H_2 + CO_2 \qquad \Delta H = -9.2 \qquad (9)$$

$$CO + 3H_2 \rightleftharpoons CH_4 + H_2O \qquad \Delta H = -52.4 \qquad (10)$$

Only four of the above are independent when the products are H_2, CO, CO_2, and CH_4, and only three if no CH_4 is produced. Equation (9) is the water-gas shift reaction, and equation (10) is the reverse of the methane/steam reforming reaction.

Considering the case in which no methane is produced, the gasification system is constrained by mass balance, as shown in Figure 6.3. The four corners of the shaded trapezium are defined by choosing (2), (3), and (4), as the independent equations, together with reaction

$$C + 2H_2O \longrightarrow CO_2 + 2H_2 \qquad \Delta H = +23.0 \qquad (11)$$

which is the sum of (4) and (9). Chemical equilibrium is not considered here.

Point X on the diagram, for example, shows that 50 mols of carbon, 20 mols of oxygen, and 30 mols of steam could react completely to CO, CO_2, and H_2, whereas point Y with 65 mols carbon, 20 mols of oxygen, and 15 mols of steam cannot react to completion because too much carbon is present to satisfy any combination of the reactions above.

In a hypothetical adiabatic gasifier, where no heat is lost or added, the heat required by the endothermic gasification reactions (4) and (10) is supplied by the combustion reactions (2) and (3). Balancing of these respectively further constrains the stoichiometry to lie along the "thermally balanced line" AB in Figure 6.3. For inlet and outlet streams at 700°F, the equations for points A and B correspond to:

$$C + 0.28\ O_2 + 0.45\ H_2O \longrightarrow CO + 0.45\ H_2 \qquad (12)$$

$$C + 0.20\ O_2 + 1.61\ H_2O \longrightarrow CO_2 + 1.61\ H_2 \qquad (13)$$

The composition of the product varies greatly along line AB and is represented by line EF in Figure 6.4. The equation of EF is given by:

$$H_2/CO = 0.45 + 1.61\ CO_2/CO \qquad (14)$$

Figure 6.3

FEED STOICHIOMETRIC AND ENERGY CONSTRAINTS ON GASIFICATION REACTIONS
(Without Methane Formation)

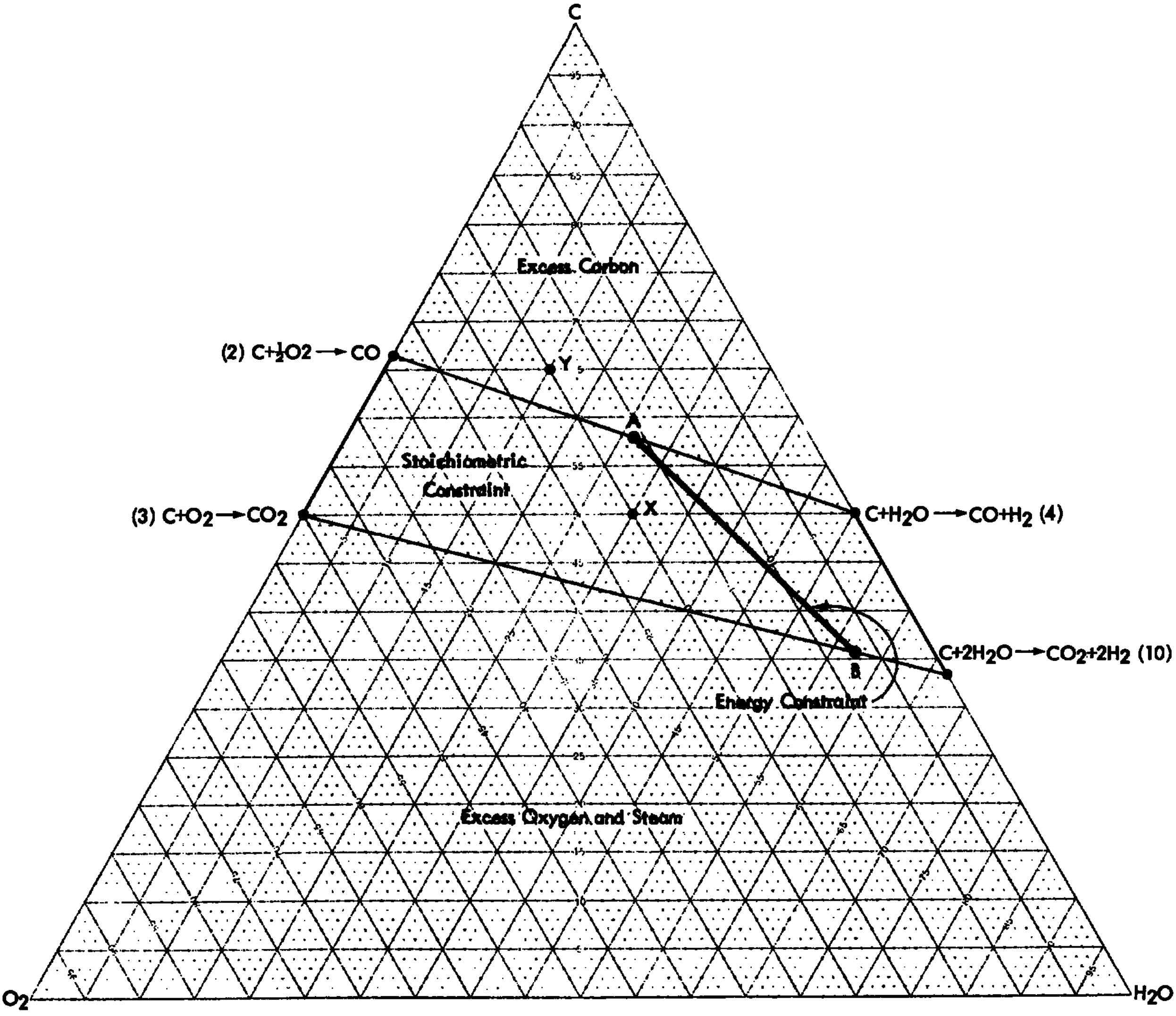
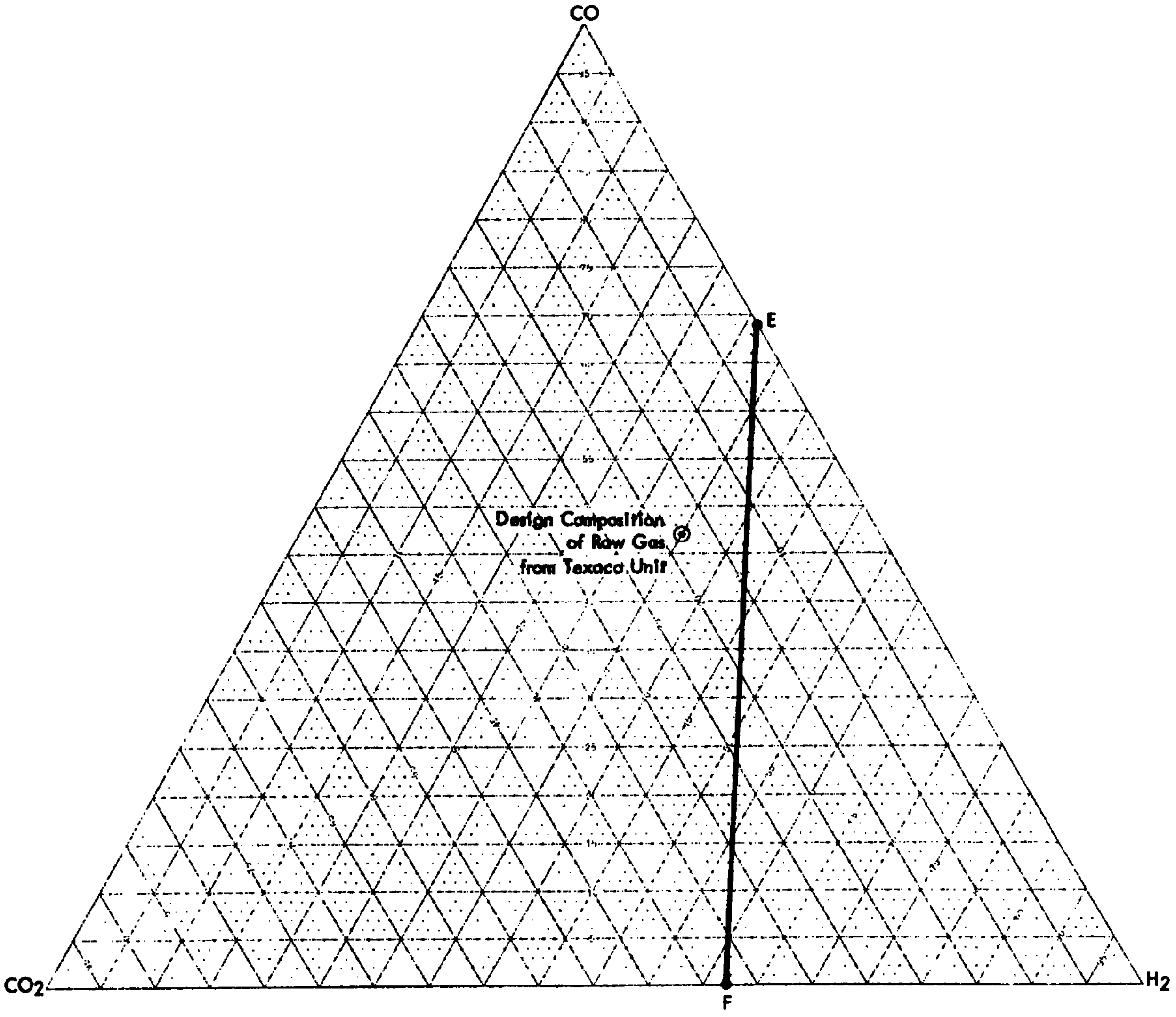


Figure 6.4

PRODUCT STOICHIOMETRIC AND ENERGY CONSTRAINTS



The minimum H_2/CO ratio attainable is thus 0.45, corresponding to operation at point A. At point B, the product is all H_2 and CO_2.

When inlet and outlet temperatures are the same, the thermal efficiency of a gasifier operating at a point on line AB is 100%. However, if one takes into account the energy needed to prepare and heat the steam and oxygen, the overall thermal efficiency of the process drops in proportion. Shinnar (472041) has made some illustrative calculations on this for a gasifier operating at a pressure of 400 psia with a 700°F inlet and outlet temperature. At these conditions, producing one mol of oxygen requires 4.1 times as much energy as producing one mol of steam. From equations (12) and (13) it follows that in moving from point A to point B, 0.08 mol less oxygen is required, while 1.16 mols more steam are used per mol of carbon. The energy required at point B is thus more than that required at point A by the equivalent of 0.83 mol of steam (1.16 - 0.08 x 4.1). In absolute terms the overall thermal efficiencies for points A and B are 81% and 72% respectively.

As a generalization, therefore, operation nearer point A with a low steam to oxygen ratio, and correspondingly a low H_2/CO product ratio, favors thermal efficiency. This is likely to apply even if in end use syngas is required with a high H_2/CO ratio. In such a case it is normally more efficient to use an external shift reaction to adjust the H_2/CO ratio upward, rather than to shift within the gasifier itself. The latter in effect entails combusting coal with oxygen to produce steam at the maximum temperature in the gasifier, and is unlikely to be optimal.

The much lower CO_2 content of the raw syngas is normally an additional advantage for a gasifier operating near point A. Besides reduction of the overall acid gas removal requirements, H_2S removal and sulfur recovery may be simplified at low CO_2 levels.

To the left of lines AB and EF (Figure 6.4), the outlet stream is hotter than the inlet, and to the right the outlet stream is cooler than the inlet. In practice the outlet stream is usually hotter than the inlet and the operation lies to the left of lines AB and EF respectively.

The effect of gasifying a coal with a nominal composition of CH_n (typically $n = 0.6$ to 0.9) rather than char, would be to shift the operating point to the right. Wei (472145) notes that, in practice, the raw gas compositions from a wide variety of gasifiers do in fact usually lie quite close to the thermally balanced line. The composition for the raw gas used in the Texaco gasifier design detailed further below, fits this pattern (see Figure 6.4).

The kinetic constraints on the reactions vary markedly with the type of gasifier. However, all of the oxygen fed is normally consumed since the combustion reactions (2) and (3) are in essence irreversible and proceed much more rapidly than the gasification reactions. The water gas shift reaction is fast and normally attains equilibrium. However, an excess of steam over the stoichiometric amount is generally needed for temperature moderation and to push the carbon-steam reaction to completion.

For conditions producing little methane, the net overall stoichiometry of the gasification process can therefore be approximated by the equation:

$$CH_n + pO_2 + qH_2O = aCO + bH_2 + cH_2O + dCO_2 \qquad (15)$$

From material balances for the elements, it readily follows that the yield of syngas ($CO + H_2$) is given by:

$$(a + b) = 2 + \frac{n}{2} - 2p \qquad (16)$$

It is interesting that the yield of syngas is thus determined by the oxygen consumption (p) and the H/C ratio of the feed (n) but is independent of the amount of steam fed. For a given reaction temperature, however, the oxygen requirement is related directly to the steam fed. Similarly high moisture, high ash content, and low heating value of the feed all increase the oxygen requirement and at the same time reduce the yield of syngas.

In practice, the yield of syngas is always slightly lower than the value calculated from equation (16) because of the incomplete conversion of carbon, the formation of methane, and the production of H_2S and COS from sulfur in the coal. It will be a good first approximation for high temperature, entrained flow gasifiers, where kinetic limitations are minimal and the equilibrium concentration of methane is small. However, syngas yields are substantially lower for countercurrent gasifiers, where methane is released from devolatilization, or for gasifiers operating below ash fusion temperatures when direct methane formation becomes appreciable. The Lurgi dry-bottom gasifier, for example, being countercurrent and operating at low temperatures produces raw gas containing more than 10% methane. The methane in a Shell/Koppers entrained flow gasifier on the other hand is essentially zero.

Some illustrative data on oxygen requirements and syngas yields for high-temperature entrained flow gasifiers are given in reference 472035 and are reproduced in Figures 6.5 and 6.6. These were derived for a gasifier fed with a low sulfur Southern Appalachia coal and operating with a combustion zone exit temperature of 2800°F.

Figure 6.5 illustrates the effect of coal heating value on coal and oxygen requirements. The data were derived by varying heating value at a constant coal composition, while in practice the heating value would in fact be a function of the coal analysis. Heating values of 11,000 Btu/lb (dry basis) or less are usually obtained with subbituminous coals and lignites (see Table 6.4). Heating values above 13,000 Btu/lb would correspond to preheated feeds. The penalty in terms of yield becomes increasingly severe as the heating value drops. Despite the disadvantage of their somewhat lower heating values, however, subbituminous coals and lignites can nevertheless be quite attractive gasification feedstocks. Their higher oxygen and volatiles contents compensate in part for the lower heating values, and their higher reactivities and noncaking properties may offer substantial

Figure 6.5

COAL AND OXYGEN REQUIREMENTS AS A FUNCTION OF COAL HEATING VALUE

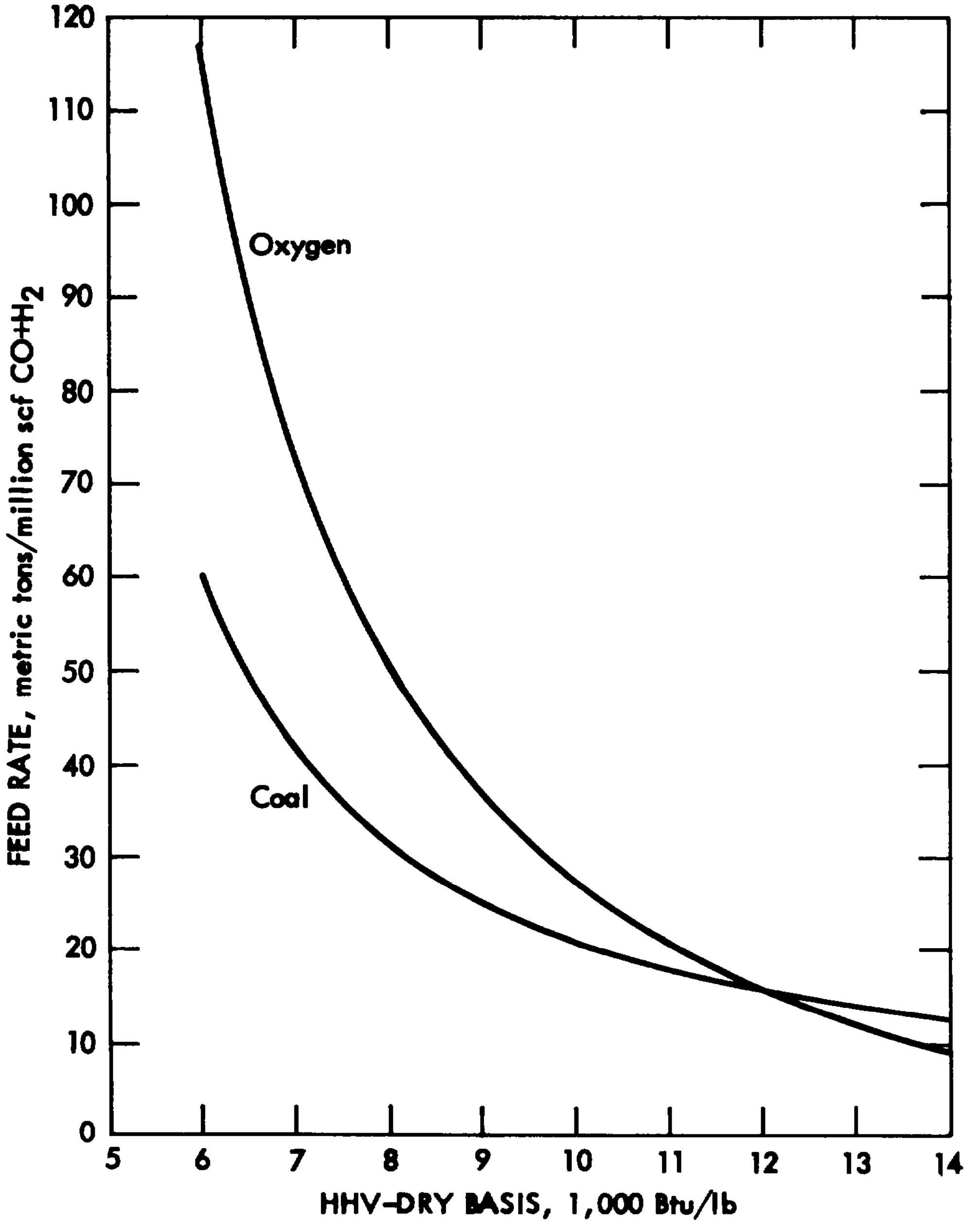
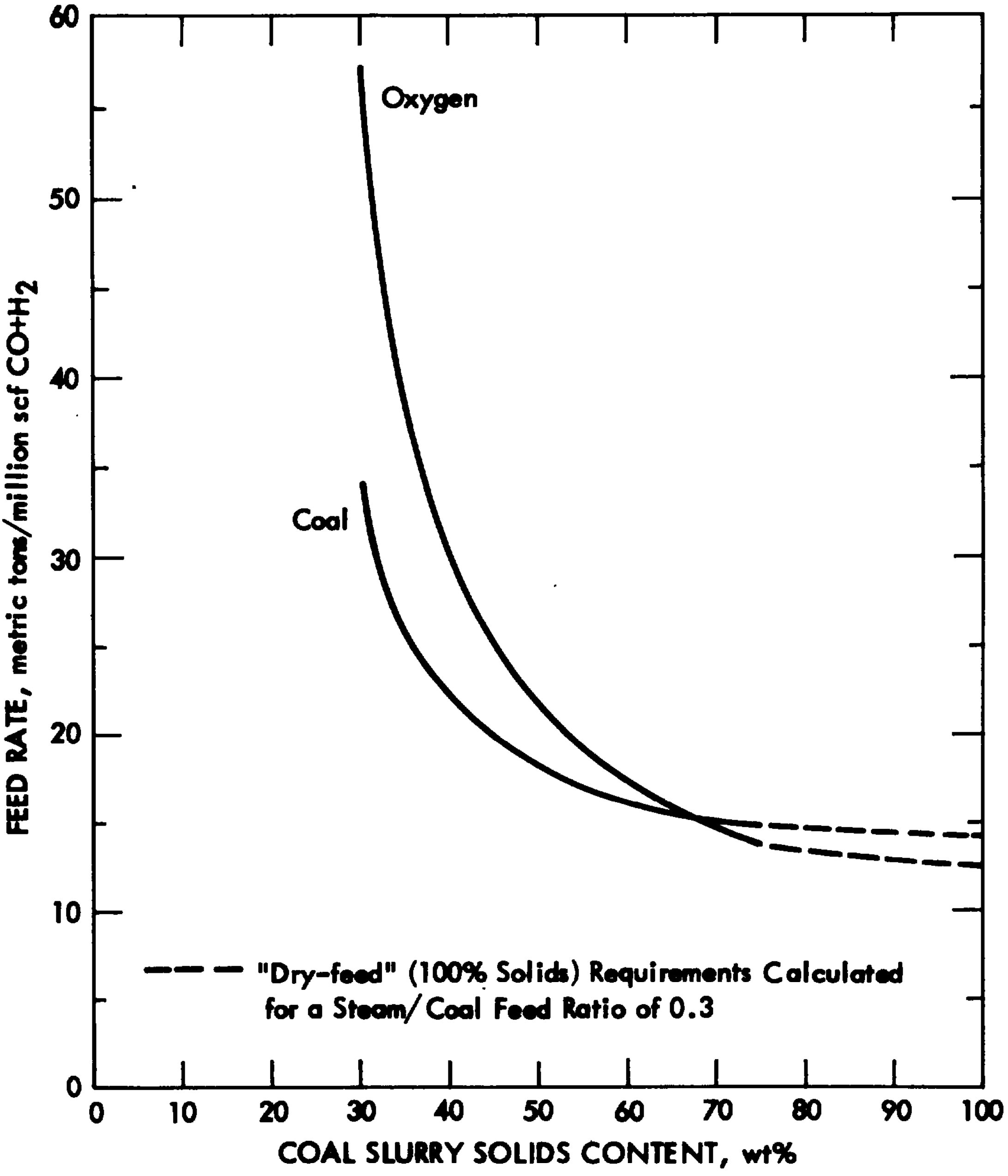


Figure 6.6

COAL AND OXYGEN REQUIREMENTS AS A FUNCTION OF SLURRY FEED SOLIDS CONTENT



advantages in certain types of gasifiers. In addition, subbituminous coals and lignites are more frequently amenable to surface mining and thus are typically cheaper than higher rank coals.

For example, subbituminous coals are far better suited for the dry ash Lurgi gasifier than are the less reactive bituminous coals, and the comparisons which are often made on the basis of Illinois No. 6 show a bias against this gasifier. The reason for this is as follows (472041): The combustion reactions (2) and (3) above are much faster than the endothermic gasification reactions (4) and (5). Therefore a very high local temperature is obtained where the combustion takes place. In the dry ash Lurgi, heat has to be removed to keep the temperature below the melting point of the ash, and a large excess of steam is used as a heat transfer medium to move this heat out of the combustion zone into the gasification zone. If the coal is more reactive, reactions (4) and (5) proceed to a larger extent inside the combustion zone, and the resultant cooling reduces the steam requirements by up to some 40%. In addition caking coals are inherently less well suited to a fixed bed gasifier.

Figure 6.6 illustrates the effect of using a water slurry to feed the coal. The data are calculated for an entrained flow gasifier operating at 2800°F and fed with a low sulfur Appalachian coal. The higher heating value of the coal is taken as 12,840 Btu/lb on a dry basis. The curve clearly illustrates the importance of being able to operate with high solids content in the slurry feed. Lignites normally have a high inherent moisture level and, unless specially treated, they also reabsorb water to high levels if dried and then slurried. They are, therefore, inherently not well suited for gasification in a slurry fed gasifier such as the Texaco. Pretreatment techniques for high moisture coals are under development, but pretreatment may not prove to be the most economic choice. For coals which can be readily slurried and fed at high solids concentrations (greater than 60 wt% solids), on the other hand, the penalty paid in terms of thermal efficiency may well be outweighed by the operability and safety advantages associated with a water slurry feed for high pressure gasification.

Selection of Base Case for Cost Evaluation

The cost data presented in this section are keyed to:

- Illinois No. 6 bituminous coal.
- Texaco gasification, Rectisol® acid gas removal, ICI methanol process.
- U.S. Gulf Coast construction costs.
- Capacity equivalent to 10,000 metric tons/day of methanol.

The scope of the present study did not permit extension of the detailed analysis to other coals, or to other gasification and downstream technology. However, the data are broken down in sufficient detail so that factors can be applied to estimate the cost impact of using other coals, process variations, or locations. Some broad guidelines are given later. Similarly, in the computer program for estimating and projecting product costs (Appendix B) the user can readily change the default values for capital and operating costs to examine sensitivities, and in effect examine also the costs of other gasification schemes. Some comments on the rationale for selecting the base case are noted below.

In practice, choice of the overall process scheme is influenced by the end uses for the gas and the scale of production. As discussed in Section 3, current chemical uses comprise a mixture of small operations such as oxo synthesis, medium scale operations such as acetic acid manufacture, and the large scale production (in chemical terms) of the primary syngas products, methanol and ammonia. Production for these various uses may be integrated to various degrees. Well publicized process developments on the horizon range from the medium scale, e.g., acetic anhydride, to the very large scale, e.g., ethylene via methanol or directly from syngas (see PEP Review 80-3-2). For a world-scale plant for ethylene, the syngas requirement in terms of methanol equivalent (ca 10,000 metric tons/day) would be roughly an order of magnitude larger than that for a typical existing methanol plant. One is here thus approaching the scale of production mooted for "mega" methanol and SNG plants for fuels production. Given the latter, one can, of course, refine the raw fuels products for chemical synthesis. In such a case, the rationale for syngas process selection and the associated economics could differ substantially from those in which syngas production is dedicated to chemical syntheses.

To set some practical limits on the present scope, we decided to aim at developing screening level economics which form a continuum across the middle ground in terms of scale (i.e., greater than that for oxo synthesis but lower than that for the mega complexes), and relate to facilities dedicated to producing syngas for chemical uses (i.e., we avoided as far as possible the added complications of assigning values to other chemical and fuels coproducts).

As discussed earlier in this section, entrained flow gasifiers produce a syngas that has no tars, is low in methane, and has a low H_2/CO ratio. This, combined with their ability to use coal fines, makes these gasifiers inherently well suited for the production of feedstock for the chemical synthesis in the above context. The status of candidate technologies for such gasifiers here appears to be as follows:

Koppers-Totzek (atmospheric, dry feed)	Operated on a commercial scale for ammonia synthesis
Texaco (pressure, slurry feed)	Several large pilot units in operation Demonstration plant under construction
Shell-Koppers (pressure, dry feed)	Advanced large scale pilot development
Saarberg-Otto (pressure, dry feed)	Large scale pilot development

The Koppers-Totzek process is in commercial operation in South Africa (472190), India, and elsewhere, and has also recently been chosen by the Tennessee Valley Authority (TVA) for its proposed commercial-scale coal gasification facilities at Murphy Hill, Alabama (472191). However, the disadvantages of operating at atmospheric pressure (see above) make it an unlikely competitor for the medium or longer term.

In terms of efficiency and the range of processable coals, the Shell-Koppers and Saarberg-Otto pressurized, dry feed, entrained flow gasifiers (PDEG) are the most attractive. However, the Saarberg-Otto process is in a relatively early stage of development. The Shell-Koppers process has undergone extensive large pilot unit (150 tons/day) testing, and proposals have been made for its commercialization (472192). A PDEG could, therefore, be demonstrated on a commercial scale in the latter half of this decade. However, the published information and the analysis regarding the Shell-Koppers technology are rather limited; resolution of one of the most intractable problems, the development of an efficient pressurized dry-feed system suitable for commercial operation, may still be some way off. (As noted earlier, Shell and Krupp-Koppers recently terminated their association, and each company is continuing development on its own.)

Of the pressurized entrained flow developments, the Texaco technology, which feeds coal as a water slurry, has progressed the furthest. Variations of this technology have been successfully piloted on a substantial scale (greater than 150 tons/day, greater than 6,500 hr) by Ruhrkohle AG/Ruhrchemie AG (RAG/RCH) (472153) and Dow (472194). Construction of a demonstration plant to gasify some 1,000 tons/day of coal (472071, 472149) is proceeding at the Cool Water generating station in Barstow, California. The latter is a project to demonstrate integrated gasification/combined-cycle (IGCC) technology for electricity generation. The project is being undertaken by a consortium comprising Southern California Edison, EPRI, Bechtel, General Electric, and Texaco. They have been recently joined by a Japanese group which includes Tokyo Electric, Toshiba, IHI, and Japan's Central Research Institute (472189). Texaco gasifiers of a similar size are under construction as part of Tennessee Eastman Company's commercial venture to produce acetic anhydride from coal derived syngas (472211) - see Section 3.

It should be noted that on another pilot project using Texaco gasification technology, namely, the TVA unit at Muscle Shoals, Alabama, the gasifier as originally designed and installed was not operable.

The problems here related primarily to the slag removal system (472193): However, the impression we gained during a visit there is broadly in line with the claim of Texaco, namely, that "the problems are not fundamental to the process; it's the way the plant is put together" (472195). As of May 1982, we understand that a redesign of the slag removal system has been implemented, and a number of test runs lasting several days have been successfully carried out.

We believe that the costs keyed to Texaco gasification are conservatively representative of what might be expected by 1990. Another advantage to our selecting Texaco technology is the large number of openly published technoeconomic studies (for projects using such gasifiers) which have been carried out by major contractors for the U.S. Department of Energy and EPRI. Availability of a selection of well honed designs and estimates by contractors with experience in this area increases confidence in the numbers.

Acid gas removal and sulfur recovery systems typically account for up to 20% of the gasification system investment. For sulfur recovery, a Claus plant with a tail gas treating unit is normally chosen. Its use is contingent on separating a stream sufficiently rich in H_2S in the acid gas removal section. Selective adsorbtion/desorbtion of the H_2S and CO_2 normally ensures the latter. Choice of the optimum acid gas removal process does not appear to be clear-cut, but the Rectisol® (Linde and Lurgi) and Selexol® (Norton Company) selective physical solvent processes have been the ones most commonly specified in proposed gasification designs. The Rectisol® process, which uses refrigerated methanol as a solvent, is commercially well established in coal gasification and other systems. It has a successful history of protecting sulfur-sensitive catalysts such as those used in methanol systems. Costs associated with it should therefore be representative for our general case.

Illinois No. 6 coal as the feedstock and the U.S. Gulf Coast as the manufacturing location, are advantageous choices because both have in many ways become standard reference points and are used widely as basis for comparison. It could be argued that despite this advantage, the combination departs too far from anticipated reality—that because of the expense of transporting coal, gasification complexes will most likely be located at the mine. We are not altogether convinced of this. Gasification economics are highly capital intensive and the extra costs and problems of setting up in a remote location, together with the transport costs of the product, could negate the advantages of the cheaper coal. Thus, particularly for chemicals production, an established manufacturing location could be the most economic site. In any case, values are here assigned to coal price and location factor, in effect, for illustration only.

The most recent in a series of studies for EPRI by Fluor Inc. (472120) presented technoeconomic data well fitted to the criteria for our base case. Fluor evaluated the production of methanol at a scale close to 10,000 metric tons/day from Illinois No. 6 bituminous coal with Texaco coal gasifiers, Rectisol® acid gas removal, and ICI methanol synthesis. Fluor's evaluation was based on design data supplied by both Texaco and ICI for their respective units, and on design and cost data supplied by Lotepro for the Rectisol® process. Both technical and economic data were presented in sufficient detail to enable breaking out costs of syngas manufacture per se. We therefore used reference 472120 as the source of our base case numbers. The base data were adjusted for a slightly different scale and scope and the costs were also escalated forward to 1981. In addition we adjusted the design to vary the H_2/CO ratio, and scaled the costs by section to arrive at overall costs for lower capacities.

Base Case Design—Methanol from Coal

Overall Plant Design

A block flow diagram of the facility is shown in Figure 6.7 (foldout at end of report). For process flow sheets, see reference 472120. Illinois No. 6 coal is gasified by Texaco partial oxidation technology. The coal is fed as a water slurry and gasified with oxygen in reactors operating at 915 psig. The gasifier effluent is processed by shift conversion, COS hydrolysis, and Rectisol® acid gas removal to produce a methanol syngas. An ICI low pressure process (800 psig) is used to produce methanol. Water formed during methanol synthesis is removed by distillation to produce methanol suitable for turbine fuel.

A mass balance for a facility using as feedstock a 60 wt% solids coal slurry and producing 10,000 metric tons/day (100% basis) of better than 99% pure methanol is given in Table 6.6. The feed and product flow rates are summarized below:

	Metric Tons/Day	lb/hr
Feed		
Coal (mf basis)	13,341	1,225,700
Oxygen (as 100%)	12,791	1,175,200
Products		
Methanol (99.1% product)	10,090	927,000
Sulfur	462	42,400
Ash to disposal (dry basis)	1,538	141,300
CO_2 vent stream (93% CO_2)	17,675	1,623,900

The support units include facilities for coal receiving, air separation, sulfur recovery, and product storage and shipping. The plant is designed to be self-sufficient in utilities, with only coal and clarified water being imported. The overall energy balance hangs on the large amount of high level process heat contained in the gasifier and shift conversion effluent streams. In the given design this heat is recovered as 1500 psig superheated steam and suffices for almost 90% of the total steam needed for electric power turbogenerators, and process equipment drives. The latter include turbine drives for the air, oxygen, and methanol synthesis unit recycle compressors. The rest of the prime steam is raised in boilers fired with purge gas from the methanol synthesis unit (see Figure 6.8, foldout at end of report). A utilities summary is shown in Table 6.7. For this design, the waste heat boilers in the Texaco unit are of the superheating type. If all the high level heat in the gasifier effluent had been used to generate

Table 6.6

METHANOL FROM COAL

STREAM FLOWS

(10,000 Metric Tons/day Methanol)

Component	Mol Wt	(1) Air to Cryo Plant		(2) Oxygen Feed to Gasifier		(3) Coal to Coal Prep		(4) Slurry Water		(5) Gasifier Product	
		lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr
Hydrogen	2	—	—	—	—	—	—	—	—	37,784	75,600
Carbon monoxide	28	—	—	—	—	—	—	—	—	51,189	1,433,300
Carbon dioxide	44	—	—	—	—	—	—	—	—	19,459	856,200
Methane	16	—	—	—	—	—	—	—	—	383	6,100
Oxygen	32	38,988	1,247,600	36,727	1,175,300	—	—	—	—	—	—
Nitrogen	28	144,815	4,054,800	116	3,200	—	—	—	—	759	21,200
Argon	40	1,866	74,600	633	25,300	—	—	—	—	633	25,300
Hydrogen sulfide	34	—	—	—	—	—	—	—	—	1,244	42,300
Carbonyl sulfide	60	—	—	—	—	—	—	—	—	83	5,000
Ammonia	17	—	—	—	—	—	—	269	4,600	269	4,600
Methanol	32	—	—	—	—	—	—	—	—	—	—
Light ends	46	—	—	—	—	—	—	—	—	—	—
Higher alcohols	46	—	—	—	—	—	—	—	—	—	—
Coal (maf)	—	—	—	—	—	—	1,085,500	—	—	—	—
Ash	—	—	—	—	—	—	140,200	—	—	*	141,300
Water (steam)	18	4,702	84,600	—	—	—	151,500	36,726	661,100	35,319	635,700
Total		190,371	5,461,600	37,476	1,203,800	—	1,377,200	36,995	665,700	147,122*	3,246,600
Gpm (60°F)		—	—	—	—	—	—	—	1,331	—	—
Million scfd		1,734	—	341	—	—	—	—	—	1,340	—
Temp (°F)		—	—	—	—	—	—	—	—	2,300– 2,600	—
Press (psig)		—	—	—	—	—	—	—	—	915	—

Component	Mol Wt	(6) Quench/Scrubbing Water		(7) To COS Hydrolysis		(8) To Shift Conversion		(9) Shifted Gas		(10) Gas From COS Hydrolysis	
		lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr
Hydrogen	2	—	—	12,883	25,800	24,901	49,800	48,555	97,100	12,883	25,800
Carbon monoxide	28	—	—	17,452	488,700	33,737	944,600	10,083	282,300	17,452	488,700
Carbon dioxide	44	—	—	6,634	291,900	12,825	564,300	36,523	1,607,000	6,661	293,100
Methane	16	—	—	130	2,100	253	4,000	253	4,000	130	2,100
Oxygen	32	—	—	—	—	—	—	—	—	—	—
Nitrogen	28	—	—	258	7,200	501	14,000	501	14,000	258	7,200
Argon	40	—	—	216	8,600	417	16,700	417	16,700	216	8,600
Hydrogen sulfide	34	—	—	425	14,400	819	27,900	863	29,400	451	15,300
Carbonyl sulfide	60	—	—	28	1,700	55	3,300	11	700	1	60
Ammonia	17	—	—	—	—	—	—	—	—	—	—
Methanol	32	—	—	—	—	—	—	—	—	—	—
Light ends	46	—	—	—	—	—	—	—	—	—	—
Higher alcohols	46	—	—	—	—	—	—	—	—	—	—
Coal (maf)	—	—	—	—	—	—	—	—	—	—	—
Ash	—	—	—	—	—	—	—	—	—	—	—
Water (steam)	18	36,790	662,200	13,302	239,400	58,807	1,058,500	35,109	632,000	13,276	239,000
Total		36,790	662,200	51,328	1,079,800	132,315	2,683,100	132,315	2,683,200	51,328	1,079,900
Gpm (60°F)		—	1,324	—	—	—	—	—	—	—	—
Million scfd		—	—	467	—	1,205	—	1,205	—	467	—
Temp (°F)		—	—	380		435		866		—	—
Press (psig)		—	—	870		890		850		—	—

Table 6.6 (Concluded)

METHANOL FROM COAL

STREAM FLOWS

(10,000 Metric Tons/day Methanol)

		(11)		(12)		(13)		(14)		(15)	
		Feed to Acid Gas Removal		Feed to Methanol Synthesis		Acid Gas to Sulfur Recovery		Tail Gas Vent to Atmosphere		Fuel Gas from Rectisol Unit	
Component	Mol Wt	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr
Hydrogen	2	61,437	122,900	61,306	122,600	3	10	4	10	124	250
Carbon monoxide	28	27,535	771,000	27,111	759,100	3	80	42	1,170	380	10,630
Carbon dioxide	44	43,183	1,900,100	2,872	126,360	2,331	102,580	34,360	1,511,850	3,620	159,280
Methane	16	383	6,100	359	5,700	—	—	6	100	17	280
Oxygen	32	—	—	—	—	—	—	—	—	—	—
Nitrogen	28	759	21,200	744	20,800	70	1,960	3,943	110,410	7	200
Argon	40	633	25,300	621	24,800	—	—	2	80	10	410
Hydrogen sulfide	34	1,314	44,700	tr	tr	1,314	44,690	5 ppm	4 ppm	—	—
Carbonyl sulfide	60	12	700	tr	tr	12	720	5 ppm	7 ppm	—	—
Ammonia	17	—	—	—	—	—	—	—	—	—	—
Methanol	32	—	—	3	100	17	550	8	240	3	100
Light ends	46	—	—	—	—	—	—	—	—	—	—
Higher alcohols	46	—	—	—	—	—	—	—	—	—	—
Coal (maf)	—	—	—	—	—	—	—	—	—	—	—
Ash	—	—	—	—	—	—	—	—	—	—	—
Water (steam)	18	230	4,100	—	—	—	—	—	—	—	—
Total		135,486	2,896,100	93,016	1,059,360	3,750	150,590	38,365	1,623,860	4,161	171,150
Gpm (60°F)		—	—	—	—	—	—	—	—	—	—
Million scfd		1,234	—	847	—	34	—	350	—	38	—
Temp (°F)		105	—	86	—	—	—	—	—	—	—
Press (psig)		815	—	768	—	—	—	—	—	—	—

		(16)		(17)		(18)		(19)		(20)	
		Crude Methanol		Methanol to HP Column		Methanol to LP Column		Fuel Gas from Methanol Unit		Methanol Product to Storage	
Component	Mol Wt	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr	lb-mols /hr	lb/hr
Hydrogen	2	9	20	4	10	5	10	1,368	2,700	—	—
Carbon monoxide	28	5	140	2	60	3	80	680	19,000	—	—
Carbon dioxide	44	127	5,590	62	2,730	65	2,860	504	22,200	1	50
Methane	16	9	140	4	60	5	80	359	5,700	—	—
Oxygen	32	—	—	—	—	—	—	—	—	—	—
Nitrogen	28	3	90	1	30	2	60	744	20,800	—	—
Argon	40	2	80	1	40	1	40	621	24,800	—	—
Hydrogen sulfide	34	—	—	—	—	—	—	—	—	—	—
Carbonyl sulfide	60	—	—	—	—	—	—	—	—	—	—
Ammonia	17	—	—	—	—	—	—	—	—	—	—
Methanol	32	28,694	918,200	13,877	444,060	14,817	474,140	22	700	28,711	918,750
Light ends	46	15	690	7	320	8	370	2	100	13	600
Higher alcohols	46	15	690	7	320	8	370	—	—	15	700
Coal (maf)	—	—	—	—	—	—	—	—	—	—	—
Ash	—	—	—	—	—	—	—	—	—	—	—
Water (steam)	18	2,387	42,970	1,155	20,790	1,232	22,180	17	300	383	6,900
Total		31,266	968,610	15,120	468,420	16,146	500,190	4,317	96,300	29,123	927,000
Gpm (60°F)		—	2,400	—	1,160	1,240	—	—	2,330	—	
Million scfd		—	—	—	—	—	—	39	—	—	—
Temp (°F)		—	—	—	—	—	—	121	—	110	—
Press (psig)		—	—	—	—	—	—	45	—	Atm	—

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*Ash free basis.

Table 6.7

METHANOL FROM COAL

UTILITIES SUMMARY

(10,000 Metric Tons/Day Methanol)

	Electric Power (kw)	Cooling Water (1,000 gpm)	Clarified Water (1,000 gpm)	Fuel Gas (Million Btu/hr HHV)	Steam (1,000 lb/hr)			
					1500 psig	600 psig	100 psig	50 psig
Coal preparation	12,830	—	—	—	—	—	—	—
Air separation	(1,470)	267	—	—	1,987	—	—	—
Gasification and heat recovery	10,130	22	—	—	(2,380)*	—	(171)	15
Shift and COS hydrolysis	1,220	3	—	—	(373)	—	(264)	(255)
Acid gas removal	9,420	24	—	(69)	—	443	(244)	224
Sulfur recovery	3,700	—	—	24	—	—	(101)	—
Methanol synthesis and refining	2,770	47	—	(397)	*	257	439	62
Boilers	—	—	—	442	(358)	28	—	—
Power generation	(65,600)	62	—	—	1,124	(728)	225	41
Misc. utilities and off-sites	27,000	(425)	9.5	—	—	—	116	(87)
Plant import			9.5					

( ) = net produced.

*736 million Btu/hr input into BFW from methanol synthesis.

saturated steam, an externally fired superheater would have been required. Total steam generation would then have exceeded the amount needed in-plant. However, some import of steam could be needed to simplify start-up of the unit.

The thermal efficiency of the overall operation is as follows:

	Flow Rate (lb/hr)	Heat of Combustion (Btu/lb)	Total Heat (10^6 Btu/hr)	Efficiency (%)	Energy Usage (10^6 Btu/metric ton methanol)
Higher heating value (HHV) basis					
Coal in (mf)	1,225,700	12,670	15,530	57.9	37.3
Methanol out	927,000	9,692	8,984		
Lower heating value (LHV) basis					
Coal in (mf)	1,225,700	12,214	14,971	52.6	35.9
Methanol out	927,000	8,502	7,881		

Since the design is balanced in terms of utilities, the thermal efficiency values noted above reflect the overall efficiency of the process. However, one should be careful in comparing these values with literature values for "thermal" or "cold gas" efficiencies. Too often these omit energy inputs such as air separation power requirements or live steam to the gasifier.

The design for 10,000 metric tons/day methanol production was based on the number of trains within each unit, as shown in Table 6.8.

Table 6.8

TRAINS PER UNIT

Coal preparation	1
Air separation	6
Coal gasification	*
COS hydrolysis	2
Shift conversion	2
Acid gas removal	4
Methanol synthesis	4
Methanol refining	4
Claus sulfur plant	2
Claus tail gas unit	2
Boiler plant	3
Turbogenerators	2

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*Information not published. We assumed for scale-down purposes that eight gasifiers and one spare unit were included.

Storage for 10 days of sulfur and methanol production and loading facilities for train and truck are provided.

A mass balance around the gasifier itself is shown in Table 6.9. It is based primarily on reference 472120, supplemented by references 472138 and 472041. It contains some minor imbalances because it is compiled from several sources. The relative amount of H_2S and COS formed, or the fraction of nitrogen converted to ammonia, does not appear to be accurately predictable at this time. A typical assumption is that 25% of the nitrogen in the coal would form ammonia, which would then be complexed as ammonium carbonate in the various process condensates (472138, 472001). Eventually these are recycled to the gasifiers, where the ammonia is likely to be destroyed.

Table 6.9

MASS BALANCE AROUND TEXACO GASIFIERS

(10,000 Metric Tons/Day Methanol)

		Wt% Basis		
	lb/hr	Maf Coal	Coal as Received	Slurry Feed
Feeds				
Coal				
Carbon	855,044	78.8	62.1	
Hydrogen	60,181	5.5	4.3	
Oxygen	108,841	10.0	7.9	
Nitrogen	18,018	1.7	1.3	
Sulfur	42,533	3.9	3.1	
Chlorine	857	0.1	0.1	
Coal (maf)	1,085,474	100.0	78.8	
Ash	140,220		10.2	
Coal (mf)	1,225,694			60.0
Moisture	151,489		11.0	7.4
Coal (as received)	1,377,183		100.0	
Slurry water				
Ammonia	4,569			
Water	661,071			
Total	665,640			32.6
Slurry feed	2,042,823			100.0
Oxidant				
Oxygen	1,175,266			
Argon	25,328			
Nitrogen	3,249			
Total	1,203,843			
TOTAL FEED	3,246,666			

	Mol Wt	lb/hr	lb-mols/hr	Mol% (Dry)	Mol% (Wet)
Products					
Raw gas product					
Hydrogen	2	75,568	37,783.8	33.8	25.7
Carbon monoxide	28	1,433,293	51,189.0	45.8	34.8
Carbon dioxide	44	856,215	19,459.4	17.4	13.2
Methane	16	6,124	382.8	0.3	0.3
Nitrogen	28	21,264	759.4	0.7	0.5
Argon	40	25,328	633.2	0.6	0.4
Hydrogen sulfide	34	42,297	1,244.0	1.1	0.8
Carbonyl sulfide	60	4,948	82.5	0.1	0.1
Ammonia	17	4,569	268.8	0.2	0.2
Total		2,469,606	111,802.9	100.0	76.0
Water	18	635,745	35,319.0		24.0
Total		3,105,351	147,121.9		100.0
Ash		141,315			
TOTAL PRODUCT		3,246,666			

The mass balance does not show trace compounds released or formed on gasification. Data on levels of trace components in the various effluent streams of the Texaco pilot units are given in reference 472137. For illustration, an analysis of the water bleed from a unit gasifying an Eastern coal is shown in Table 6.10.

Table 6.10

WATER QUALITY DATA

BLEED STREAM - EASTERN COAL	
pH	7.7
TDS (ppm)	1,708
COD (ppm)	405
TOC (ppm)	215
Ammonia (ppm)	1,270
Anions (ppm)	
Bromide	<1
Chloride	740
Fluoride	175
Cyanide	8
Formate	522
Nitrate	9
Sulfide	316
Sulfate	21
Thiocyanate	8
Trace organics (ppb)	
Benzene	3.0
Toluene	2.0
Anthracene	0.5
Fluoranthene	0.5
Naphthalene	2.0
Pyrene	0.7
Phenanthrene	0.02
Phenols	<10

As noted previously, an inherent advantage of the entrained bed gasifier is that the high temperature operation keeps undesirable by-products to a minimum.

Process Description

Washed -1.5 inch Illinois No. 6 coal, delivered to the plant in unit trains, is stored in piles. A crusher reduces it to less than 3/4 inch. It is then stored and fed forward to two-stage grinding units. The ground coal is slurried with recycled process and makeup water to give a 60 wt% solids coal slurry. The coal slurry is pumped by charge pumps to the gasifiers.

Oxygen of 98% purity is produced by air separation in six 2,095 metric tons/day units. The units also supply nitrogen for the acid gas removal section. Air and oxygen are compressed in centrifugal machines driven by condensing-type steam turbines. The technology is conventional. Both long term liquid storage and short term gaseous oxygen surge are provided. Air separation systems in general and their specific application with Texaco gasifiers are reviewed respectively in references 483000 and 472188.

Details of the Texaco gasification and ash recovery system are proprietary. A number of arrangements are described in journals and patents (see also below under Process Discussion). The scheme in the present evaluation is broadly as follows.

The coal-water slurry is fed, together with oxygen, through special burners into a vertical gasification reactor. The burners are located at the top and feed downward into a refractory lined chamber, where partial combustion takes place at 915 psig and 2300 to 2800°F. The product gas consists primarily of CO, H_2, CO_2, and steam. Most of the sulfur in the coal is converted to H_2S, and the rest to COS. The product is essentially free of uncombined oxygen. The gas contains some unconverted carbon and all of the ash, in the form of molten slag.

The bulk of the crude gas produced in the gasification zone separates from most of the molten slag, and is led from the gasification chamber to a mixing chamber, where it is quenched with cool scrubbed recycle gas. This lowers the bulk temperature below the softening point of the entrained ash; part of the solidified ash may drop out at this point. The gas is then fed forward to waste heat boilers of the superheating type to generate 1500 psig, 900°F steam. After further indirect cooling, it is scrubbed with a large quantity of process condensate to remove the last traces of entrained particulates.

A small portion of the gas formed in the gasification zone passes straight down into the bottom section of the gasifier. This stream carries with it the bulk of the larger slag particles, which are quenched with water and discharged via a lock-hopper. The ash is dewatered and sent to disposal. Water recovered from the ash is recycled to the slag quench and coal slurrying units. A bleed stream of this water is purged to a treating unit to prevent buildup of ultrafine solids, dissolved metals, ammonia, and traces of other impurities.

The raw gas has an H_2/CO mol ratio of about 0.75:1, whereas for methanol synthesis a more optimal ratio is above 2 (i.e., close to the stoichiometric ratio). A shift reactor is therefore used to adjust the ratio upward by the exothermic water-gas shift reaction:

$$CO + H_2O \rightleftharpoons H_2 + CO_2$$

Use of a sulfur tolerant cobalt-molybdate catalyst enables the shift to be carried out before acid gas removal.

The design adopted aims to maximize heat recovery while providing for effective control of H_2/CO ratio as the catalyst ages and/or gasifier effluent compositions fluctuate. To this end the net particulate-free raw gas is split into two streams. About two-thirds is sent to the shift converter and shifted to give an H_2/CO ratio close to 5. The rest of the gas is bypassed around the shift unit and sent to a COS hydrolysis reactor, where COS is converted to H_2S over an activated alumina catalyst. The shift reaction is exothermic and a substantial amount of high pressure steam is generated by initial cooling of the gas from the converter. An integrated scheme entailing condensate heating and low pressure steam production is provided to recover the maximum amount of the rest of the heat remaining in the shift and hydrolysis reactor products, which are eventually combined and sent to acid gas removal.

The combined cooled gas stream is processed in a Rectisol® unit for acid gas removal. In this process, refrigerated methanol is used to absorb sulfur compounds and carbon dioxide. The absorbed gases are stripped from the methanol in a three-step regeneration entailing pressure letdown, and thermal and nitrogen stripping. This yields two CO_2-rich off-gas streams and an H_2S-rich acid gas stream suitable for sulfur recovery in a Claus plant. One of the CO_2-rich off-gas streams contains substantial amounts of CO and hydrogen and is used as fuel in the boiler plant. The other off-gas stream, consisting primarily of CO_2 and nitrogen, can be discharged directly to the atmosphere. The treated product gas leaves the unit essentially free of sulfur compounds. The system is designed to leave some 3% of CO_2 in the product gas. This represents an optimum level for methanol synthesis, where the CO_2 enhances the activity of the catalyst.

The H_2S-rich stream from the Rectisol® unit is sent to a conventional Claus plant for converting H_2S to elemental sulfur. The chemistry entails the combustion of one-third of the H_2S to SO_2, followed by reaction of the H_2S and SO_2 over an alumina catalyst to form elemental sulfur. The sulfur is produced as a liquid and then is flaked for shipment.

A Beavon process treating unit reduces the sulfur content of the Claus plant tail-gas stream to an environmentally acceptable level and produces additional elemental sulfur. The first step here comprises catalytic hydrogenation of all sulfur species to H_2S. The second step entails use of a Stretford unit to convert the H_2S to elemental sulfur. The Stretford process employs a treating solution containing anthraquinone disulfonic acid and vanadium salts which adsorb H_2S, then promote the oxidation of H_2S to sulfur in an air-blowing operation. Sulfur is separated from the solution as a broth, then filtered and melted to obtain a high purity product. Exhaust gas from the Beavon plant is suitable for discharge to the atmosphere. Overall sulfur recovery in the Claus tail-gas units exceeds 99.9%.

The syngas from the Rectisol® unit contains traces of sulfur compounds and is sent through a sulfur guard system to ensure adequate protection for the methanol synthesis copper-based catalyst. The guard system consists of drums filled with zinc oxide, which is replaced about every six months.

The methanol synthesis units employ ICI "low pressure" technology. The design used comprises a multibed quench converter followed by a single bed adiabatic converter. The nominal operating pressure of the reaction loop is 800 psig, or about 54 atmospheres. The primary reaction is the exothermic hydrogenation of CO to give methanol, namely:

$$CO + 2H_2 = CH_3OH$$

$$\Delta H_{700} = -21.1 \text{ kcal/g-mol}$$

Much of the heat of reaction is recovered as preheat for high pressure boiler feedwater. The water in the product derives from the CO_2 in the syngas. Recent studies confirm that the CO_2 activates the catalyst and is itself converted to methanol, primarily by first undergoing the reverse shift reaction back to CO (487019). In addition to water, some dimethyl ether and higher alcohols comprise the primary impurities.

Syngas is available at pressure and a separate syngas compression stage is thus not needed. Fresh feed from the guard beds is combined with recycle gas and fed to the reactors by the synthesis loop recycle compressor. To limit buildup of the inerts (Ar, N_2, CH_4), gas is purged from the synthesis loop. Because the design purge exceeds the amount of fuel gas needed for boiler fuel, a PSA unit is included to recover hydrogen, which is recycled to the methanol synthesis loop. The residual purge gas is used as boiler fuel.

The crude methanol from the synthesis unit is refined to a fuel grade methanol (99+ wt%) by distilling off water and light ends. Each of the refining units consists of a two-column fractionating system.

For energy efficiency the two columns are designed to operate at different pressure, with the high pressure column overhead serving to reboil the low pressure column bottoms.

The product methanol is stored in floating roof tanks before shipment (by rail or truck).

Process Discussion

Gasification

A key factor in the economics of a slurry fed process such as the Texaco is the attainable solids concentration in the slurry. The dependence of coal and oxygen consumption on slurry concentration was discussed above and illustrated in Figure 6.6. The investment similarly increases as the slurry solids concentration is reduced. For example, reference 472003 presents data on investment and total costs as a function of slurry concentration for a lignite based process; increasing the concentration from 43% to 55% reduced the total investment by some 26%. The present design was based on feeding a 60% solids slurry of Illinois No. 6 coal. This is representative of currently demonstrated technology and thus in effect is a conservative assumption. With additional development, satisfactory operation with slurry concentrations of up to 70% may well be possible for similar coals.

The gasifier design is also keyed to the use of superheating waste heat boilers (WHB's) for extracting heat directly from the high temperature gasifier effluent. Designs under development for such service have yet to be demonstrated as being commercially viable. Alternative designs which use direct water quench to solidify the slag before heat recovery are available. However, with direct water quench, a significant penalty is paid in overall thermal efficiency. To solidify the slag, quenching to about 1600°F is typically required. As Shinaar et al. (472041) illustrate, this can shift the quality of the steam produced to a point where too much low pressure steam, and not enough high pressure steam is produced to supply the drive requirements of the oxygen plant. Additional coal is then needed for power generation. By comparison with the data given in reference 472045, we estimate very roughly that a design with a water quench may require some 10% more coal feed for methanol production. However, the WHB's are of somewhat esoteric design and are costly. Comparative cost estimates given in reference 472138 indicate that the gasifier and gas cooling unit costs would be more than double for a system with superheating WHB's as compared with a water quench design. For a methanol facility, the net investment for the water quench case may be some 5% less when due allowance is made for the extra boilers needed. WHB designs therefore may not always have a clear-cut advantage over the water quench designs, particularly where process steam is needed downstream for the shift reaction.

The pressure level of 915 psig for the gasifiers was set indirectly by considerations relating to oxygen compression, namely, the choice of centrifugal compressors available from existing product lines. This set the oxygen discharge pressure at about 1050 psig. This pressure is somewhat lower than that typically selected for methanol synthesis based on natural gas, but still in the range for a practical design without the need for feed gas compression. The Ruhrkhole/Ruhrchemie pilot gasifiers at Oberhausen have to date only been operated at pressures up to 500 psig. However, with a slurry feed there should be no inherent problem in designing for higher operating pressures. In gasifying hydrocarbons, Texaco partial oxidation reactors typically operate at pressures up to 1200 psig.

If the Cool Water gasifier is successfully demonstrated, the scale-up for the present design would likely be much less than a factor of 2.

Shift, COS Hydrolysis, and Acid Gas Removal

The shift reaction requires steam and is highly exothermic. For good thermal efficiency, therefore, careful integration of the heat balance with upstream and downstream processes is needed. There are choices of shifting before or after sulfur removal, in varying the fraction of gas to shift, in selecting the shift temperature(s), and in matching the operation to alternative acid gas removal processes. Many possible schemes thus exist. The optimum one depends on individual circumstances and its selection may not be clear-cut.

In the present study, Rectisol® acid gas removal schemes are used both in the partial oxidation designs of Section 5 and the gasification scheme evaluated here. The arrangement of the shift/acid gas removal sequence however, is different in each case. The selection was keyed more to the availability of a set of consistent design and cost data for each case, than to the intrinsic merit of the schemes themselves. Evaluation of the latter is outside the present scope. However, we feel that the overall economics are only marginally affected by the specific arrangement selected, and that the choice is not critical for this study.

The present scheme, which shifts before removing sulfur, aims to maximize heat recovery, is environmentally sound, and uses in essence demonstrated technology. It should, therefore, be conservatively representative for the general case. Although the Rectisol® process is capable of COS removal, a more complex and expensive design is needed if most of the COS is to report with the H_2S-rich gas fed to the Claus unit. A COS hydrolysis unit is therefore included to convert COS to H_2S in the gas bypassed around shift conversion. Because hydrolysis of COS occurs over the shift catalyst, a separate stage for COS conversion is not needed for the shifted stream.

Methanol Synthesis and Refining

ICI methanol technology, one of the two leading commercial technologies, was selected for the evaluation on the basis of convenience. Costs for a design utilizing Lurgi technology would be expected to be very similar.

For production of 10,000 metric tons/day methanol, the design consists of four trains. Each train is somewhat larger than the largest built to date, but is considered to be within the limits for conventional design. Field fabrication of the reactors would be required.

The two-column purification system rejects water to a level of less than 1% and produces a methanol product suitable as turbine fuel. The methanol contains a small amount of other impurities, and does not meet the U.S. specification for chemical grade methanol. However, it is likely to be more than pure enough to serve as feedstock for many of the proposed methanol based chemical syntheses noted in Section 3. Purification of raw methanol streams is discussed in Section 4, where some differential cost data are presented. The incremental capital cost for purification is seen to be relatively small, while the incremental production cost hinges on the value assigned to the low level energy used in the distillation.

Cost Estimates—Methanol from Coal

Capital Investment

The cost estimates presented here are, as discussed above, based primarily on data developed for the Electric Power Research Institute (EPRI) by Fluor Inc. (472120).

The total fixed capital (TFC) breakdown for a 10,000 metric tons/day methanol-from-coal facility is shown in Table 6.11 together with scaled-down costs for smaller capacities. An across-the-board contingency of 25% is included in the TFC. (In the EPRI study, process and project contingencies were allocated individually to each section, and in the final analyses these amounted to some 26% of the total.)

Our cost numbers are for a U.S. Gulf Coast location, assuming "instant construction" as at mid-1981 (PEP Cost Index = 400). It is estimated that in practice from date of order to completion would take some 5 years, with cumulative cash expenditures as follows:

Table 6.11

METHANOL FROM COAL

TOTAL FIXED CAPITAL

Location: U.S. Gulf Coast
PEP Cost Index: 400 (mid 1981)

	Capacity (metric tons/day)		
	10,000	2,500	625
Investment (million $)			
Coal storage and preparation	21	8	3
Air separation	264	75	24
Gasification and heat recovery	260	91	34
Shift and COS hydrolysis	42	13	5
Acid gas removal	132	35	13
Sulfur recovery	21	6	2
Methanol synthesis and refining	126	34	12
	866	262	93
Contingency, 25%	216	65	23
BATTERY LIMITS INVESTMENT	1,082	327	116
Steam and power generation	56	16	6
Other utilities	46	5	1.5
Storage	19	12	4.5
General service facilities	71	41	23
	192	74	35
Contingency, 25%	48	19	9
OFF-SITES INVESTMENT	240	93	44
TOTAL FIXED CAPITAL	1,322	420	160

Year	Cumulative % Cash Expended
1	10
2	30
3	60
4	80
5	100

Our TFC does not include land, start-up costs, or working capital. Royalties are also excluded (they are estimated to amount to some 0.3%).

The number of trains making up each unit in a 10,000 metric tons/day methanol facility is given above in Table 6.8. Information on the number of gasifiers included in the design was not published. However, in previous studies for EPRI (472138, 472016) entailing similar Texaco gasification schemes, the gasifier designs were for processing about 2,000 metric tons/day coal at somewhat lower pressures. For scale-down, we therefore assumed that eight gasifiers and one spare were used for the 10,000 metric tons/day base case. The minimum number of gasifiers at lower capacities was taken as two, plus one spare.

Costs for plant capacities below 10,000 metric tons/day methanol were obtained by applying scaling exponents to each section. For reduction in the number of trains in a given unit, we used a 0.95 exponent; for reduction in the size of a given train, the exponent was taken as 0.75 down to 1/8 of the scale, and 0.7 below that. An exception here was the scaling down of the general service facilities, for which an exponent of 0.4 gave more realistic results. The exponents noted above are broadly in line with the considerations given in Section 8 of PEP Report 119, Construction Costs. The resulting overall scaling exponents for the complete facility are shown in Table 6.12. The TFC requirements per daily metric ton of methanol are illustrated in Figure 6.9. It is seen that the capital requirements per metric ton rise very rapidly at capacities much below 5,000 metric tons/day.

The variation of total capital requirements with capacity is illustrated in Figure 6.10. The data points are given in Table 6.12.

Table 6.12

METHANOL FROM COAL

INVESTMENT AS A FUNCTION OF CAPACITY

Capacity (metric tons/day)	Battery Limits Investment (million $)	Off-sites Investment (million $)	Total Fixed Capital (million $)	TFC per Daily Ton ($1,000)	Capacity Exponent for Scale-down of TFC
10,000	1,082	239	1,322	132	0.86
5,000	580	147	727	145	0.79
2,500	327	93	420	168	0.75
1,250	188	62	250	200	0.64
625	116	44	160	256	—

The percentage breakdown of the battery limits investment for the 10,000 metric tons/day facility is shown below:

	Million $	%
Coal storage and preparation	21	2.4
Air separation	264	30.5
Gasification and heat recovery	260	30.0
Shift and COS hydrolysis	42	4.8
Acid gas removal	132	15.2
Sulfur recovery	21	2.4
Methanol synthesis and refining	126	14.5
Subtotal	866	100.0
Contingency (25%)	216	25.0
Battery limits investment	1,082	125.0

Figure 6.9

METHANOL FROM COAL

Variation of Unit Capital Requirements with Scale

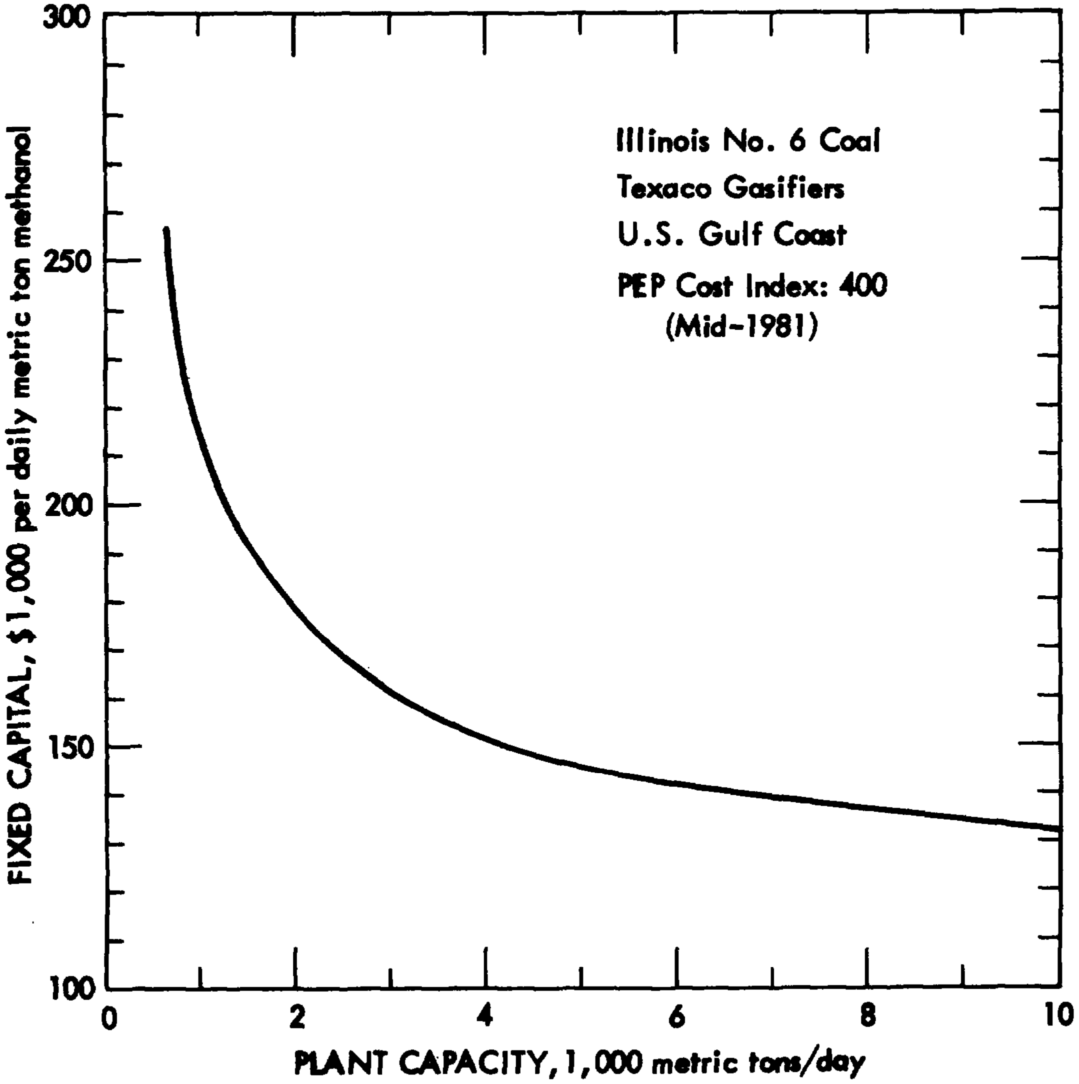
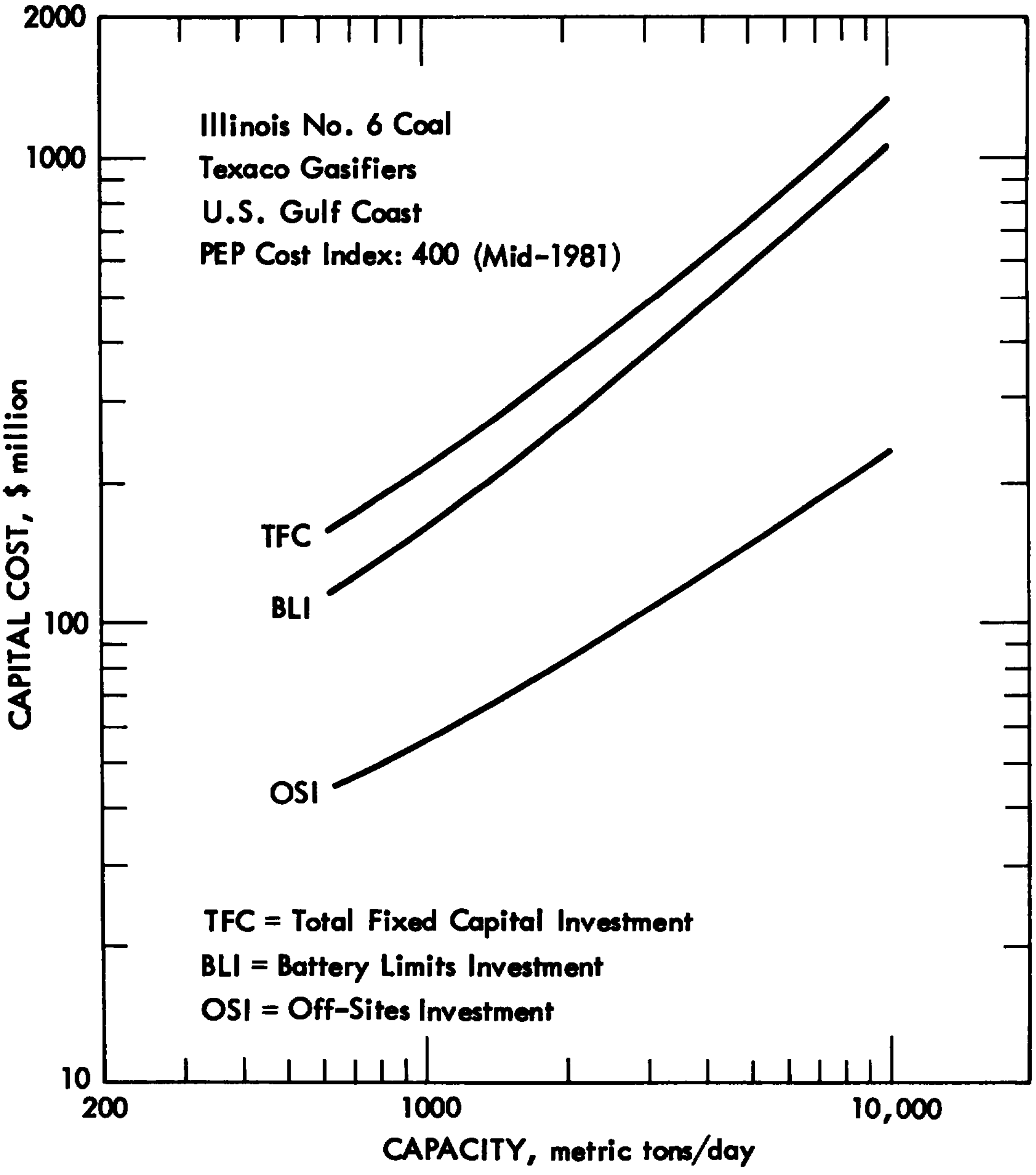


Figure 6.10

METHANOL FROM COAL

Variation of Capital Costs with Capacity



It is seen that the gasifier and the facilities for heat recovery and particulate cleanup directly associated with it comprise about one-third of the battery limits investment. However, for any given coal, the gasifier selection also indirectly determines the selection and design of much of the equipment in the rest of the facility.

Production Costs and Product Value

The production costs for various capacities are shown in Table 6.21 at the end of this section. They are presented in the traditional format based on a single year, with a standard allowance for depreciation and pretax return on investment (ROI). The estimates are for the U.S. Gulf Coast in mid-1981.

As discussed above, the methanol plant designs evaluated are self-sufficient in all utilities except for clarified water. For the illustrative economics shown in the tables, the price of Illinois No. 6 coal is taken as \$32.3/metric ton (\$29.4/short ton) at the mine, with an allowance of \$15.0/metric ton for transport to the Gulf Coast. The total price therefore breaks down as follows:

	\$/short ton	\$/metric ton	\$/MM Btu
Coal at mine	29.4	32.3	1.3
Transport to site	13.6	15.0	0.6
Total	43.0	47.3	1.9

i.e., a delivered price of 1.9 \$/million Btu (HHV basis).

A cost of \$5.00/metric ton (dry basis) is allowed for the transport and disposal of ash off-site.

A credit of \$100/metric ton is allowed for the sulfur recovered from the acid gases. The facility also vents very large quantities of CO_2 and some nitrogen. In certain circumstances these products also have value, but are given no credit here.

It is assumed that the annual variable costs decrease in direct proportion to the capacity of the plant, i.e., remain the same per unit of product irrespective of capacity or stream factor. In practice this would not hold quite true and these costs will be somewhat higher at the lower capacities and stream factors. However, because our prime concern here is with the gasification economics at the larger capacities, the approximation was considered acceptable.

The production cost calculations shown are based on the PEP standard stream factor of 0.9. This corresponds to 328.5 days' operation per calendar year, or some 5 weeks' total downtime for maintenance.

For the prototype versions of the coal based plants, this is likely to be an optimistic assumption. However, for mature plants and adequate sparing, stream factors should be attainable which are comparable with those of existing petrochemicals plants based on gas and liquid feedstocks. Because the production from coal based plants is capital intensive, production economics are very sensitive to downtime (see also below).

To reflect the higher levels of maintenance expected with coal based plants, maintenance costs are taken as 4% of the battery limits investment (BLI) and divided 40% labor and 60% materials. This compares with the value of 3% of BLI used for the natural gas based processes in Section 4.

The coal based plants also have a much higher operating and maintenance labor force at a given production capacity. However, the administrative and support labor costs do not increase in direct proportion. The plant overhead for the coal based plants is estimated at about 30% of operating and maintenance labor, compared with the PEP standard of 80% for petrochemical plants. The general and administrative (G&A), sales and research costs are taken as 5% of the main product value, in line with PEP standards for bulk chemical products.

A traditional charge for depreciation of 10%/yr of the total fixed capital (TFC) is included in the production cost. A 25%/yr return on the TFC is then added to the net production costs to arrive at a product value (PV). The PV used here for comparison is thus equivalent to the initial sales price that would be needed to give a 25%/yr simple return on the TFC, before tax. The PV's for production of methanol from coal are shown in Table 6.21, and the variation with capacity is illustrated in Figure 6.11.

Before we look at the trends, some comments on the rationale of comparisons in terms of PV's seem worthwhile.

ROI and Profitability

As a general yardstick for comparison of the overall economic attractiveness of competing processes, PEP uses the concept of a product value, i.e., a unit production cost plus an annual capital charge. The capital charge traditionally included by PEP has been a simple 25%/yr before-tax return on total fixed capital (TFC), sometimes loosely referred to as a "25% ROI." We feel that it remains an adequate and preferred measure for the types of comparisons being made in this study. In contrast, much of the published work dealing with coal gasification economics has recourse to complex criteria for return on capital invested, and often places great emphasis on "creative" financing arrangements to lower the cost of capital.

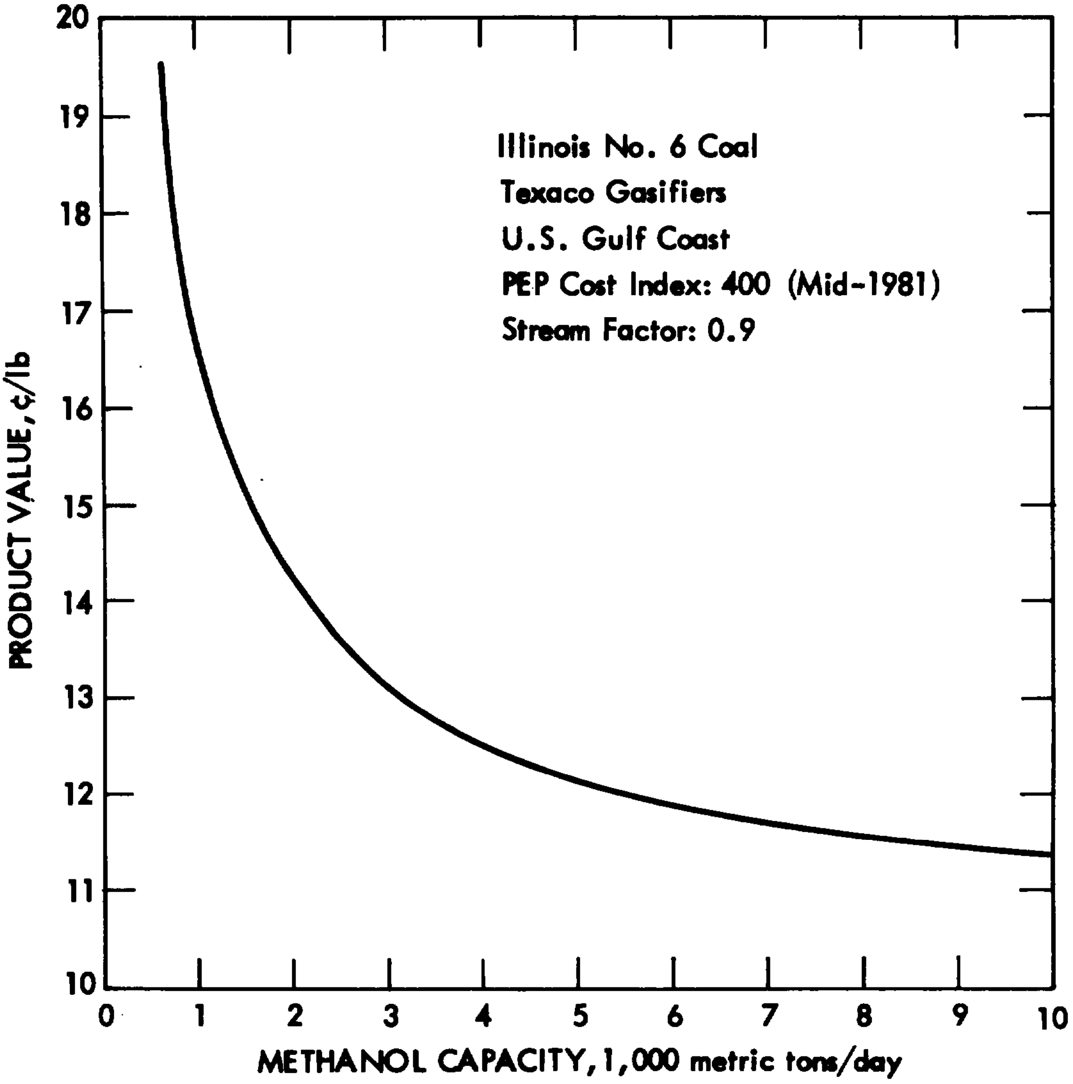
Because the coal based plants require large amounts of capital per unit of production, the level of return required on that capital is a key factor determining the competitiveness of such plants. Availability of low cost financing will thus obviously result in lower revenue requirements. Similarly any investment credits and accelerated depreciation allowed for tax purposes would have a very significant impact on the price required for the product. For any specific project, therefore, a detailed analysis of the projected cash flow picture as a function of possible financing arrangements is indispensible.

The aim of this study, however, is to provide cost numbers for general screening level evaluations and projections. A prime advantage of using a capital charge based on a simple ROI is in fact

Figure 6.11

METHANOL FROM COAL

Product Values



the simplicity of the approach. It is unambiguous, easily calculated, and readily understood. For a set of projects in which the associated parameters such as construction periods, capacity buildup rates, etc., are comparable, the correlations between the discounted-cash-flow (DCF) yields and the ROI will be very similar for all of the projects. For such projects comparisons in terms of ROI mirror closely the comparisons in terms of DCF yield. For gas- versus coal-based plants, construction periods and other constraints will differ, and a given ROI will not represent quite the same DCF yield in each case. However, the correlation is expected to be close enough in general to justify retaining the simple ROI yardstick as a realistic measure of profitability.

The level of return on capital that should be expected is, of course, open to debate. For the constraints associated with a typical petrochemical plant, the cash flow represented by a 10%/yr depreciation allowance and a 25%/yr pretax ROI generally is equivalent to a DCF yield of 12-17%. To aim for 15% yield on a constant dollar basis used to be traditional for screening level analyses of petrochemical projects. In recent times expectations have perhaps diminished. For a risky project such as a coal based facility, a higher than average return on equity might normally be allowed for. However, many of the published analyses base project value calculations on real yields on capital of less than 10%/yr.

Discussion of Costs

In our judgment the screening level costs presented here are likely to be representative of the costs associated with large coal conversion plants that could be operating by the end of the decade. The accelerated development work and the many studies on the topic in recent years bring such estimates into more realistic focus. However, since substantial development during the start-up may be needed for prototype commercial facilities, higher contingencies than included here should be allowed for first-time plants.*

The base case economics are for a facility producing 10,000 metric tons/day of methanol. This is roughly the amount of methanol that would be needed for two 750 million lb/yr ethylene plants based on the Mobil Zeolite process. If used as fuel, the methanol would be equivalent to about 37,000 barrels/day of oil. In terms of technology the scale is substantial but not excessive. However, it should also be noted that the base case plant size exceeds the total in-place methanol capacity in the United States in 1980, and obviously does not relate to present day chemical usage.

Scaling down of costs by means of exponents becomes increasingly uncertain as the ratio of capacities increases. In the present instance, therefore, the absolute cost numbers should be considered as increasingly tentative below the 2,500 metric tons/day level. However, the trend is clear. In the longer term plants of capacities much below 5,000 metric tons/day methanol equivalent are unlikely to be competitive for the production of feedstocks for bulk chemicals manufacture.

The calculations are shown for a stream factor of 0.9, i.e. 328.5 operating days/yr. The product value would increase sharply if the amount of downtime increased, for example:

Stream Factor	Operating days/yr	Product Value for 10,000 metric tons/day ¢/lb	¢/U.S. gal	$/metric ton	$/MM Btu
0.9	328.5	11.4	75	251	11.7
0.7	255	13.7	90	303	14.0
0.5	182.5	18.0	119	396	18.4

---

*Continuing evaluation of gasification designs and discussions with industry lead us to believe that these costs may be somewhat on the optimistic side even for more mature plants. In the computerized data base (see Section 2) we have therefore allowed for a more conservative design which increases these estimates by about 20%.

The cost components of the base case product value of 11.4¢/lb can be segregated as follows:

	¢/lb	%
Coal-related costs	3.2	28
Labor-related costs	1.1	10
Capital-related costs	7.1	62
	11.4	100

The present analysis and the above breakdown is keyed to a relatively high coal price (by U.S. standards), and U.S. Gulf Coast construction costs. The sensitivity of the product value to coal price and capital is shown in Figure 6.12.

Whether a location at the mine would show better economics can only be determined in a given case. The product value is much more sensitive to capital costs than to coal price, and costs of construction at the mine are generally likely to be significantly higher. In addition, there are costs of transport for the product which could approach those of transporting the coal. In the illustrative numbers presented here about 1/3 of the coal-related cost comprises coal transport. If, for example, the coal price is reduced by 1/3, and the capital charges increased by 15%, the product value remains unchanged. The location factor could well be in excess of 1.15 for a plant at the mine, particularly if there is substantial expense for infrastructure. In such a case, therefore, the U.S. Gulf Coast economics would look better.

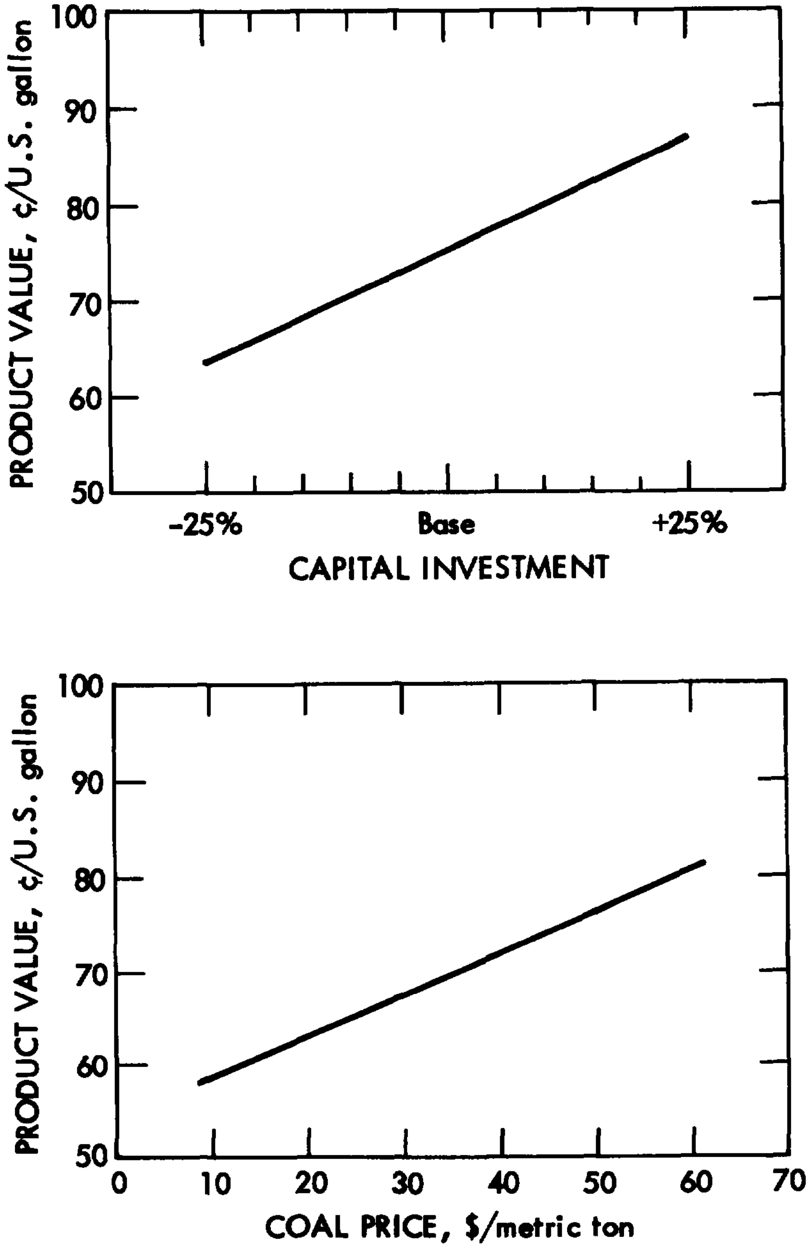
For some comparisons of costs of product from coal based with costs from gas and oil based facilities, refer to Section 2.

The present study did not examine in any detail capital requirements for facilities based on other types of gasifiers or other types of coals. However, some very approximate guidelines are noted below.

Figure 6.12

SENSITIVITY OF METHANOL PRODUCT VALUE TO CAPITAL INVESTMENT AND COAL PRICE

10,000 metric tons/day Methanol
Mid-1981, U.S. Gulf Coast
Texaco Gasifiers



For facilities based on dry-feed entrained flow gasifiers, such as the Shell-Koppers, somewhat higher overall thermal efficiencies and lower capital costs would be expected than for facilities based on slurry-fed gasifiers. Some screening work done at SRI indicates that savings of about 5% in both coal consumption and capital investment might be achieved by dry feeding when gasifying a bituminous coal such as the Illinois No. 6. As regards other widely available U.S. coal types, the following approximate factors were estimated for a methanol facility based on a dry-feed gasifier:

Coal*	Relative Capital for Coal-to-Methanol Facility	Relative Coal Consumption†		Typical Coal Price at Mine ($/Metric Ton)
		HHV Basis	Weight Basis	
Illinois No. 6	1.00	1.00	1.00	32
Powder River subbituminous	0.98	0.93	1.25	10
Texas lignite	1.13	1.05	1.66	15

---

*See Table 6.4 for compositions.

†On an as-received basis including ash and moisture.

Of these three types, the Powder River coal thus appears to be inherently best suited for dry feed, entrained flow gasification. Both the Powder River subbituminous and the Texas lignite have high intrinsic moisture levels which make them unattractive for slurry-fed gasifiers. For the latter, subbituminous coals with a much lower moisture content would probably be an optimal choice.

Some rough comparisons with methanol facilities based on other types of gasifiers can be made using the data published by Brown and Hargreaves of Humphries & Glasgow Ltd. (472045). In that study screening designs and estimates were made for production of 1,000 metric tons/day of methanol from a subbituminous coal in facilities based on four types of gasifier. The facilities were designed to feed a 50 wt% solids slurry and use a water quench to cool the gasifier effluent.

Private communication with the authors indicates that the estimate for this unit was somewhat low. Making some approximate adjustments to allow for the above differences in comparison with the present design we arrive at the following:

Process	Relative Coal Consumption	Relative Capital for Coal-to-Methanol Facility
Koppers-Totzek	1.57	1.4
Winkler	1.31	1.3
BGC/Lurgi Slagger	1.25	1.2
Texaco 50% slurry, water-quench	1.27	1.1
Texaco 60% slurry, WHB	1.00	1.0

The factors illustrate the penalty for gasification at close to atmospheric pressure, viz, the K-T and Winkler systems. The BGC/Lurgi Slagger is not inherently well suited for methanol or syn gas production because of its high methane make. Given that the K-T and Winkler systems are commercially proven, the numbers also serve to set in better perspective the likely economics at the present and projected state of the art.

Derived Cost Modules

To obtain the economics of producing syngas rather than methanol from coal, we divided the flow sheet for the methanol unit described above into sections and allocated the capital and utilities to each of the sections. The shift and acid gas removal sections were then scaled to estimate costs for various H_2/CO ratios in the product gas. To estimate the costs of producing hydrogen, we modified the design to also include a two-stage low temperature shift unit following the high temperature shift, plus a methanation stage following acid gas removal.

Some of the many rationales for allocating costs to the various sections are discussed below, together with an outline of what we did here. The net result here was that a methanol-from-syngas module became in effect a small exporter of high pressure steam, while the syngas-from-coal and hydrogen-from-coal modules became net importers of high pressure steam. The hydrogen facilities produced a surplus of low pressure steam for which no credit was taken in the present calculations. With the present base case design—which entails some quench cooling, a sulfur tolerant high temperature shift, and COS hydrolysis—the shifting of the raw gas to higher H_2/CO ratios was estimated to result only in rather marginal increases in overall capital and production costs. The major influence on costs is the scale of production.

Rationale for Cost Allocations

In estimating the costs of the syngas production steps (gasification; shift, if any; and purification) there are two broad options: either design and cost an independent unit ("stand-alone module") that produces syngas of a certain specification, or design an integrated facility in which an identical syngas is used as an intermediate stream, and allocate costs to the syngas portion of the process ("cut-out module"). The answers will differ.

The reason for the differences is that both the syngas generation process and the typical user processes operate at elevated temperatures and produce large amounts of heat. Normally, substantial compression is required in each portion of the process. The way that the heat recovery and power production are integrated makes significant differences in the overall thermal efficiency of the total process, as well as in the capital requirements. To some extent the method of integrating depends not only on the end product but also on the scale of operation.

There appears to be no clear-cut advantage to either the stand-alone or the cut-out module costing options for the generalized case. Also the best means of allocating value to the heat content of streams crossing the boundaries of a given module is somewhat moot. However, provided the design and cost allocations are made judiciously, either approach should yield costs which are satisfactory for general screening purposes. For a higher order of accuracy there is no alternative but to include customized syngas generation in any given user process.

In the present study we have used both stand-alone and cut out modules. The criteria for choosing were somewhat subjective, with the least complicated option normally being given preference. Thus in Section 4, stand-alone modules were designed for syngases of various ratios produced from natural gas, while the raw syngas costs were cut out from an integrated natural gas-to-methanol design.

In the present section, the syngas cost data are derived from the integrated methanol-to-coal design described above. Given below is a very general outline of how the syngas and methanol production steps are integrated, and how costs are allocated to separate syngas and methanol modules.

The coal-to-methanol plant is designed so that heat and power requirements are in overall balance. (See Table 6.7.) High level process heat from the shift and gasification units is recovered as 1500 psig steam. The waste heat boilers in the Texaco unit superheat this steam to 900°F. These sources furnish close to 90% of the total steam requirement for electric power generation (in a turbogenerator) and for mechanical drives for the process equipment including the air, oxygen, and methanol compressors. The remainder of the prime steam is raised in gas fired boilers which burn purge gas from the methanol synthesis unit and gas or methanol during start-up.

The utilities requirements for the methanol synthesis and purification units are also shown in Table 6.7. Integration with the rest of the plant is as follows:

- The product stream from the methanol synthesis reactor preheats the boiler feedwater which goes to generate the high pressure steam. The heat input of 750 million Btu is equivalent to some 20% of the total heat input to the high pressure steam.
- Low pressure steam (100 psig and 50 psig) supplies heat for the methanol purification columns.
- 600 psig extraction steam from the turbogenerator supplies the intermediate pressure level demands, which include the turbine drive of the methanol recycle compressor. (See Figure 6.8 above.)
- Purge gas from methanol synthesis is used to fire package boilers raising high pressure steam. In terms of heating value it could alternatively produce medium pressure steam (600 psi) somewhat in excess of that needed to drive the methanol recycle compressors.

Methanol-from-Syngas Unit

The methanol unit is separated from the complex as follows:

The heat for export as high pressure BFW preheat is first reduced by the amount of heat imported as low pressure steam. Such a trade-off is not unreasonable given the overlap of temperature levels. The balance of this heat is then credited to the methanol unit at the value of the high pressure steam that is ultimately produced from the BFW stream. The rationale for using such a "phantom steam" credit is that it is more likely to reflect the actual end result than any other allocation.

The 600 psi steam requirement for the recycle compressor drive is taken to be supplied directly from the purge gas boilers (at 85% efficiency), while the balance of the purge gas heating value is credited as high pressure steam.

The value used for crediting high pressure (1500 psi, 900°F) steam for transfer purposes is estimated as $7.73/1,000 lb on the basis of firing coal. (See Table 6.13.)

Inside the battery limits, the high pressure boiler feedwater heater was included with the methanol unit. The utilities and offsites were prorated according to battery limits capital, except as follows: methanol storage and shipping were allocated to the methanol unit; capital for the purge gas boilers was estimated and allocated to the methanol unit.

Syngases of Various H_2:CO Ratios, and Hydrogen

For syngas with H_2/CO ratios different from that of the methanol syngas, we adjusted the split between shift and COS hydrolysis to give the desired overall H_2/CO ratio. Production of hydrogen represents a limiting case in which all of the raw gas is sent to the high temperature shift and no COS hydrolysis stage is used. For hydrogen, a low temperature shift and a methanation stage were also added to the design. In the other limit, all of the raw gas ($H_2/CO = 0.74$) is processed in the COS hydrolysis unit and the shift reactors are eliminated entirely.

A breakdown of costs as between the shift and hydrolysis sections was estimated and the costs scaled in proportion to flow rates. Because of the requirement for COS hydrolysis, the capital savings resulting directly from elimination of the shift reactors are relatively minor. More substantial savings associated with the elimination of the shift reaction result indirectly from the decrease in acid gas removal requirements. For present purposes very approximate estimates of the change in the capital and operating costs for the latter were made by assuming that the cost changes would be proportional to the

Table 6.13

HIGH PRESSURE STEAM PRODUCTION COST

Steam: 1500 psig, 950°F
Capacity: 500,000 lb/hr
Boiler: Pulverized coal fired
PEP Cost Index: 400
Reference: PEP Report 136, p. 156

Total Fixed Capital (TFC): $38.2 million

	$1,000/yr	$/1,000 lb
Labor		
Operating (17.50 $/hr, 4/shift)	614	
Maintenance (2% TFC)	764	
Control lab (20% op. labor)	123	
Total labor	1,501	
Materials		
Chemicals	46	
Maintenance (2% TFC)	764	
Operating (10% op. labor)	61	
Total materials	871	
Utilities		
Boiler feedwater	249	
Electricity (3.6¢/kwh)	1,204	
Coal ($1.90/million Btu)	11,339	
Total utilities	12,792	
Plant overhead (80% total labor)	1,200	
Total operating costs	16,364	4.15
Taxes and insurance (2% TFC)	764	
Depreciation (10% TFC)	3,820	
Total capital charges	4,584	1.16
Op. costs and cap. charges	20,948	5.31
25% ROI	9,550	2.42
PRODUCT VALUE	30,498	7.73

average of the factors by which the acid gas flow (CO_2 + H_2S) and the total gas flows to acid gas removal had changed.

Because the heat balance of the integrated facilities is fairly complex, we made some approximations and simplifications in modifying the base case design. High pressure steam is a key factor.

In the base case design for methanol syngas ($H_2/CO = 2.26$) the heat produced in the high temperature shift reaction is used to raise HP steam, and the complex is in overall utilities balance. Cutting back on the amount of shift (cases in which $H_2/CO \leq 2.0$), therefore, results in an HP steam debit, and increasing the amount of shift (for hydrogen) gives an HP steam credit. Steam is also needed for the shift reaction itself and is provided by saturating the shift feedstream at the quench stage. As a conservative approximation we did not take any HP steam credit for potential savings here as the amount of shift is cut back (for $H_2/CO \leq 2.0$ cases), but did allow an equivalent HP steam debit for increased quench requirements (when making hydrogen).

The net result is that the HP steam requirement is not overly sensitive to the fraction of raw gas shifted. This is in contrast to what happens in the type of shift/acid gas scrubbing arrangement used in the partial oxidation design of Section 5. There, the raw gas undergoes sulfur removal before shift and is thus cooled and dried. For shifting, addition of HP steam to the reactor feed is therefore necessary, while none of the heat in the reactor product is recovered as HP steam. The HP steam required then increases in direct proportion to the fraction of raw gas shifted. To compensate, such an arrangement simplifies acid gas removal and sulfur recovery.

The net changes in the overall heat balance for the acid gas removal section resulting from the design variations are relatively much smaller; we made some rough trade-offs to simplify the picture. These included balancing out fuel gas debits with 600 psi steam credits, and balancing out some steam requirements irrespective of pressure level. The inaccuracies introduced will have but minor effect on the overall syngas economics.

In the hydrogen design there is also an excess of low pressure steam produced from both the high and low temperature shift units. In the illustrative calculations below, this is shown as a low pressure steam equivalent, but is credited at no value.

Capital requirements were scaled on the basis of total gas flow rates for the shift section. For the acid gas removal section the average of the acid gas and total gas flow ratios was used as a scaling parameter. For hydrogen production, costs were also estimated for a low temperature shift unit and a methanation unit and added to the modified battery limits investment.

Adjustments were made to the utilities and off-sites capital in proportion to the changes in the battery limits investment.

1. Methanol Syngas from Coal (Module 13)

This module comprises the front end of the methanol-to-coal complex described above. The product is a clean syngas with an H_2/CO ratio of 2.26 containing about 3 vol% of carbon dioxide and available at 53 atmospheres. (See stream 12 in Figure 6.7 and Table 6.6.) For consistency with the other modules the costs are expressed on the basis of the H_2 and CO contained in the gas.

The capital requirements are shown in Table 6.14 and Figure 6.13. The battery limits investment (BLI) for the syngas module comprises some 85% of the BLI for the methanol complex.

Table 6.14

METHANOL SYNGAS FROM COAL

INVESTMENT AND PRODUCT VALUE AS A FUNCTION OF CAPACITY

Capacity		Capital (million $)			
Million scfd of Contained CO + H_2	Metric Tons/Day Methanol Equivalent	Battery Limits Investment	Off-sites Investment	TFC	Product Value (¢/mscf)
805.3	10,000	924	178	1,102	278
402.6	5,000	498	110	608	297
201.3	2,500	285	73	358	334
101	1,250	165	50	213	382
50	625	100	36	136	467

The product value for a production capacity of 805 million scfd of contained carbon monoxide and hydrogen is estimated at 278¢/1,000 mscf or $104/1,000 Nm^3. This breaks down approximately as follows:

Cost Component	¢/mscf	%
Coal related	88.2	32
Labor related	25.2	9
Capital related	162.6	58
Miscellaneous	2.4	1
Total	278.4	100

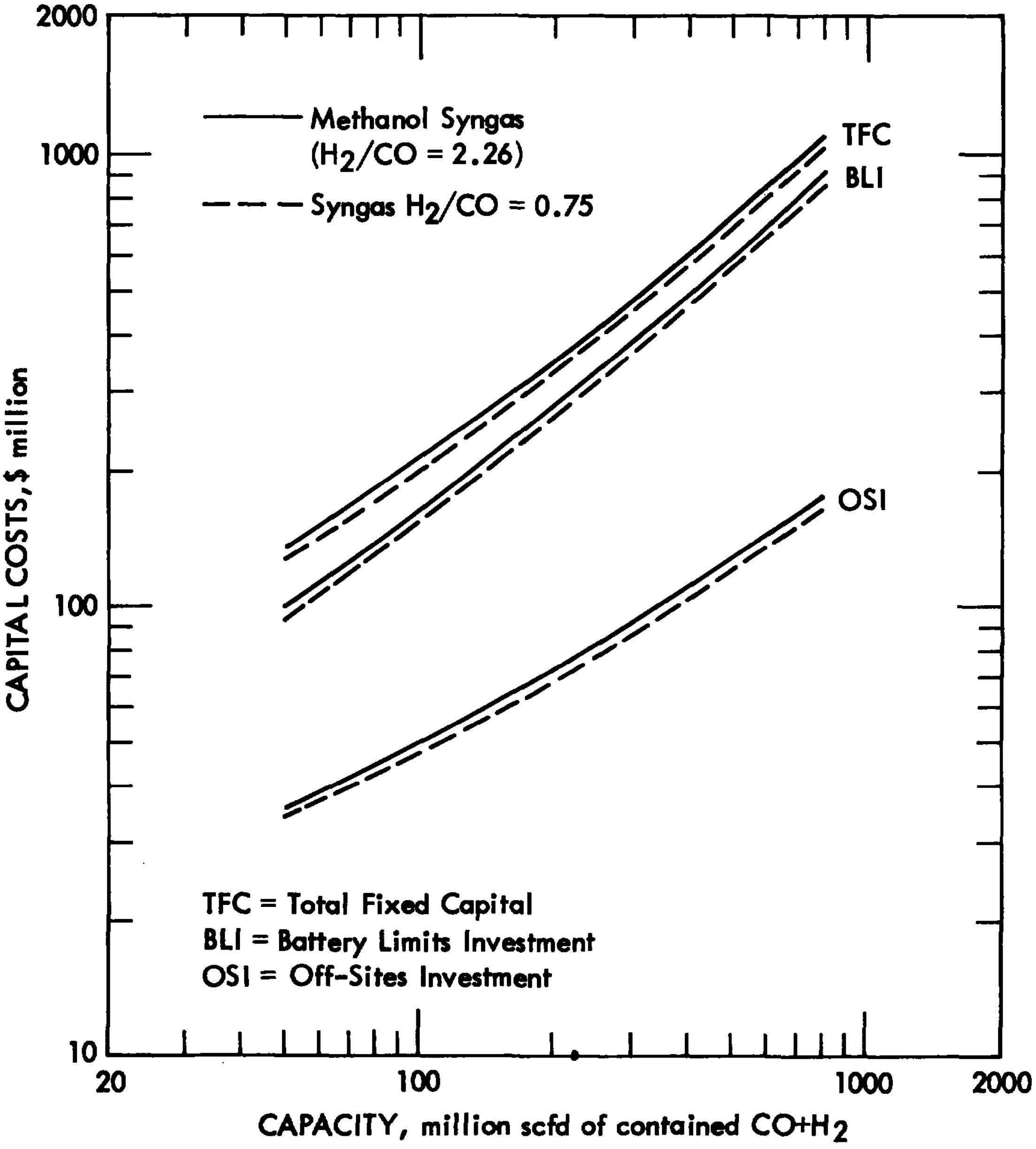
The product value of the syngas comprises close to 90% of the product value of the methanol produced from it. The considerations relating to plant design, scale-up, production cost parameters, etc., are essentially the same as those discussed in relation to the overall methanol complex above.

Detailed breakdowns of the production costs and product values are shown in Table 6.22 at the end of this section. Product values are

Figure 6.13

SYNGAS FROM COAL
Variation of Capital Costs with Capacity

Illinois No. 6 Coal
Texaco Gasifiers
U.S. Gulf Coast
PEP Cost Index: 400 (Mid-1981)



also plotted as a function of capacity in Figure 6.14, and summarized in Table 6.14.

The allowance for G&A, sales, and research costs is taken at 5% of the syngas value, i.e., the same as for the methanol estimates. This contrasts with the 3% allowance used in the syngas cost estimates further below. The G&A allowances are to some extent arbitrary, and the rationale here was to keep with the standard PEP conventions which class methanol and hence methanol syngas as a commodity, and syngas per se as a captive chemical.

2. Methanol from Coal-Derived Syngas (Module 27)

This module comprises the cut-out methanol synthesis and purification sections, i.e., the tail-end of the methanol-to-coal complex described above. Adding together this module and the methanol syngas module (13) thus gives the costs for production of methanol from coal.

The capital requirements are shown in Table 6.15, and Figure 6.15. The battery limits investment (BLI) for the methanol synthesis and purification accounts for some 15% of the BLI for the total methanol complex.

Table 6.15

METHANOL FROM COAL-DERIVED SYNGAS

INVESTMENT AS A FUNCTION OF CAPACITY

	Capital (million $)		
Capacity Metric Tons/Day	Battery Limits Investment	Off-Sites Investment	TFC
10,000	158	62	220
5,000	82	37	119
2,500	42	20	62
1,250	25	12	37
625	16	8	24

Figure 6.14

METHANOL SYNGAS ($H_2/CO = 2.26$) FROM COAL

Product Values as a Function of Capacity

Illinois No. 6 Coal
Texaco Gasifiers
U.S. Gulf Coast
PEP Cost Index: 400 (Mid-1981)
Stream Factor: 0.9

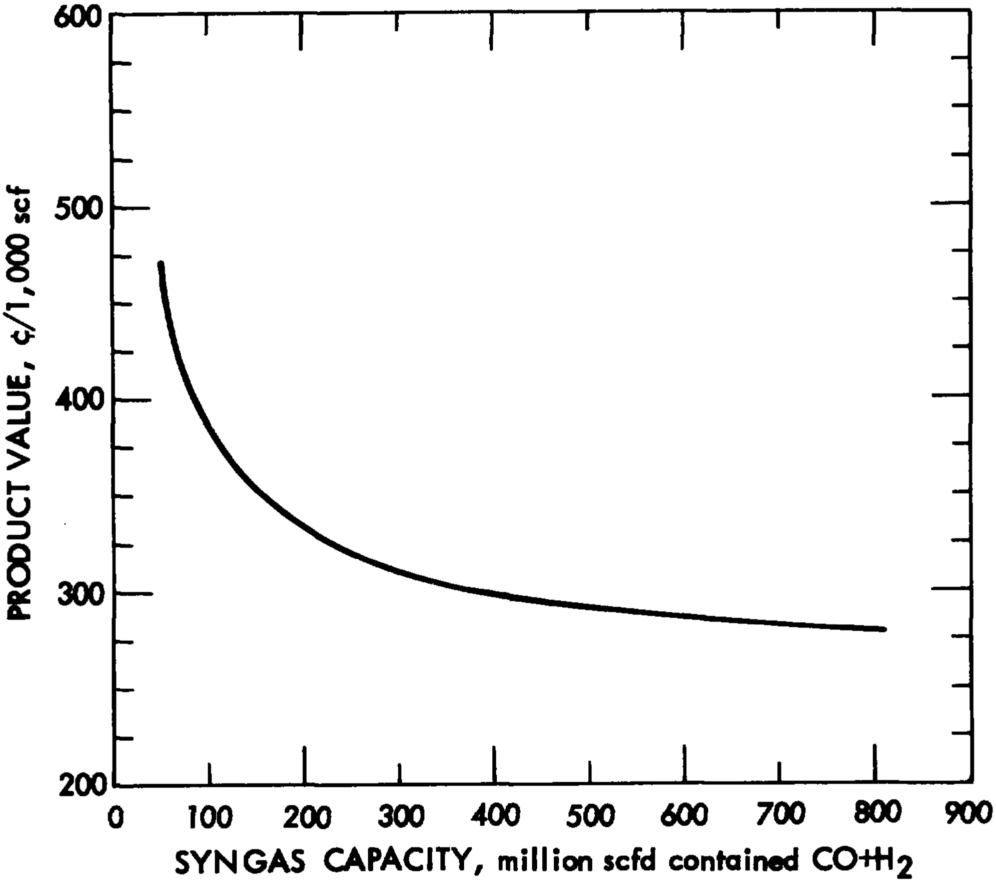
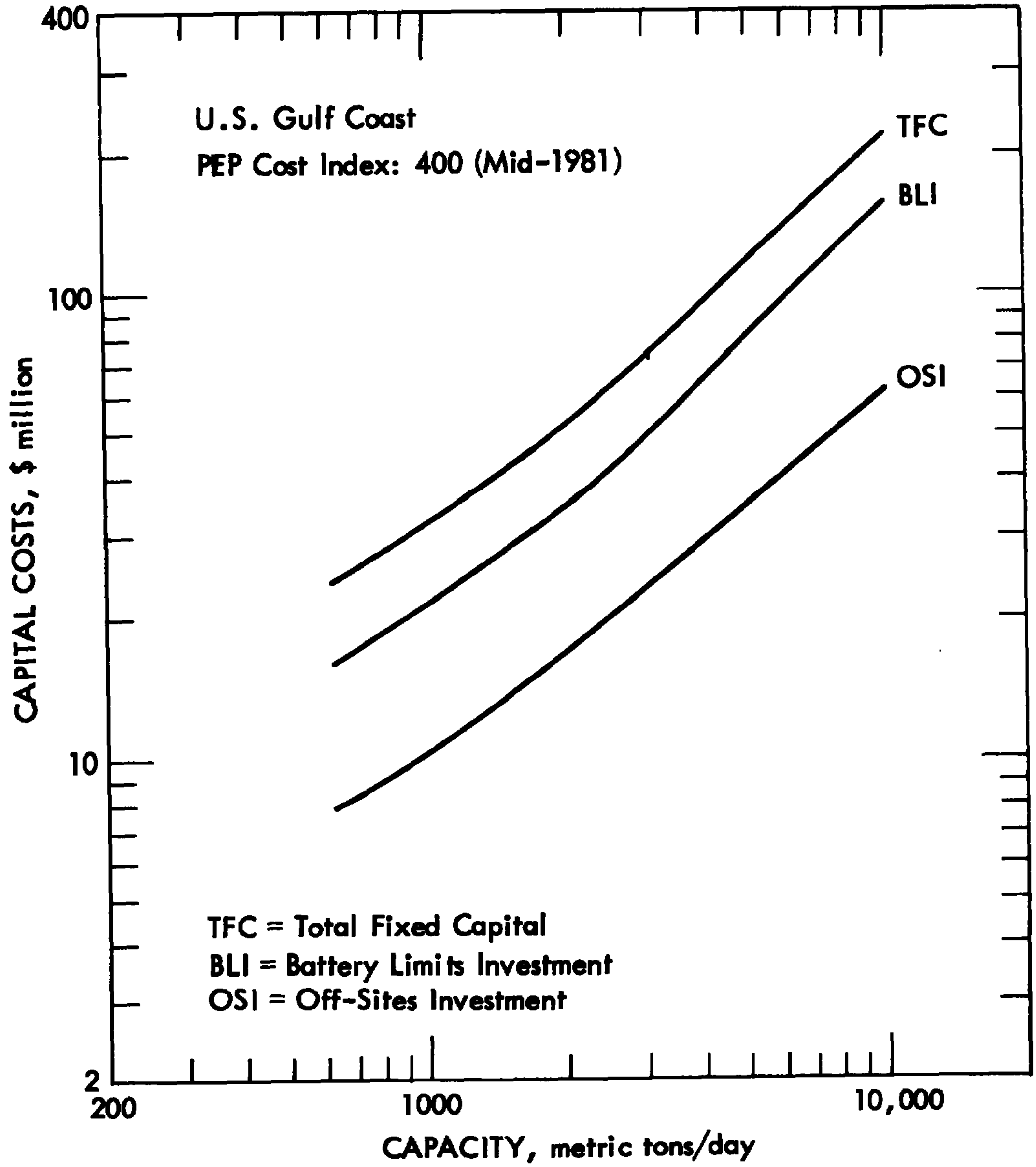


Figure 6.15

METHANOL FROM COAL DERIVED SYNGAS

Variation of Capital Costs with Capacity



The production costs and product values are shown in Table 6.23 at the end of this section.

To maintain consistency between the parts and the whole, the G&A charges here were based on the product value added to the syngas rather than on the methanol product value. In the instance where the size of the gasification facility is matched to the size of the methanol facility, the plot of product value as a function of capacity for the overall methanol complex (Figure 6.11) applies here as well.

Because the cost of the syngas dominates the methanol production cost, it is the scale of the syngas manufacture which has the major effect on the cost of the methanol. Thus, for example, a methanol unit of 1,250 metric tons/day, fed with syngas from a unit producing 805 million scfd, would produce methanol at a product value of 11.9¢/lb. This compares with the value of 15.7¢/lb calculated for the case in which the syngas production is matched to the smallish methanol unit. Obviously, the economics of manufacturing most chemicals from coal based syngas will be very much improved if this can be done in a complex based on a central large scale gasification facility.

3. Syngas (H_2:CO = 0.75) from Coal (Module 1)

A H_2/CO mol ratio of 0.75 in the product is the lowest that can be attained directly with the 60% solids slurry fed gasifiers used for the present base case design. The gas is cleaned up and all of it is sent to the COS hydrolysis reactors. No water-gas shift reaction is carried out.

In practice, such a design would probably yield a product gas with a somewhat variable H_2/CO ratio because the facility to adjust this readily by varying the split between hydrolysis and shift is eliminated. The nominal composition of the gas is shown in Table 6.1 at the beginning of this section.

As discussed in Section 3, syngases with H_2/CO ratios as low as 0.75 are unlikely to be needed on any large scale for chemical synthesis. The requirement for carbon monoxide per se is normally on a much smaller scale, as are the requirements for highly CO-rich syngases (e.g., vinyl acetate synthesis requiring methanol plus a syngas with a 0.58 H_2/CO ratio). The optimal way to produce this in a given case will most likely entail separation or skimming from a hydrogen-rich syngas being produced for some other major end use (see Sections 3 and 7).

However, should syngases very rich in CO be required on a large scale, dry-feed entrained-bed gasifiers would inherently be more suitable. The Shell/Koppers process typically produces a syngas with an H_2/CO ratio of about 0.5. An even lower ratio can be attained by using carbon dioxide as part of the feedstock (cf. steam reforming), but little has been published on the operation of gasifiers in such a mode.

For production of intermediate Btu gas (IBG) for fuel, there would be no need to shift, or to remove carbon dioxide from the product. Acid gas recovery would therefore be simplified. Costs for the production of IBG would therefore be even lower than those for the syngas considered here.

The capital requirements for producing the 0.75 H_2/CO ratio gas are shown in Table 6.16 and in Figure 6.13.

The detailed production costs and product values for various capacities are given in Table 6.24 at the end of this section. Product values are summarized in Table 6.16 and also plotted as a function of capacity in Figure 6.16.

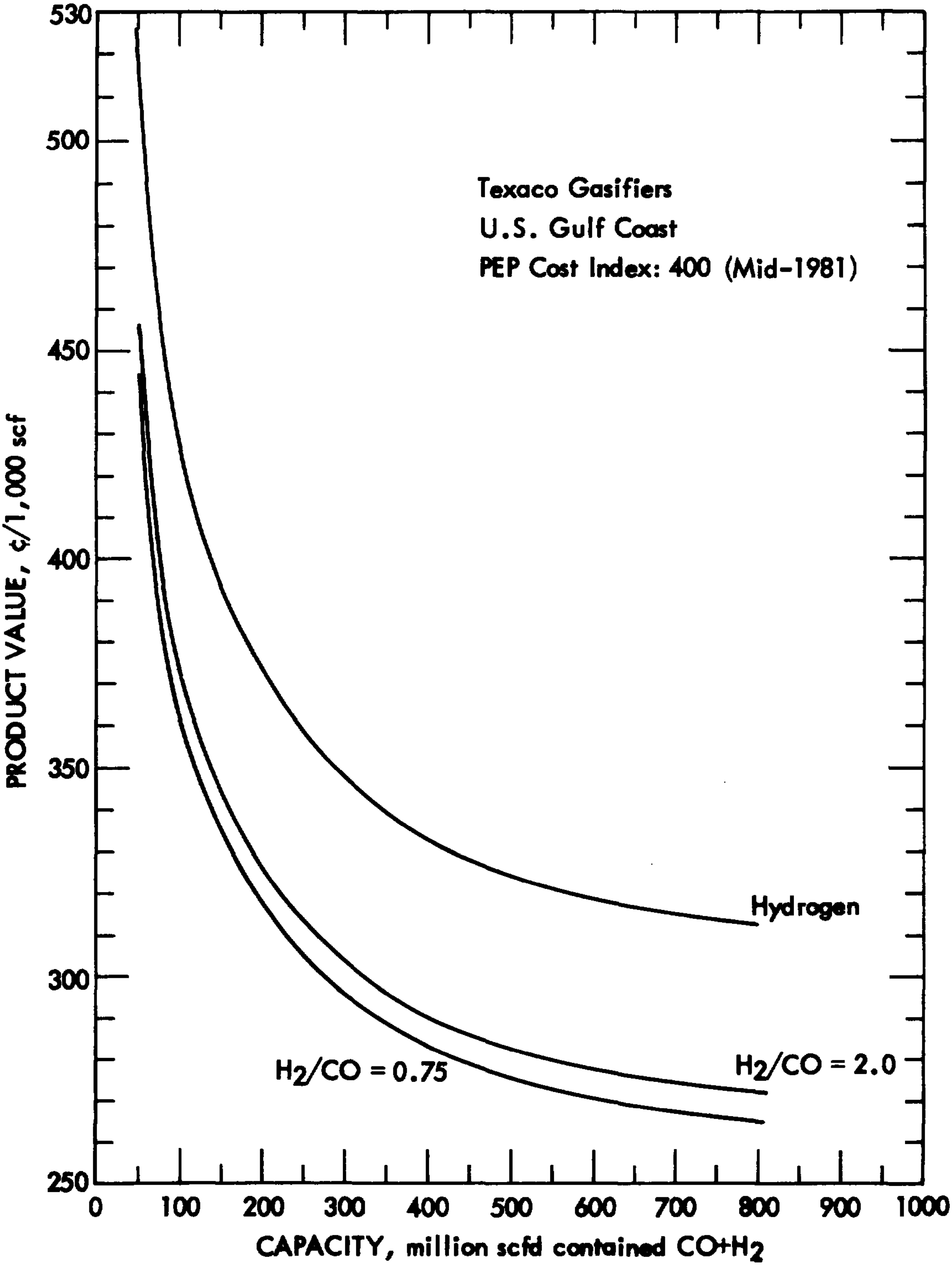
The product value for a production capacity of 802 million scfd of contained CO and hydrogen is estimated at 265¢/1,000 scf or $99/1,000 Nm^3. This breaks down approximately as follows:

Cost Component	¢/mscf	%
Coal related	88.4	33
Labor related	18.8	7
Capital related	152.8	58
Miscellaneous	5.4	2
Total	265.4	100

Figure 6.16

SYNGAS FROM COAL

Product Value as a Function of Capacity



In line with PEP standards, the allowance for G&A, sales, and research costs was set at 3% of the syngas product value, syngas being considered a captive chemical. This contrasts with the 5% allowance used for methanol and methanol syngas.

Table 6.16

SYNGAS (H_2:CO = 0.75) FROM COAL

INVESTMENT AND PRODUCT VALUE AS A FUNCTION OF CAPACITY

Capacity		Capital (million $)			
Million scfd* of Contained CO + H_2	Metric Tons/Day Methanol Equivalent*	Battery Limits Investment	Off-Sites Investment	Total Fixed Capital	Product Value (¢/mscf)
802	10,000	863	169	1,032	265
401	5,000	467	104	571	283
201	2,500	269	69	338	318
100	1,250	153	47	200	362
50	625	94	34	128	442

---

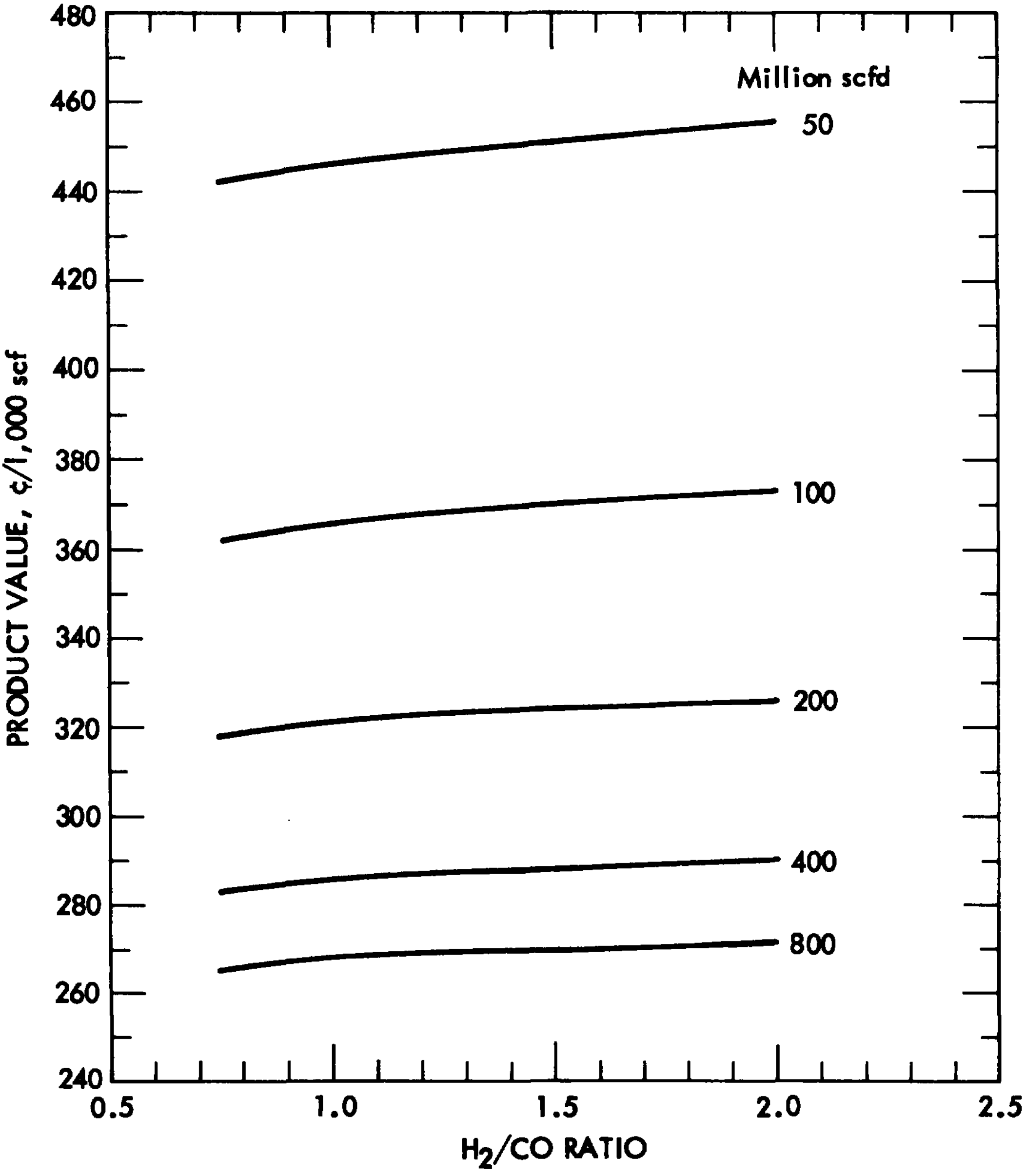
*Basis equivalent gasifier capacity.

As compared with the base case (methanol syngas, H_2/CO = 2.26) costs are reduced primarily because of the reduction in acid gas scrubbing requirements. (The major change in product value, however, here in fact derives from the arbitrary allocation of a different level of G&A, sales, and research costs.) Because of the reduced shift requirements there also appears to be some potential for backing out some of the quench cooling and recovering more of the sensible heat in the form of high pressure steam. No allowance was made for this here, but maximum savings of the order of 10¢/1,000 scf might be possible. With optimization of the overall design in each given instance, the syngas product values may therefore be somewhat more sensitive to the H_2/CO ratio than shown in Figure 6.17.

Figure 6.17

SYNGAS FROM COAL

Product Value as a Function of H_2/CO Ratio and Scale of Production



The literature often quotes Cold Gas Efficiencies (CGE), for gasification processes. A typical definition of CGE is:

$$\frac{\text{Heating value of syngas produced}}{\text{Heating value of feedstock consumed}}$$

In Europe the net or lower heating value (LHV) is usually used for reference, while in the United States it is more normal to sell fuels and calculate efficiencies on the basis of the gross or higher heating value (HHV). The CGE is not an efficiency in a thermodynamic sense, but rather a statement of yield. Provided a design is balanced in terms of all energy inputs, the CGE can be used as a rough comparative measure of its overall efficiency in utilizing feedstock. Its meaning, however, becomes very ambiguous if a large amount of energy flows either into or out from the system. In the present instance a CGE of about 70% is calculated if the relatively minor imbalance in steam and electricity is neglected. If an allowance is made for the latter, the CGE drops to about 68.5%.

4. Syngases (H_2:CO = 1.0, 1.5, 2.0) from Coal (Modules 2, 7, 8)

For production of syngases with H_2/CO mol ratios of 1.0, 1.5, and 2.0, respectively, 18%, 43%, and 59% of the raw gas stream is sent to the high temperature shift reactor and shifted to give an H_2/CO ratio of 4.8. The rest of the raw gas in each case is processed in the COS hydrolysis reactors. The two streams are eventually remixed to give the desired overall H_2/CO ratio.

An outline of how the base case design was modified and costs allocated in these schemes was given above under Rationale for Cost Allocations.

The capital requirements are shown in Tables 6.17–6.19. At the maximum capacity the TFC for the 2.0 ratio syngas is some 6% greater than for the 0.75 ratio syngas where no shifting takes place. On the plot of Figure 6.13, the capital requirements for the whole range of syngas compositions covered here will lie within the relatively narrow bands shown.

Table 6.17

SYNGAS (H_2:CO = 1.0) FROM COAL

INVESTMENT AND PRODUCT VALUE AS A FUNCTION OF CAPACITY

Capacity		Capital (million $)			
Million scfd of Contained CO + H_2	Metric Tons/day Methanol Equivalent*	Battery Limits Investment	Off-Sites Investment	Total Fixed Capital	Product Value (¢/mscf)
803.2	10,000	883	172	1,055	268
402	5,000	477	106	583	286
201	2,500	274	70	344	321
100	1,250	156	48	204	366
50	625	96	34	130	446

---

*Basis equivalent gasifier capacity.

Table 6.18

SYNGAS (H_2:CO = 1.5) FROM COAL

INVESTMENT AND PRODUCT VALUE AS A FUNCTION OF CAPACITY

Capacity		Capital (million $)			
Million scfd of Contained CO + H_2	Metric Tons/Day Methanol Equivalent*	Battery Limits Investment	Off-Sites Investment	Total Fixed Capital	Product Value (¢/mscf)
804.3	10,000	905	175	1,080	270
402	5,000	488	108	596	288
201	2,500	280	71	351	324
101	1,250	160	49	209	370
50	625	98	35	133	451

---

*Basis equivalent gasifier capacity.

Table 6.19

SYNGAS (H_2:CO = 2.0) FROM COAL

INVESTMENT AND PRODUCT VALUE AS A FUNCTION OF CAPACITY

Capacity		Capital (million $)			
Million scfd of Contained CO + H_2	Metric Tons/Day Methanol Equivalent*	Battery Limits Investment	Off-Sites Investment	Total Fixed Capital	Product Value (¢/mscf)
805	10,000	919	177	1,096	272
402.5	5,000	495	110	605	290
201	2,500	284	72	356	326
101	1,250	162	50	212	373
50	625	100	35	135	456

---

*Basis equivalent gasifier capacity.

The detailed production costs and product values for various capacities are shown in Tables 6.25, 6.26, and 6.27 at the end of this section. Product values are also plotted in Figure 6.17 as a function of both H_2/CO ratio and capacity. As noted before, optimization of the gasifier product cooling design and the high pressure steam balance could lead to somewhat lower product values for the lower H_2/CO ratio syngases than shown in Figure 6.17.

For the 2.0 ratio syngas at a production scale of 805 million scfd contained H_2 and CO, the product value is estimated at 272¢/1,000 scf, or $101.5/1,000 Nm^3, for a 0.9 stream factor. This breaks down approximately as follows:

Cost Component	¢/mscf	%
Coal related	88.2	32.4
Labor related	19.4	7.1
Capital related	161.7	59.5
Miscellaneous	2.7	1.0
Total	272.0	100.0

Again, the allowance for G&A, sales, and research costs was set at 3% of the syngas product value compared with 5% for the methanol syngas.

Because of the high proportion of fixed costs the product value is very sensitive to the stream factor, and increases substantially as the downtime increases.

Stream Factor	Operating Days/yr	Product Value ¢/mscf	 $/million Btu	 Ratio
0.9	328.5	272	8.3	1.0
0.7	255	324	9.9	1.19
0.5	182.5	417	12.8	1.53

The present analysis and the above breakdowns are keyed to a relatively high coal price (by U.S. norms), and to U.S. Gulf Coast construction costs. The sensitivity of the product value to coal price and capital is illustrated in Figure 6.18 for the 2.0 ratio syngas.

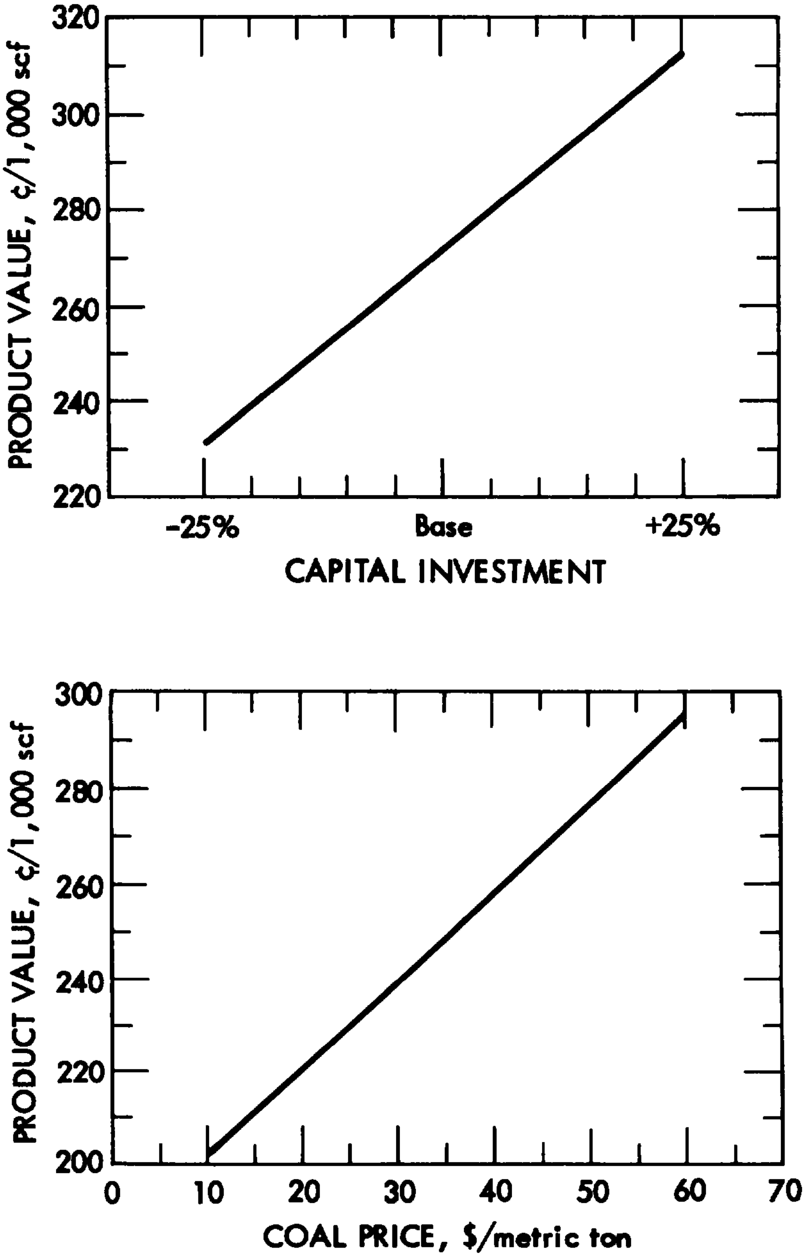
The more extensive discussion of costs in the section on methanol is also relevant here. For some comparisons with costs related to gas and oil based facilities, refer to Section 2.

5. Hydrogen from Coal (Module 22)

The analysis was extended to include cost estimates for production of hydrogen over the same capacity range as the syngases (50-800 million scfd). This is, of course, a very large scale for hydrogen production. Currently a large unit for on-purpose refinery hydrogen typically produces less than 100 million scfd. Alternatively 100 million scfd could be used to produce some 1,350 metric tons per day of ammonia. The size of facilities being envisaged for synfuels manufacture by direct coal liquefaction is often of the order of 50,000 barrels per day, and would typically require some 200-300 million scfd of hydrogen. The product values estimated below thus represent the lower

Figure 6.18

SENSITIVITY OF SYNGAS PRODUCT
Value to Capital Investment and Coal Price



Texaco Gasifiers
U.S. Gulf Coast, Mid-1981
805 Million scfd Syngas
$H_2/CO = 2.0$

limits of the cost of hydrogen produced on a very large scale from coal.

To estimate screening level costs we modified the base-case methanol syngas design to include a low temperature shift stage following the high temperature shift. All of the raw gas is shifted and the COS hydrolysis section is eliminated entirely. An optimization of the steam balance was not attempted. A methanation stage was added after acid gas removal to reduce the CO below 10 ppmv. The acid gas removal section costs were scaled simply on the basis of flow rates. Selective acid gas separation becomes more difficult as the CO_2 level in the raw gas increases (415023), and in practice, a somewhat more complex design may be needed than in the methanol syngas case. However, for present purposes we believe that a simple scaling is adequate.

The hydrogen product composition is shown as stream 6 in Table 6.1. The hydrogen purity is 97 vol% on a dry basis, with methane, inerts, and water composing the main impurities in roughly equal amounts. This purity would typically be adequate for chemical grade hydrogen used for example in refinery hydrogenations.

The capital requirements are shown in Table 6.20 and Figure 6.19.

The detailed product costs and product values for various capacities are given in Table 6.28 at the end of this section. Product values are also summarized in Table 6.20 below, and plotted as a function of capacity in Figure 6.16. As for the syngases, the allowance for G&A costs was taken as 3% of the product value. The surplus of low pressure steam produced was given no credit.

Figure 6.19

LARGE SCALE HYDROGEN FROM COAL

Variation of Capital Costs with Capacity

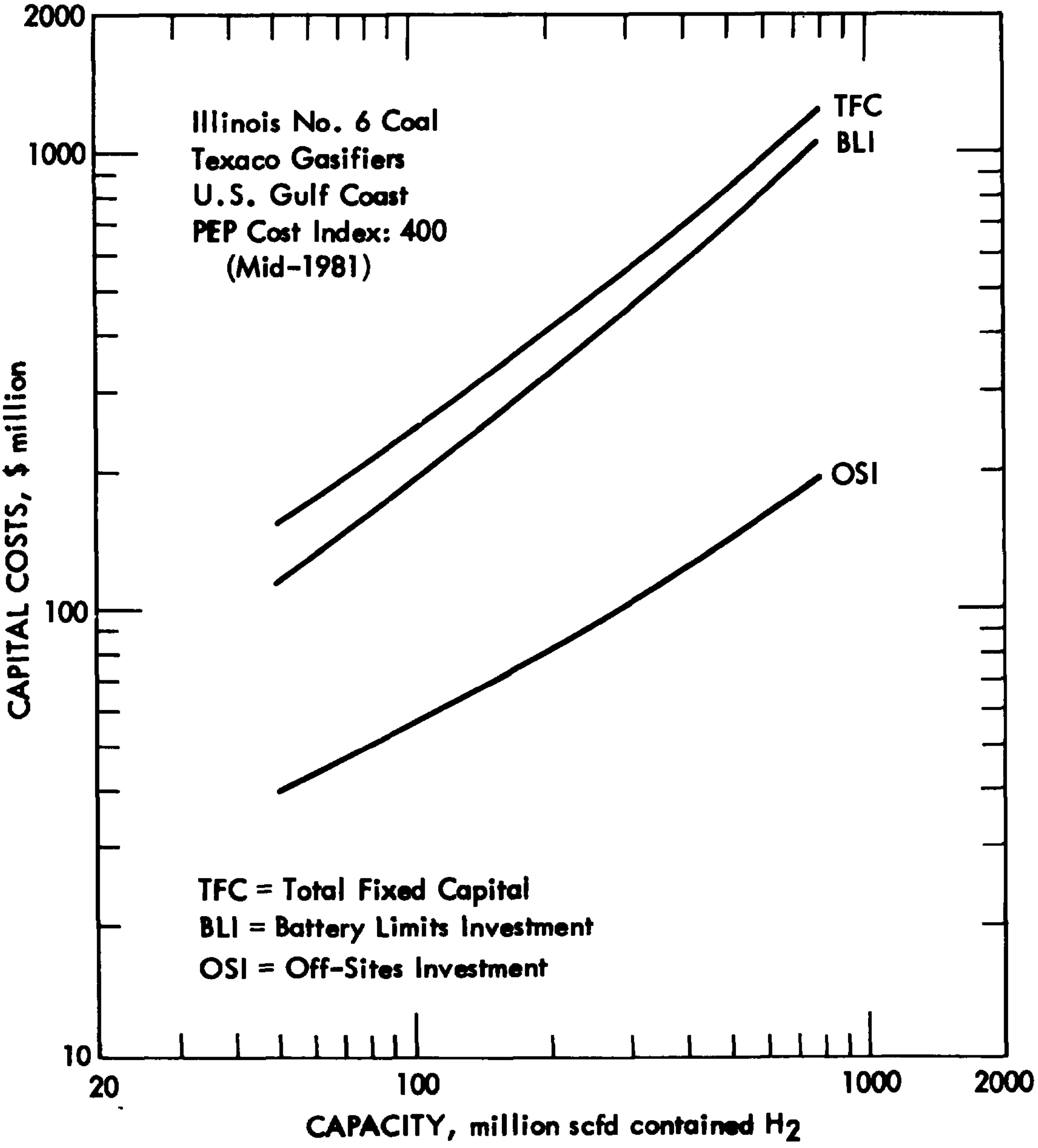


Table 6.20

LARGE SCALE HYDROGEN PRODUCTION FROM COAL

INVESTMENT AND PRODUCT VALUE AS A FUNCTION OF CAPACITY

Capacity		Capital (million $)				
Million scfd*	Metric Tons/Day Methanol Equivalent†	Battery Limits Investment	Off-Sites Investment	Total Fixed Capital	Product Value (¢/mscf)	Product Value (¢/lb)
781	10,000	1,049	194	1,243	313	59.4
391	5,000	563	121	684	334	63.4
195	2,500	322	80	402	375	71.2
98	1,250	184	56	240	430	81.6
49	625	114	39	153	526	99.8

---

*Based on contained hydrogen.

†Basis equivalent gasifier capacity.

Conclusions

In this section we have outlined some background considerations on the gasification of coal as a starting point for large scale chemicals production, and presented screening level economics for syngas, hydrogen, and methanol production. An example on separating out carbon monoxide from coal based methanol syngas is analyzed in Section 7.

The basis for the economic analysis was second generation gasification, which is close to demonstration on a commercial scale. The scale of operation considered was one in which the facilities could be dedicated to bulk chemicals production rather than used primarily for synthetic fuels manufacture.

It was seen that within these constraints, entrained flow gasification has inherent advantages. It produces a CO-rich synthesis gas low in methane and tars which is readily suited to chemical synthesis. Adjusting the H_2/CO ratio upward by the water gas shift reaction is a relatively simple and economic operation. Because gasification and associated facilities are very capital intensive, it is essential to take advantage of the economies of scale; the size of the production facilities needs to be substantial. A central syngas complex feeding several types of downstream units would be a likely arrangement.

Regarding investment estimates, the intent of the current work is to present screening level costs for large coal conversion plants that could be operating by the end of the decade. As such they should be applicable to demonstrated technology and not to "first-time" facilities. Costs for the latter would be expected to be substantially higher. Economics of eventual chemicals production from syngases produced in even larger syn fuels complexes should, on the other hand, be more favorable.

We initially thought that the design in the Fluor study (472120) would serve the present purpose. However, continuing evaluation of gasification facilities, and discussions with industry have led us to conclude that a somewhat more conservative design basis should be adopted to match the assumed stream factor of 0.9 (328.5 days per year), even for a mature plant. In particular, sparing on the gasifier and heat recovery section should be increased to about 50%. In addition more extensive facilities for coal storage and preparation, and for auxiliary steam generation would be required. We estimate that such changes would increase the total fixed capital for syngas production by close to 25% in the base case. In the computerized version of the present data base therefore, namely, the SYNCOST Program, the capital requirements for coal-based facilities have been increased in line with these more conservative design assumptions (see Table 2.3 in Section 2.) The numbers in the present section should thus be considered to represent an optimistic scenario.

Some comparisons of the costs of coal derived syngas with those of syngas made from natural gas and residue are also given in Section 2.

However, the comparisons should only be viewed as selected illustrations. The main objective of the present work is to establish a framework and a data base which can be used to project and examine various scenarios in the future. The point at which coal based feedstocks will become competitive will depend primarily on the relative rates of escalation of crude oil and capital costs, projections of both of which are particularly moot at the present time. Because of the large sums of capital placed at risk in constructing gasification complexes, the actual crossover point is also likely to lag the theoretical one.

Table 6.21

METHANOL FROM COAL

PRODUCTION COSTS

Time:	Mid-1981
Location:	U.S. Gulf Coast
PEP Cost Index:	400

Capacity: 10,000 Metric Tons/Day (100% Methanol Basis)
3,285,000 Metric Tons/yr
7,243 Million lb/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	15,000 metric tons/day as received Illinois No. 6
2. Air separation	12,800 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	810 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	534 million scfd (CO + H_2)
5. COS hydrolysis	276 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	1,234 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	462 metric tons/day sulfur
8. Methanol synthesis (ICI process)	10,000 metric tons/day (100% basis)
9. Methanol purification (99% fuel grade)	10,000 metric tons/day (100% basis)

Investment (million $)

Battery limits (BLI)	1,082
Off-sites	240
Total fixed capital (TFC)	1,322

Variable Cost Summary

	Unit Cost	Consumption per metric ton	¢/lb	$/metric ton	$1,000/yr
Raw materials					
Coal at mine	32.3 $/metric ton	1.5	2.20	48.45	159,158
Coal transport	15.0 $/metric ton	1.5	1.02	22.50	73,913
Ash disposal	5.0 $/metric ton	0.15	0.03	0.75	2,464
Methanol catalyst	4.0 $/lb	0.4	0.07	1.60	5,256
Misc. cat. and chem.	1.0 $/unit	0.6	0.03	0.60	1,971
			3.35	73.90	242,762
By-product					
Sulfur	100$/metric ton	(0.046)	(0.21)	(4.60)	(15,111)
Imported utilities					
Clarified water	0.68 $/1,000 gal	1.37	0.04	0.93	3,055
Total variable costs			3.18	70.23	230,706

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

10,000 Metric Tons/Day

	¢/lb	$/metric ton	$1,000/yr
Production costs			
Raw materials	3.35	73.90	272,762
By-product credit	(0.21)	(4.60)	(15,111)
Imported utilities	0.04	0.93	3,055
Variable costs	3.18	70.23	230,706
Operating labor (62/shift; 17.50 $/hr)	0.13	2.89	9,505
Maintenance labor (1.6% BLI)	0.24	5.27	17,312
Control lab. labor (20% op. labor)	0.03	0.58	1,901
Total direct labor	0.40	8.74	28,718
Maintenance materials (2.4% BLI)	0.36	7.91	25,968
Operating supplies (10% op. labor)	0.01	0.29	951
	0.37	8.20	26,919
Plant overhead (30% total labor)	0.12	2.62	8,615
Taxes and insurance (2% TFC)	0.37	8.05	26,440
Depreciation (10% TFC)	1.82	40.24	132,200
	2.31	50.91	167,255
Subtotal: plant gate cost	6.26	138.08	453,598
G&A, sales, research (5% PV)	0.57	12.56	41,268
ROI before taxes (25% TFC)	4.56	100.61	330,500
Product value (PV)	11.39	251.25	825,366
¢/gallon (U.S.)*	75.2		
$/million Btu*	11.65		

---

*Basis 6.6 lb/gallon,
9,690 Btu/lb (HHV) of 99.1% methanol.

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

Time: Mid-1981
Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity: 5,000 Metric Tons/Day (100% Methanol Basis)
1,642,500 Metric Tons/yr
3,622 Million lb/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	7,500 metric tons/day as received Illinois No. 6
2. Air separation	6,400 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	405 million scfd ($CO + H_2$)
4. Shift conversion (4.8 H_2/CO ratio)	267 million scfd ($CO + H_2$)
5. COS hydrolysis	138 million scfd ($CO + H_2$)
6. Acid gas removal (Rectisol process)	617 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	231 metric tons/day sulfur
8. Methanol synthesis (ICI process)	5,000 metric tons/day (100% basis)
9. Methanol purification (99% fuel grade)	5,000 metric tons/day (100% basis)

Investment (million $)

Battery limits (BLI)	580
Off-sites	147
Total fixed capital (TFC)	727

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

5,000 Metric Tons/Day

	¢/lb	$/metric ton	$1,000/yr
Production costs			
Raw materials	3.35	73.90	121,381
By-product credit	(0.21)	(4.60)	(7,556)
Imported utilities	0.04	0.93	1,528
Variable costs	3.18	70.23	115,353
Operating labor (34/shift; 17.50 $/hr)	0.14	3.17	5,212
Maintenance labor (1.6% BLI)	0.26	5.66	9,280
Control lab. labor (20% op. labor)	0.03	0.63	1,042
Total direct labor	0.43	9.46	15,534
Maintenance materials (2.4% BLI)	0.38	8.47	13,920
Operating supplies (10% op. labor)	0.02	0.32	521
	0.40	8.79	14,441
Plant overhead (30% total labor)	0.13	2.84	4,660
Taxes and insurance (2% TFC)	0.40	8.85	14,540
Depreciation (10% TFC)	2.01	44.26	72,700
	2.54	55.95	91,900
Subtotal: plant gate cost	6.55	144.43	237,228
G&A, sales, research (5% PV)	0.61	13.43	22,051
ROI before taxes (25% TFC)	5.02	110.65	181,750
Product value (PV)	12.18	268.51	441,029
¢/gallon (U.S.)	80.4		
$/million Btu	12.45		

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

Time:	Mid-1981
Location:	U.S. Gulf Coast
PEP Cost Index:	400

Capacity: 2,500 Metric Tons/Day (100% Methanol Basis)
821,250 Metric Tons/yr
1,811 Million lb/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	3,750 metric tons/day as received Illinois No. 6
2. Air separation	3,200 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	202 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	133 million scfd (CO + H_2)
5. COS hydrolysis	69 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	308 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	115 metric tons/day sulfur
8. Methanol synthesis (ICI process)	2,500 metric tons/day (100% basis)
9. Methanol purification (99% fuel grade)	2,500 metric tons/day (100% basis)

Investment (million $)

Battery limits (BLI)	327
Off-sites	93
Total fixed capital (TFC)	420

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

2,500 Metric Tons/Day

	¢/lb	$/metric ton	$1,000/yr
Production costs			
Raw materials	3.35	73.90	60,690
By-product credit	(0.21)	(4.60)	(3,778)
Imported utilities	0.04	0.93	764
Variable costs	3.18	70.23	57,676
Operating labor (24/shift; 17.50 $/hr)	0.20	4.48	3,679
Maintenance labor (1.6% BLI)	0.29	6.37	5,232
Control lab. labor (20% op. labor)	0.04	0.90	736
Total direct labor	0.53	11.75	9,647
Maintenance materials (2.4% BLI)	0.43	9.55	7,848
Operating supplies (10% op. labor)	0.02	0.45	368
	0.45	10.00	8,216
Plant overhead (30% total labor)	0.18	4.07	3,341
Taxes and insurance (2% TFC)	0.46	10.23	8,400
Depreciation (10% TFC)	2.32	51.14	42,000
	2.97	65.44	53,741
Subtotal: plant gate cost	7.13	157.42	129,280
G&A, sales, research (5% PV)	0.68	15.01	12,330
ROI before taxes (25% TFC)	5.80	127.85	105,000
Product value (PV)	13.61	300.28	246,610
¢/gallon (U.S.)	89.8		
$/million Btu	13.92		

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

Time:	Mid-1981
Location:	U.S. Gulf Coast
PEP Cost Index:	400

Capacity: 1,250 Metric Tons/Day (100% Methanol Basis)
410,625 Metric Tons/yr
905 Million lb/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	1,875 metric tons/day as received Illinois No. 6
2. Air separation	1,600 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	101 million scfd ($CO + H_2$)
4. Shift conversion (4.8 H_2/CO ratio)	67 million scfd ($CO + H_2$)
5. COS hydrolysis	34 million scfd ($CO + H_2$)
6. Acid gas removal (Rectisol process)	154 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	58 metric tons/day sulfur
8. Methanol synthesis (ICI process)	1,250 metric tons/day (100% basis)
9. Methanol purification (99% fuel grade)	1,250 metric tons/day (100% basis)

Investment (million $)

Battery limits (BLI)	188
Off-sites	62
Total fixed capital (TFC)	250

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

1,250 Metric Tons/Day

	¢/lb	$/metric ton	$1,000/yr
Production costs			
Raw materials	3.35	73.90	30,345
By-product credit	(0.21)	(4.60)	(1,889)
Imported utilities	0.04	0.93	382
Variable costs	3.18	70.23	28,838
Operating labor (20/shift; 17.50 $/hr)	0.34	7.47	3,066
Maintenance labor (1.6% BLI)	0.33	7.32	3,008
Control lab. labor (20% op. labor)	0.07	1.49	613
Total direct labor	0.74	16.28	6,687
Maintenance materials (2.4% BLI)	0.50	10.99	4,512
Operating supplies (10% op. labor)	0.04	0.75	307
	0.54	11.74	4,819
Plant overhead (30% total labor)	0.22	4.89	2,006
Taxes and insurance (2% TFC)	0.55	12.18	5,000
Depreciation (10% TFC)	2.76	60.88	25,000
	3.53	77.95	32,006
Subtotal: plant gate cost	7.99	176.20	72.350
G&A, sales, research (5% PV)	0.78	17.28	7,097
ROI before taxes (25% TFC)	6.90	152.21	62.500
Product value (PV)	15.67	345.69	141,947
¢/gallon	103.4		
$/million Btu	16.0		

Table 6.21 (Continued)

METHANOL FROM COAL

PRODUCTION COSTS

Time: Mid-1981
Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity: 625 Metric Tons/Day (100% Methanol Basis)
205,300 Metric Tons/yr
453 Million lb/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	938 metric tons/day as received Illinois No. 6
2. Air separation	800 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	51 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	34 million scfd (CO + H_2)
5. COS hydrolysis	17 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	77 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	29 metric tons/day sulfur
8. Methanol synthesis (ICI process)	625 metric tons/day
9. Methanol purification (99% fuel grade)	625 metric tons/day

Investment (million $)

Battery limits (BLI)	116
Off-sites	44
Total fixed capital (TFC)	160

Table 6.21 (Concluded)

METHANOL FROM COAL

PRODUCTION COSTS

625 Metric Tons/Day

	¢/lb	$/metric ton	$1,000/yr
Production costs			
Raw materials	3.35	73.90	15,172
By-product credit	(0.21)	(4.60)	(944)
Imported utilities	0.04	0.93	191
Variable costs	3.18	70.23	14,419
Operating labor (19/shift; 17.50 $/hr)	0.64	14.19	2,913
Maintenance labor (1.6% BLI)	0.41	9.04	1,856
Control lab. labor (20% op labor)	0.13	2.84	583
Total direct labor	1.18	26.07	5,352
Maintenance materials (2.4% BLI)	0.61	13.56	2,784
Operating supplies (10% op. labor)	0.06	1.42	291
	0.67	14.98	3,075
Plant overhead (30% total labor)	0.35	7.82	1,606
Taxes and insurance (2% TFC)	0.72	15.59	3,200
Depreciation (10% TFC)	3.53	77.93	16,000
	4.60	101.34	20,806
Subtotal: plant gate cost	9.64	212.62	43,652
G&A, sales, research (5% PV)	0.97	21.44	4,402
ROI before taxes (25% TFC)	8.84	194.84	40,000
Product value (PV)	19.45	428.90	88,054
¢/gallon	128.4		
$/million Btu	19.88		

Table 6.22

METHANOL SYNGAS FROM COAL (H_2:CO = 2.26)

PRODUCTION COSTS

Time: Mid-1981
Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity: 805.3 x 10^6 scfd (contained CO + H_2)*
88,400 lb-mols/hr (contained CO + H_2)
264.4 x 10^9 scf/yr (contained CO + H_2)

Stream Factor: 0.9

Process units include:

1. Coal preparation	15,000 metric tons/day as received Illinois No. 6
2. Air separation	12,800 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	810 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	534 million scfd (CO + H_2)
5. COS hydrolysis	276 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	1,234 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	462 metric tons/day sulfur

---

*Represents "front-end" of a 10,000 metric ton/day methanol unit. Syngas contains 3% CO_2.

Investment (million $)

Battery limits (BLI)	924
Off-sites	178
Total fixed capital (TFC)	1,102

Variable Cost Summary

	Unit Cost	Consumption per 10^6 scf	¢/1,000 scf	$/1,000 Nm^3	$1,000/yr
Raw materials					
Coal at mine	32.3$/metric ton	18.64	60.2	22.5	159,158
Coal transport	15.0$/metric ton	18.64	28.0	10.4	73,913
Ash disposal	5.0$/metric ton	1.86	0.9	0.3	2,464
Misc. cat. and chem.	1.0$/unit	6.16	0.6	0.2	1,630
			89.7	33.4	237,165
By-product					
Sulfur	100$/metric ton	0.57	(5.7)	(2.1)	(15,111)
Imported utilities					
Clarified water	0.68$/1,000 gal	15.12	1.0	0.4	2,718
Electricity	3.6¢/kwh	(82.5)	(0.3)	(0.1)	(785)
Steam (HP)	7.73$/1,000 lb	7.6	5.9	2.2	15,533
			6.6	2.5	17,466
Total variable costs			90.6	33.8	239,520

Table 6.22 (Concluded)

METHANOL SYNGAS FROM COAL (H_2:CO = 2.26)

PRODUCTION COSTS

805.3×10^6 scfd

	¢/1,000 scf	\$/1,000 Nm^3	\$1,000/yr
Production costs			
Raw materials	89.7	33.4	237,165
By-product credit	(5.7)	(2.1)	(15,111)
Imported utilities	6.6	2.5	17,466
Variable costs	90.6	33.8	239,520
Operating labor (42/shift; 17.50 \$/hr)	2.4	0.9	6,439
Maintenance labor (1.6% BLI)	5.6	2.1	14,784
Control lab. labor (20% op. labor)	0.5	0.2	1,288
Total direct labor	8.5	3.2	22,511
Maintenance materials (2.4% BLI)	8.4	3.1	22,176
Operating supplies (10% op. labor)	0.2	0.1	644
	8.6	3.2	22,820
Plant overhead (30% total labor)	2.6	1.0	6,753
Taxes and insurance (2% TFC)	8.3	3.1	22,040
Depreciation (10% TFC)	41.7	15.6	110,200
	52.6	19.7	138,993
Subtotal: plant gate cost	160.3	59.9	423,844
G&A, sales, research (5% PV)	13.9	5.2	36,808
ROI before taxes (25% TFC)	104.2	38.9	275,500
Product value (PV)	278.4	104.0	736,152
\$/million Btu*	8.51		
¢/lb (CO + H_2)*	10.59		

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*0.327 million Btu/mscf (CO + H_2) - HHV.
38.03 scf/lb (CO + H_2).

Table 6.23

METHANOL FROM COAL-DERIVED SYNGAS

PRODUCTION COSTS

Time: Mid-1981
Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity: 10,000 Metric Tons/Day (100% Methanol Basis)
3,285,000 Metric Tons/yr
7,243 Million lb/yr

Stream Factor: 0.9

Process units include:

1. Methanol synthesis.
2. Methanol purification.

Investment (million $)

Battery limits (BLI)	158
Off-sites	62
Total fixed capital (TFC)	220

Variable Cost Summary

	Unit Cost	Consumption per metric ton	¢/lb	$/metric ton	$1,000/yr
Raw materials					
Syngas (H_2/CO = 2.26)	2.78$/mscf	80.5	10.16	224.09	736,152
Methanol catalyst	4.0$/lb	0.4	0.07	1.60	5,256
Misc. cat. and chem.	1.0$/unit	0.1	—	0.10	341
			10.23	225.79	741,749
Imported utilities					
Clarified water	0.68$/1,000 gal	0.15	—	0.10	337
Electricity	3.6¢/kwh	6.63	0.01	0.24	785
Steam (HP)	7.73$/1,000 lb	(0.61)	(0.21)	(4.73)	(15,533)
			(0.20)	(4.39)	(14,411)
Total variable costs			10.03	221.40	727,338

Table 6.23 (Concluded)

METHANOL FROM COAL-DERIVED SYNGAS

PRODUCTION COSTS

10,000 Metric Tons/Day

	¢/lb	$/metric ton	$1,000/yr
Production costs			
Raw materials	10.23	225.79	741,749
By-product credit	—	—	—
Imported utilities	(0.20)	(4.39)	(14,411)
Variable costs	10.03	221.40	727,338
Operating labor (20/shift; 17.50 $/hr)	0.04	0.93	3,066
Maintenance labor (1.6% BLI)	0.04	0.77	2,528
Control lab. labor (20% op. labor)	0.01	0.19	613
Total direct labor	0.09	1.89	6,207
Maintenance materials (2.4% BLI)	0.05	1.16	3,792
Operating supplies (10% op. labor)	0.01	0.09	307
	0.06	1.25	4,099
Plant overhead (30% total labor)	0.03	0.57	1,862
Taxes and insurance (2% TFC)	0.06	1.34	4,400
Depreciation (10% TFC)	0.30	6.70	22,000
	0.39	8.61	28,262
Subtotal: plant gate cost	10.57	233.15	765,906
G&A, sales, research (5% PVA)*	0.06	1.36	4,460
ROI before taxes (25% TFC)	0.76	16.74	55,000
Product value (PV)	11.39	251.25	825,366
¢/gallon (U.S.)†	75.2		
$/million Btu†	11.65		

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*5% of product value added (PVA) by process to syngas.

†Basis 6.6 lb/gallon and 9,690 Btu/lb of 99.1% methanol.

Table 6.24

SYNGAS (H_2:CO = 0.75) FROM COAL

PRODUCTION COSTS

Time:	Mid-1981
Location:	U.S. Gulf Coast
PEP Cost Index:	400

Capacity: Basis contained (CO + H_2) 802.4×10^6 scfd
88,100 lb-mol/hr
263.6×10^9 scf/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	15,000 metric tons/day as received Illinois No. 6
2. Air separation	12,800 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	810 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	--
5. COS hydrolysis	810 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	1,018 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	462 metric tons/day sulfur

Investment (million $)

Battery limits (BLI)	863
Off-sites	169
Total fixed capital (TFC)	1,032

Variable Cost Summary

	Unit Cost	Consumption per 10^6 scf	¢/1,000 scf	$/1,000 Nm^3	$1,000/yr
Raw materials					
Coal at mine	32.3 $/metric ton	18.68	60.4	22.5	159,158
Coal transport	15.0$/metric ton	18.68	28.0	10.5	73,913
Ash disposal	5.0$/metric ton	1.86	1.0	0.3	2,646
Misc. cat. and chem.	1.0$/unit	5.14	0.5	0.2	1,356
			89.9	33.5	237,073
By-product					
Sulfur	100$/metric ton	(0.57)	(5.7)	(2.1)	(15,111)
Imported utilities					
Clarified water	0.68$/1,000 gal	14.83	1.0	0.4	2,658
Electricity	3.6¢/kwh	(181)	(0.7)	(0.2)	(1,718)
Steam (HP)	7.73$/1,000 lb	12	9.3	3.4	24,451
			9.6	3.6	25,391
Total variable costs			93.8	35.0	247,353

Table 6.24 (Concluded)

SYNGAS (H_2:CO = 0.75) FROM COAL

PRODUCTION COSTS

802.4 x 10^6 scfd

	¢/1,000 scf	$/1,000 Nm^3	$1,000/yr
Production costs			
Raw materials	89.9	33.5	237,073
By-product credit	(5.7)	(2.1)	(15,111)
Imported utilities	9.6	3.6	25,391
Variable costs	93.8	35.0	247,353
Operating labor (42/shift; 17.50 $/hr)	2.5	0.9	6,439
Maintenance labor (1.6% BLI)	5.2	2.0	13,808
Control lab. labor (20% op. labor)	0.5	0.2	1,288
Total direct labor	8.2	3.1	21,535
Maintenance materials (2.4% BLI)	7.9	2.9	20,712
Operating supplies (10% op. labor)	0.2	0.1	644
	8.1	3.0	21,356
Plant overhead (30% total labor)	2.4	0.9	6,461
Taxes and insurance (2% TFC)	7.8	2.9	20,640
Depreciation (10% TFC)	39.2	14.6	103,200
	49.4	18.4	130,301
Subtotal: plant gate cost	159.5	59.5	420,545
G&A, sales, research (3% PV)	8.0	3.0	20,986
ROI before taxes (25% TFC)	97.9	36.5	258,000
Product value (PV)	265.4	99.0	699,531
$/million Btu*	8.14		
¢/lb (CO + H_2)*	5.97		

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*0.326 million Btu/mscf (HHV). 22.5 scf/lb.

Table 6.25

SYNGAS (H_2:CO = 1.0) FROM COAL

PRODUCTION COSTS

Time:	Mid-1981
Location:	U.S. Gulf Coast
PEP Cost Index:	400

Capacity: Basis contained (CO + H_2) - 803.2×10^6 scfd
88,200 lb-mol/hr
263.9×10^9 scf/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	15,000 metric tons/day as received Illinois No. 6
2. Air separation	12,800 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	810 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	144 million scfd (CO + H_2)
5. COS hydrolysis	666 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	1,077 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	462 metric tons/day sulfur

Investment (million $)

Battery limits (BLI)	883
Off-sites	172
Total fixed capital (TFC)	1,055

Variable Cost Summary

	Unit Cost	Consumption per 10^6 scf	¢/1,000 scf	$/1,000 Nm^3	$1,000/yr
Raw materials					
Coal at mine	32.3$/metric ton	18.66	60.3	22.5	159,158
Coal transport	15.0$/metric ton	18.66	28.0	10.5	73,913
Ash disposal	5.0$/metric ton	1.86	1.0	0.3	2,646
Misc. cat. and chem.	1.0$/unit	5.42	0.6	0.2	1,432
			89.9	33.5	237,149
By-product					
Sulfur	100$/metric ton	0.57	(5.7)	(2.1)	(15,111)
Imported utilities					
Clarified water	0.68$/1,000 gal	14.91	1.0	0.4	2,676
Electricity	3.6¢/kwh	(153)	(0.6)	(0.2)	(1,454)
Steam (HP)	7.73$/1,000 lb	11	8.5	3.2	22,440
			8.9	3.4	23,662
Total variable costs			93.1	34.8	245,700

Table 6.25 (Concluded)

SYNGAS (H_2:CO = 1.0) FROM COAL

PRODUCTION COSTS

	¢/1,000 scf	\$/1,000 Nm^3	\$1,000/yr
Production costs			
Raw materials	89.9	33.5	237,149
By-product credit	(5.7)	(2.1)	(15,111)
Imported utilities	8.9	3.4	23,662
Variable costs	93.1	34.8	245,700
Operating labor (42/shift; 17.50 \$/hr)	2.4	0.9	6,439
Maintenance labor (1.6% BLI)	5.4	2.0	14,128
Control lab. labor (20% op. labor)	0.5	0.2	1,288
Total direct labor	8.3	3.1	21,855
Maintenance materials (2.4% BLI)	8.0	3.0	21,192
Operating supplies (10% op. labor)	0.2	0.1	644
	8.2	3.1	21,836
Plant overhead (30% total labor)	2.5	0.9	6,556
Taxes and insurance (2% TFC)	8.0	3.0	21,100
Depreciation (10% TFC)	40.0	14.9	105,500
	50.5	18.8	133,156
Subtotal: plant gate cost	160.1	59.8	422,547
G&A, sales, research (3% PV)	8.0	3.0	21,226
ROI before taxes (25% TFC)	100.0	37.3	263,750
Product value (PV)	268.1	100.1	707,523
\$/million Btu*	8.20		
¢/lb (CO + H_2)*	6.78		

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*0.327 million Btu/mscf (HHV).
25.3 scf/lb.

Table 6.26

SYNGAS (H_2:CO = 1.5) FROM COAL

PRODUCTION COSTS

Time:	Mid-1981
Location:	U.S. Gulf Coast
PEP Cost Index:	400

Capacity: Basis contained (CO + H_2) - 804.3 x 10^6 scfd
88,300 lb-mol/hr
264.2 x 10^9 scf/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	15,000 metric tons/day as received Illinois No. 6
2. Air separation	12,800 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	810 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	346 million scfd (CO + H_2)
5. COS hydrolysis	464 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	1,158 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	462 metric tons/day sulfur

Investment (million $)

Battery limits (BLI)	905
Off-sites	175
Total fixed capital (TFC)	1,080

Variable Cost Summary

	Unit Cost	Consumption per 10^6 scf	¢/1,000 scf	$/1,000 Nm^3	$1,000/yr
Raw materials					
Coal at mine	32.3$/metric ton	18.64	60.2	22.5	159,158
Coal transport	15.0$/metric ton	18.64	28.0	10.5	73,913
Ash disposal	5.0$/metric ton	1.86	1.0	0.3	2,646
Misc. cat. and chem.	1.0$/unit	5.81	0.6	0.2	1,536
			89.8	33.5	237,253
By-product					
Sulfur	100$/metric ton	(0.57)	(5.7)	(2.1)	(15,111)
Imported utilities					
Clarified water	0.68$/1,000 gal	15.02	1.0	0.4	2,698
Electricity	3.6¢/kwh	(116)	(0.4)	(0.2)	(1,103)
Steam (HP)	7.73$/1,000 lb	9	7.0	2.6	18,380
			7.6	2.8	19,975
Total variable costs			91.7	34.2	242,117

Table 6.26 (Concluded)

SYNGAS (H_2:CO = 1.5) FROM COAL

PRODUCTION COSTS

	¢/1,000 scf	$/1,000 Nm^3	$1,000/yr
Production costs			
Raw materials	89.8	33.5	237,253
By-product credit	(5.7)	(2.1)	(15,111)
Imported utilities	7.6	2.8	19,975
Variable costs	91.7	34.2	242,117
Operating labor (42/shift; 17.50 $/hr)	2.4	0.9	6,439
Maintenance labor (1.6% BLI)	5.5	2.0	14,480
Control lab. labor (20% op. labor)	0.5	0.2	1,288
Total direct labor	8.4	3.1	22,207
Maintenance materials (2.4% BLI)	8.2	3.1	21,720
Operating supplies (10% op. labor)	0.2	0.1	644
	8.4	3.2	22,364
Plant overhead (30% total labor)	2.5	0.9	6,662
Taxes and insurance (2% TFC)	8.2	3.1	21,600
Depreciation (10% TFC)	40.9	15.3	108,000
	51.6	19.3	136,262
Subtotal: plant gate cost	160.1	59.8	422,950
G&A, sales, research (3% PV)	8.1	3.0	21,431
ROI before taxes (25% TFC)	102.2	38.1	270,000
Product value (PV)	270.4	100.9	714,381
$/million Btu*	8.27		
¢/lb (CO + H_2)*	8.27		

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*0.327 million Btu/mscf (HHV).
30.60 scf/lb.

Table 6.27

SYNGAS (H_2:CO = 2) FROM COAL

PRODUCTION COSTS

Time: Mid-1981
Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity: Basis contained (CO + H_2) - 805.0 x 10^6 scfd
88,400 lb-mol/hr
264.4 x 10^9 scf/yr

Stream Factor: 0.9

Process units include:

1. Coal preparation	15,000 metric tons/day as received Illinois No. 6
2. Air separation	12,800 metric tons/day oxygen (100% basis)
3. Coal gasification (Texaco with WHB)	810 million scfd (CO + H_2)
4. Shift conversion (4.8 H_2/CO ratio)	480 million scfd (CO + H_2)
5. COS hydrolysis	330 million scfd (CO + H_2)
6. Acid gas removal (Rectisol process)	1,212 million scfd feed gas
7. Sulfur recovery (Claus & Beavon processes)	462 metric tons/day sulfur

Investment (million $)

Battery limits (BLI)	919
Off-sites	177
Total fixed capital (TFC)	1,096

Variable Cost Summary

	Unit Cost	Consumption per 10^6 scf	¢/1,000 scf	$/1,000 Nm^3	$1,000/yr
Raw materials					
Coal at mine	32.3$/metric ton	18.64	60.2	22.5	159,158
Coal transport	15.0$/metric ton	18.64	28.0	10.5	73,913
Ash disposal	5.0$/metric ton	1.86	1.0	0.3	2,646
Misc. cat. and chem.	1.0$/unit	6.07	0.6	0.2	1,604
			89.8	33.5	237,321
By-product					
Sulfur	100$/metric ton	(0.57)	(5.7)	(2.1)	(15,111)
Imported utilities					
Clarified water	0.68$/1,000 gal	15.09	1.0	0.4	2,713
Electricity	3.6¢/kwh	(91.0)	(0.3)	(0.1)	(866)
Steam (HP)	7.73$/1,000 lb	8	6.1	2.3	16,207
			6.8	2.6	18,054
Total variable costs			90.9	33.9	240,264

Table 6.27 (Concluded)

SYNGAS (H_2:CO = 2) FROM COAL

PRODUCTION COSTS

	¢/1,000 scf	\$/1,000 Nm^3	\$1,000/yr
Production costs			
Raw materials	89.8	33.5	237,321
By-product credit	(5.7)	(2.1)	(15,111)
Imported utilities	6.8	2.5	18,054
Variable costs	90.9	33.9	240,264
Operating labor (42/shift; 17.50 \$/hr)	2.4	0.9	6,439
Maintenance labor (1.6% BLI)	5.6	2.1	14,704
Control lab. labor (20% op. labor)	0.5	0.2	1,288
Total direct labor	8.5	3.2	22,431
Maintenance materials (2.4% BLI)	8.3	3.1	22,056
Operating supplies (10% op. labor)	0.2	0.1	644
	8.5	3.2	22,700
Plant overhead (30% total labor)	2.5	0.9	6,729
Taxes and insurance (2% TFC)	8.3	3.1	21,920
Depreciation (10% TFC)	41.5	15.5	109,600
	52.3	19.5	138,249
Subtotal: plant gate cost	160.2	59.8	423,644
G&A, sales, research (3% PV)	8.2	3.0	21,576
ROI before taxes (25% TFC)	103.6	38.7	274,000
Product value (PV)	272.0	101.5	719,220
\$/million Btu*	8.32		
¢/lb (CO + H_2)*	9.68		

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*0.327 million Btu/mscf (HHV).
35.58 scf/lb.

Table 6.28

HYDROGEN (97%) FROM COAL

PRODUCTION COSTS

Time:	**Mid-1981**
Location:	**U.S. Gulf Coast**
PEP Cost Index:	**400**

Capacity: 781×10^6 scfd (100% basis)
256.6×10^9 scf/yr
1,352 million lb/yr
613,000 metric tons/yr

Stream Factor: 0.9

Process units include:

1.	Coal preparation	15,000 metric tons/day as received Illinois No. 6
2.	Air separation	12,800 metric tons/day oxygen (100% basis)
3.	Coal gasification (Texaco with WHB)	810 million scfd ($CO + H_2$)
4.	High and low temp. shift	810 million scfd ($CO + H_2$)
5.	COS hydrolysis	—
6.	Acid gas removal (Rectisol process)	1,475 million scfd feed gas
7.	Sulfur recovery (Claus & Beavon processes)	462 metric tons/day sulfur
8.	Methanation	803 million scfd feed gas

Investment (million $)

Battery limits (BLI)	1,049
Off-sites	194
Total fixed capital (TFC)	1,243

Variable Cost Summary

	Unit Cost	Consumption per 10^6 scf	¢/lb	¢/1,000 scf	$1,000/yr
Raw materials					
Coal at mine	32.3$/metric ton	19.19	11.77	62.0	159,158
Coal transport	15.0$/metric ton	19.19	5.47	28.8	73,913
Ash disposal	5.0$/metric ton	1.92	0.18	1.0	2,464
Misc. cat. and chem.	1.0$/unit	15.32	0.29	1.5	3,930
			17.71	93.3	239,465
By-product					
Sulfur	100$/metric ton	(0.59)	(1.12)	(5.9)	(15,111)
Imported utilities					
Clarified water	0.68$/1,000 gal	16.0	0.21	1.1	2,788
Electricity	3.6¢/kwh	30.7	0.02	0.1	284
Steam (HP)	7.73$/1,000 lb	16.3	2.48	13.1	33,522
Steam (LP)	—	(16.9)	—	—	—
			2.71	14.3	36,594
Total variable costs			19.30	101.7	260,948

Table 6.28 (Concluded)

HYDROGEN (97%) FROM COAL

PRODUCTION COSTS

	¢/lb	¢/1,000 scf	$1,000/yr
Production costs			
Raw materials	17.71	93.3	239,465
By-product credit	(1.12)	(5.9)	(15,111)
Imported utilities	2.71	14.3	36,594
Variable costs	19.30	101.7	260,948
Operating labor (46/shift; 17.50 $/hr)	0.53	2.8	7,052
Maintenance labor (1.6% BLI)	1.24	6.5	16,784
Control lab. labor (20% op. labor)	0.10	0.5	1,410
Total direct labor	1.87	9.8	25,246
Maintenance materials (2.4% BLI)	1.86	9.8	25,176
Operating supplies (10% op. labor)	0.05	0.3	705
	1.91	10.1	25,881
Plant overhead (30% total labor)	0.56	3.0	7,574
Taxes and insurance (2% TFC)	1.84	9.7	24,860
Depreciation (10% TFC)	9.19	48.4	124,300
	11.59	61.1	156,734
Subtotal: plant gate cost	34.67	182.7	468,809
G&A, sales, research (3% PV)	1.78	9.4	24,110
ROI before taxes (25% TFC)	22.98	121.1	310,750
Product value (PV)	59.43	313.2	803,669
$/1,000 Nm^3	116.9		
$/million Btu*	9.67		

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*0.324 million Btu/mscf (HHV).

7 CARBON MONOXIDE SEPARATION FROM SYNGAS

As outlined in Section 3, in some applications of syngas the overall reaction chemistry requires purified carbon monoxide in addition to CO/H_2 mixtures. Notable examples are the synthesis of acetic acid and acetic anhydride. Both these cases entail carbonylation with CO. Thus, the well established Monsanto acetic acid process carbonylates methanol. The Eastman/Halcon technology for acetic anhydride (due for commercialization in 1983) first synthesizes methyl acetate by esterification of methanol with acetic acid. The acetic anhydride then follows from the carbonylation of methyl acetate. There are also many other applications for CO such as the production of phosgene (by reaction of CO with Cl_2).

For all these applications the CO is generally separated from syngas. The separation can be effected cryogenically or by selective absorption of CO in a solvent. Two examples of these methods, which are well proven commercially, are evaluated in Section 4 for their use in adjusting H_2:CO ratios of syngas by "skimming" some of the hydrogen. These are the cryogenic, liquid methane wash system and the Cosorb® process, which uses a selective solvent consisting of cuprous aluminum chloride ($CuAlCl_4$) dissolved in toluene. Both these methods are capable of producing a 99%+ (vol) CO, with hydrogen (or a hydrogen-rich stream) as the principal coproduct. The other methods considered for "hydrogen skimming," (pressure swing adsorption and that using Monsanto's Prism® separators) do not yield CO of sufficient purity to be relevant in the present context. The economics of CO production depend not only on the costs for the separation itself and the unit cost (or transfer price) of the syngas but also in a significant way on the credits for the hydrogen coproduct. This was illustrated in PEP Report 123, "Carbon Monoxide Recovery," July 1979. In that report SRI examined the recovery of CO from syngas derived from natural gas (H_2:CO ratio = 3.4) cryogenically and the separation of CO from blast furnace gases by Cosorb®.

This section examines the economics of CO production from various syngases produced from each of the three basic feedstocks; natural gas, a heavy petroleum oil fraction, and coal. For both oil and coal we took an initial mixture that corresponds to a methanol synthesis stream, cost data for which are presented in Sections 5 and 6. For natural gas the choice was not clear; we arbitrarily chose two streams—a syngas with an H_2:CO ratio = 3 and a crude methanol-synthesis feed. The former corresponds to the "stoichiometric ratio" obtained in the steam reforming of natural gas (i.e., without any CO_2 import but with CO_2 recycle as shown in Section 4). Both these streams are evaluated for production costs at the large scale (300 million scfd) in Section 4. The details of the cost modules that we developed for CO are given in Table 7.1. We took the production scale of CO at 150 million lb/yr (approx. 6 million scfd) to match a typical world-size acetic acid plant with a capacity of about 300 million lb/yr. The syngas feed and CO product compositions for the cost modules listed in Table 7.1 are shown in Table 7.2.

We used the methanol syngas stream to illustrate the economics when CO production for acetic acid is integrated with methanol manufacture. However, when methanol is made by the steam reforming of natural gas, it is not always practical to integrate the required CO production with the main syngas generation. This is because methanol syngas, made by the steam reforming of natural gas is (in a stoichiometric sense) deficient in carbon. It is usual to import CO_2, where this is possible, to make up for this deficiency. The removal of CO for acetic acid synthesis would therefore work in the opposite direction. In such a situation, it has been the standard practice to have an independent syngas generation as a source of CO, e.g., as in the Celanese methanol facilities at Bishop and Clear Lake, Texas and in those of Monsanto at Texas City, Texas. When coal or a heavy oil fraction is the feedstock in syngas generation for methanol synthesis, integration with CO production becomes feasible because both the partial oxidation of a heavy oil fraction and the gasification of coal readily yield a syngas that has the necessary surplus carbon to furnish CO for carbonylation. The recently commissioned Du Pont-U.S. Industrial Chemical Company facility at

Table 7.1

DETAILS OF COST MODULES EXAMINED FOR PRODUCTION OF CARBON MONOXIDE

	Module 7.1	Module 7.2	Module 7.3
Syngas source	MeOH syngas from steam reforming of natural gas	Same as for Module 7.1	Syngas with H_2:CO ratio = 3 from natural gas steam reforming with CO_2 recycle
Constituent stages of module	(1) CO_2 removal by MEA scrubbing. (2) Molecular sieving to remove traces of CO_2/H_2O. (3) Cryogenic separation.	(1) Molecular sieving to remove H_2O. (2) Cosorb® separation (inc. recompression of CO).	Same as (1) and (2) in Module 7.2 plus (3) Methanation of H_2 product.
Syngas usage (scf/lb CO)	100.9	95.9	54.8
Coproducts			
H_2 product (lb/lb CO)	0.375	82.1 scf/lb CO of 85 vol% H_2	0.2107
Fuel stream (Btu/lb CO)	3,898	—	86.9

	Module 7.4	Module 7.5	Module 7.6
Syngas source	Same as for Module 7.3.	Partial oxidation of vacuum residue to give H_2:CO ratio = 2 by use of CO shift.	MeOH syngas from gasification of coal.
Constituent stages of module	(1) CO_2, H_2O removal by molecular sieves. (2) Cryogenic separation.	Same as for Module 7.4.	(1) Molecular sieving to remove H_2O. (2) Cosorb® separation.
Syngas usage (scf/lb CO)	55.1	42.5	46.8
Coproducts			
H_2 product (lb/lb CO)	0.207	0.143	3.22 scf/lb CO of 93 vol% H_2
Fuel stream (Btu/lb CO)	491	368	—

Table 7.2

SYNGAS AND CARBON MONOXIDE PRODUCT COMPOSITIONS FOR COST MODULES

	Syngas Feed Composition (vol%) CO						Product Composition (vol%)					
	CH_4	CO_2	CO	H_2	N_2	H_2O	CH_4	CO_2	CO	H_2	N_2	H_2O
Module 7.1 (Crude syngas from natural gas + cryogenic)	3.69	7.78	14.87	73.08	0.19	0.39	0.12	<1 ppm	99.0	0.35	0.53	<1 ppm
Module 7.2 (Crude syngas from natural gas + Cosorb®)	As for Module 7.1 above.						0.14	0.32	96.57	2.89	tr	—
Module 7.3 (3/1 syngas from natural gas + Cosorb®)	1.32	0.01	24.73	73.08	0.19	0.67	tr	tr	99.75	0.25	tr	<1 ppm
Module 7.4 (3/1 syngas from natural gas + cryogenic)	As for Module 7.3 above.						0.12	<1 ppm	99.0	0.35	0.53	<1 ppm
Module 7.5 (2/1 syngas from vac. residue + cryogenic)	0.32	0.01	32.87	65.74	1.06	tr	0.17	<1 ppm	97.13	0.37	2.33	<1 ppm
Module 7.6 (Coal derived MeOH syngas + Cosorb®)	0.39	3.09	29.15	65.91	1.46	tr	tr	0.01	99.75	0.23	tr	<1 ppm

Deer Park, Texas (using partial oxidation of a heavy, sour residue) and Eastman's projected coal-based complex for acetic anhydride at Kingsport, Tennessee (due onstream in 1983) are examples of such integration.

Main Features of Separation Modules

A schematic block diagram for each of the modules and the main mass balances are presented in Figures 7.1-7.6. The detailed flow diagrams for the key separation methods used in the modules (methods based on cryogenic and Cosorb® processes) are described in Section 4 for their application in adjusting H_2:CO ratios.

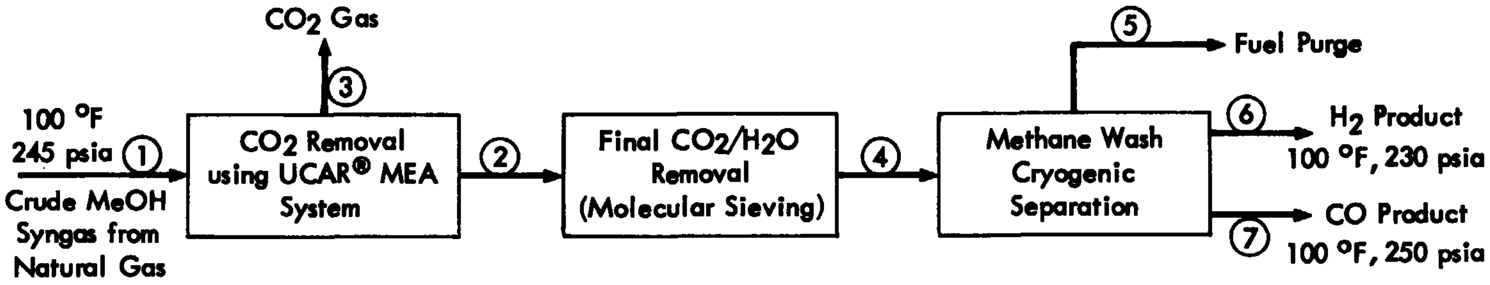
In terms of the final CO product purity the cryogenic method is limited by economics to about 99 vol% but when appreciable nitrogen is present (as in our assumed syngas derived from vacuum residue by partial oxidation), virtually all this N_2 appears in the CO product, owing to its similar volatility. With Cosorb® the final CO purity is not influenced by the presence of N_2 (because the solvent used in CO absorption has low N_2 solubility).

With the cryogenic separation a hydrogen product with less than 10 ppm CO (which is acceptable for chemical applications) can be easily made. Tenneco states that this is also possible with Cosorb® but we judge that it would be more economical to reduce CO levels to about 0.1 vol% and include an additional stage for methanating residual carbon oxides, e.g., in Module 7.3. This approach will not apply to H_2 rich streams which contain appreciable levels of CO_2 (Modules 7.2. and 7.6). The use of methanation in these cases will be practical only after prior removal of CO_2.

Both processes require the prior removal of water to 0.1 ppm and the cryogenic method requires such a rigorous removal of CO_2 as well. In the Cosorb® method the small amount of water present leads to the formation of HCl by reaction with the absorbent. When HCl at the relatively low levels formed cannot be tolerated, further treatment of the CO product becomes necessary, e.g., by an adsorption stage to remove HCl. The cost of this additional step is marginal.

Figure 7.1

SCHEMATIC DIAGRAM AND MASS BALANCES FOR CO SEPARATION FROM CRUDE METHANOL SYNGAS (DERIVED FROM NATURAL GAS) BY UCAR® CO2 REMOVAL/CRYOGENIC SEPARATION SYSTEMS (MODULE 7.1)

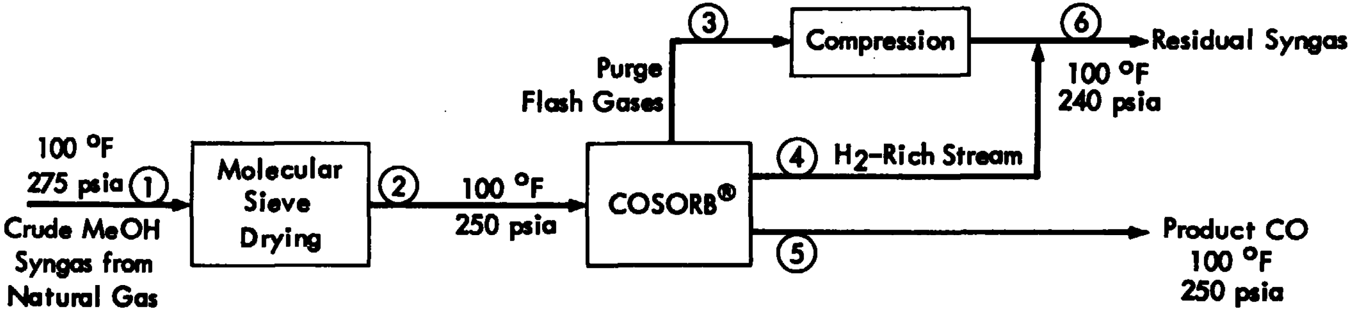


Stream Flows (lb-mols/hr, 150 million lb/yr CO)

Component	(1) Crude Syngas	(2) CO_2 Lean Syngas	(3) CO_2 Stream	(4) Sieved Syngas	(5) Fuel Purge	(6) H_2 Product	(7) CO Product
Methane	186.56	186.56		186.56	135.93	49.81	0.82
CO_2	393.39	0.46	392.93	Tr			
CO	751.56	751.56		751.56	71.16		676.41
H_2	3,694.81	3,694.81		3,694.81	136.92	3,555.49	2.39
N_2(+ Inerts)	9.63	9.63		9.63	16.80	4.33	3.62
H_2O	19.87	19.83		Tr			
Total	5,055.82	4,662.89	392.93	4,642.60	360.81	3,009.63	683.24

Figure 7.2

SCHEMATIC DIAGRAM AND MASS BALANCES FOR CO SEPARATION FROM CRUDE METHANOL SYNGAS (DERIVED FROM NATURAL GAS) BY COSORB® METHOD (MODULE 7.2)

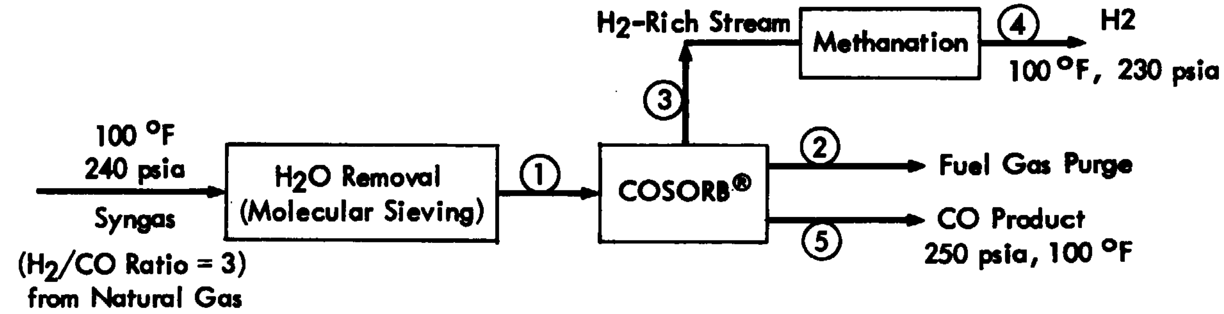


Stream Flows (lb-mols/hr, 150 million lb/yr CO)

Component	(1) Crude Syngas	(2) Dried Crude Syngas	(3) Purge	(4) H2-Rich Product	(5) CO Product	(6) Residual Syngas
Methane	177.27	177.27	1.43	174.78	1.05	176.21
CO_2	373.78	373.78	3.02	368.54	2.22	371.56
CO	714.11	714.11	34.68	3.03	676.41	37.71
H_2	3,510.69	3,510.69	28.37	3,461.45	20.86	3,489.82
N_2(+Inerts)	9.15	9.15	0.07	9.02	0.06	9.09
H_2O	18.88					
Total	4,803.88	4,785.00	76.52	4,016.82	700.60	4,084.39

Figure 7.3

SCHEMATIC DIAGRAM AND MASS BALANCES FOR CO SEPARATION FROM SYNGAS (H2:CO RATIO = 3:1, DERIVED FROM NATURAL GAS) BY COSORB® METHOD (MODULE 7.3)

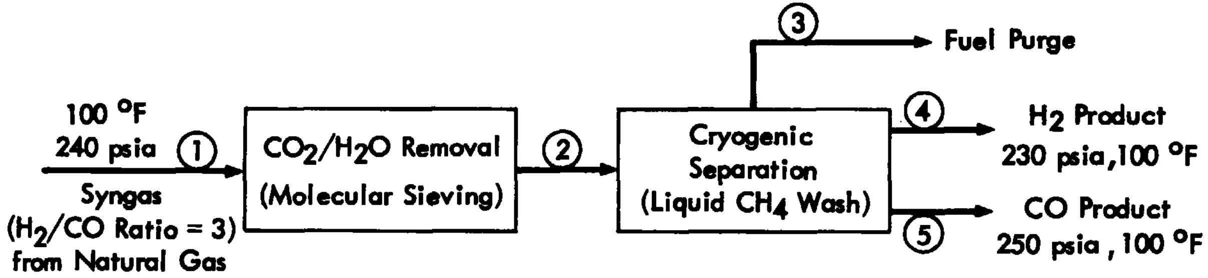


Stream Flows (lb-mols/hr, 150 million lb/yr CO)

Component	(1) Dried Syngas	(2) Fuel Purge	(3) H_2 Product	(4) Methanated H_2	(5) CO Product
CH_4	36.26	0.17	36.06	37.21	0.03
CO_2	0.34		0.34	Tr	Tr
CO	680.54	3.32	0.81	Tr	676.41
H_2	2,010.93	9.66	1,999.59	1,995.80	1.68
N_2	5.29	0.03	5.25	5.25	0.01
H_2O				1.49	
Total	2,733.36	13.18	2,042.05	2,039.75	678.13

Figure 7.4

SCHAMATIC DIAGRAM AND MASS BALANCES FOR CO SEPARATION FROM SYNGAS (H_2:CO RATIO = 3:1, DERIVED FROM NATURAL GAS) BY CRYOGENIC METHOD (MODULE 7.4)

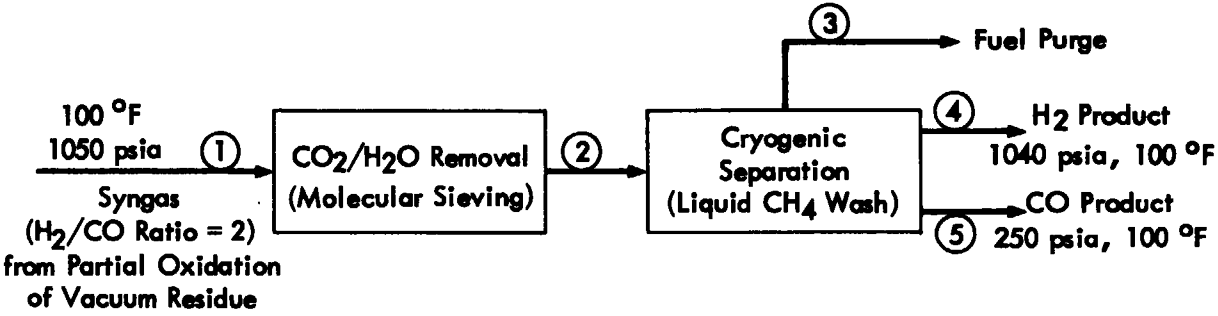


Stream Flows (lb-mols/hr, 150 million lb/yr CO)

Component	(1) 3/1 Syngas	(2) Purged Syngas	(3) Fuel Purge	(4) H_2 Product	(5) CO Product
CH_4	36.40	36.40	6.29	29.29	0.82
CO_2	0.34	Tr	–	–	–
CO	683.24	683.24	6.83	Tr	676.41
H_2	2,018.91	2,018.91	53.77	1,962.75	2.39
N_2	5.31	5.31	1.09	0.60	3.62
H_2O	18.56	Tr	–	–	–
Total	2,762.76	2,743.86	67.98	1,992.64	683.24

Figure 7.5

SCHEMATIC DIAGRAM AND MASS BALANCES FOR CO SEPARATION FROM SYNGAS (H_2:CO RATIO = 2:1, DERIVED FROM PARTIAL OXIDATION OF VACUUM RESIDUE) BY CRYOGENIC METHOD (MODULE 7.5)

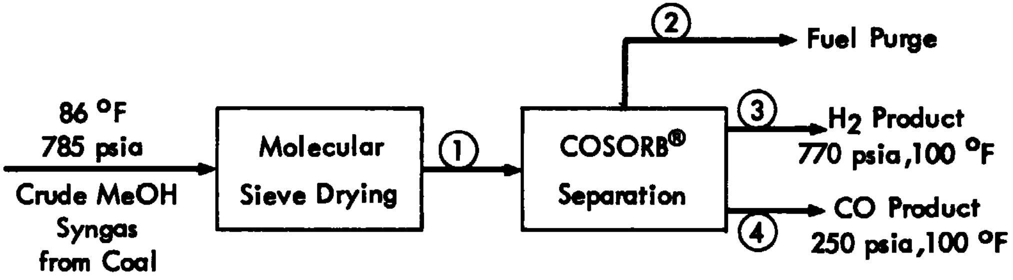


Stream Flows (lb-mols/hr, 150 million lb/yr CO)

Component	(1) Syngas	(2) Sieved Syngas	(3) Fuel Purge	(4) H_2 Product	(5) CO Product
CH_4	6.75	6.75	1.03	4.56	1.16
CO_2	0.21	Tr	–	Tr	Tr
CO	697.33	697.33	20.92	Tr	676.41
H_2	1,394.66	1,394.66	36.15	1,355.91	2.60
N_2	22.48	22.48	2.67	3.55	16.26
H_2O	Tr	Tr	–	–	Tr
Total	2,121.43	2,121.22	60.77	1,364.02	696.43

Figure 7.6

SCHEMATIC DIAGRAM AND MASS BALANCES FOR CO SEPARATION FROM CRUDE METHANOL SYNGAS (DERIVED FROM COAL) BY COSORB®METHOD (MODULE 7.6)



Stream Flows (lb-mols/hr, 150 million lb/yr CO)

Component	(1) Dried Syngas	(2) Fuel Purge	(3) H_2 Product	(4) CO Product
CH_4	9.01	0.05	8.95	0.01
CO_2	72.09	0.43	71.59	0.07
CO	680.54	3.34	0.79	676.41
H_2	1,538.90	9.17	1,528.14	1.59
N_2	34.26	0.20	34.02	0.04
H_2O	< 1 ppm	–	–	–
Total	2,334.80	13.19	1,643.49	678.12

Cost Estimates

The production costs for the six cases (or modules) examined are summarized in Table 7.3. Details are presented in Tables 7.4-7.9. The unit costs for the various syngases are those presented in the relevant Sections 4, 5, and 6 for the three basic feedstocks. For illustration the H_2 product is shown as a chemical credit when this is justified by its purity. The value of 50¢/lb H_2 (equivalent to $2.64/1,000 scf) that we used is consistent with production costs from $4.17/million Btu natural gas at typical world scales in the region of 200 million lb/yr. In two of the cases examined, the separation of CO from crude syngases (those derived from natural gas and coal, Modules 1 and 6), the H_2-rich streams are not chemical grade. We credited these streams at the initial unit price of the syngas. In one of the cases, the cryogenic separation of CO from a natural gas derived methanol syngas, some CO_2 is produced in the upstream monoethanolamine scrubbing. Again, for illustration we used a credit of 1.5¢/lb, which (as discussed in Section 4) relates to liquid CO_2 for refrigeration.

Table 7.3

CARBON MONOXIDE COSTS FROM VARIOUS SEPARATION MODULES

	Crude Syngas From Nat. Gas + Cryogenic	Crude Syngas From Nat. Gas + Cosorb®	3/1 Syngas From Nat. Gas + Cosorb®	3/1 Syngas From Nat. Gas + Cryogenic	2/1 Syngas From Vac. Resid. Partial Oxidation + Cryogenic	Coal Derived MeOH Syngas + Cosorb®
CO scale (million lb/yr)	150	150	150	150	150	150
Fixed capital for module ($ million)	19.7	14.0	9.9	5.5	6.0	9.7
Unit syn gas price[*] ($/mscf)	1.90	1.90	2.46	2.46	2.78	2.78
H_2 coproduct purity (vol%)	98.5	86.2	98.0	98.5	99.4	93.0
Assumed H_2 coproduct[†] credit ($/mscf)	2.64	1.90	2.64	2.64	2.64	2.78
Variable costs for CO						
Excluding by-product credits (¢/lb)	21.37	19.63	14.61	14.31	12.44	13.60
Including by-product credits (¢/lb)	-0.37	4.03	4.04	3.76	5.14	5.04
Product value (inc. 25% ROI)	6.57	8.83	7.75	6.25	7.77	8.71

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[*] Unit costs are the product values of these streams.

[†] A unit cost of $2.64/mscf is equivalent to 50¢/lb H_2, expressed on a 100% basis.

Table 7.4

CARBON MONOXIDE BY CRYOGENIC SEPARATION OF CRUDE SYNGAS FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Crude syngas	190¢/mscf	0.1009 mscf	19.17
Misc. chemicals			0.21
Gross raw materials			19.38
By-products			
Carbon dioxide	1.5¢/lb	-0.91 lb	-1.36
Hydrogen (98.5%)	50¢/lb	-0.375 lb	-18.75
Fuel gas	0.417¢/1,000 Btu	-3,898 Btu	-1.63
Total by-products			-21.74
Utilities			
Cooling water	5.4¢/1,000 gal	19 gal	0.10
Steam	$5.44/1,000 gal	1.15 lb	0.63
Electricity	3.6¢/kwh	0.35 kwh	1.26
Total utilities			1.99

Table 7.4 (Concluded)

CARBON MONOXIDE BY CRYOGENIC SEPARATION OF CRUDE SYNGAS FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)*	75	150†	300
Investment ($ million)			
Battery limits	11.4	17.9	28.1
Off-sites	1.2	1.8	2.8
Total fixed capital	12.6	19.7	30.9
Scaling exponents		0.65	0.65
Production costs (¢/lb)			
Raw materials	19.38	19.38	19.38
By-products	-21.74	-21.74	-21.74
Utilities	1.99	1.99	1.99
Variable costs	-0.37	-0.37	-0.37
Operating labor, 4/shift§, $17.50/hr	0.82	0.41	0.20
Maintenance labor, 2%/yr of BL inv	0.30	0.24	0.19
Control lab labor, 20% of op labor	0.16	0.08	0.04
Labor costs	1.28	0.73	0.43
Maintenance materials, 2%/yr of BL inv	0.30	0.24	0.19
Operating supplies, 10% of op labor	0.08	0.04	0.02
TOTAL DIRECT COSTS	1.29	0.64	0.27
Plant overhead, 80% of labor costs	1.03	0.58	0.35
Taxes and insurance, 2%/yr of TFC	0.33	0.26	0.21
Depreciation, 10%/yr of TFC	1.67	1.31	1.03
Plant gate cost	4.32	2.79	1.86
G&A, sales, research	0.50	0.50	0.50
NET PRODUCTION COST	4.82	3.29	2.36
ROI before taxes, 25%/yr of TFC	4.20	3.28	2.57
PRODUCT VALUE	9.02	6.57	4.93

---

*Of carbon monoxide.

†Base case.

§For base case; may be different for other capacities.

Table 7.5

CARBON MONOXIDE BY COSORB® SEPARATION OF CRUDE SYNGAS FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Crude syngas	190¢/mscf	0.0959 mscf	18.22
Misc. chemicals			0.15
Gross raw materials			18.37
By-product			
Hydrogen-rich product	190¢/mscf	-0.0821 mscf	-15.60
Utilities			
Cooling water	5.4¢/1,000 gal	3.5 gal	0.02
Steam	$5.44/1,000 gal	1.21 lb	0.66
Electricity	3.6¢/kwh	0.16 kwh	0.58
Total utilities			1.26

Table 7.5 (Concluded)

CARBON MONOXIDE BY COSORB® SEPARATION OF CRUDE SYNGAS FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)*	75	150†	300
Investment ($ million)			
Battery limits	6.6	10.4	16.3
Off-sites	2.3	3.6	5.7
Total fixed capital	8.9	14.0	22.0
Scaling exponents		0.65	0.65
Production costs (¢/lb)			
Raw materials	18.37	18.37	18.37
By-products	-15.60	-15.60	-15.60
Utilities	1.26	1.26	1.26
Variable costs	4.03	4.03	4.03
Operating labor, 2/shift§, $17.50/hr	0.41	0.20	0.10
Maintenance labor, 2%/yr of BL inv	0.18	0.14	0.11
Control lab labor, 20% of op labor	0.08	0.04	0.02
Labor costs	0.67	0.38	0.23
Maintenance materials, 2%/yr of BL inv	0.18	0.14	0.11
Operating supplies, 10% of op labor	0.04	0.02	0.01
TOTAL DIRECT COSTS	4.92	4.57	4.38
Plant overhead, 80% of labor costs	0.53	0.31	0.19
Taxes and insurance, 2%/yr of TFC	0.24	0.19	0.15
Depreciation, 10%/yr of TFC	1.19	0.93	0.73
Plant gate cost	6.88	6.00	5.45
G&A, sales, research	0.50	0.50	0.50
NET PRODUCTION COST	7.38	6.50	5.95
ROI before taxes, 25%/yr of TFC	2.97	2.33	1.83
PRODUCT VALUE	10.35	8.83	7.78

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*Of carbon monoxide.

†Base case.

§For base case; may be different for other capacities.

Table 7.6

CARBON MONOXIDE BY COSORB® SEPARATION OF SYNGAS (H_2:CO RATIO = 3:1) FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Syngas (3/1 ratio)	246¢/mscf	0.0548 mscf	13.47
Misc. chemicals			0.13
Gross raw materials			13.60
By-products			
Hydrogen (98%)	50¢/lb	-0.2107 lb	-10.53
Fuel gas	0.417¢/1,000 Btu	-86.9 Btu	-0.04
Total by-products			-10.57
Utilities			
Cooling water	5.4¢/1,000 gal	3 gal	0.02
Steam	$5.44/1,000 gal	1.03 lb	0.56
Electricity	3.6¢/kwh	0.12 kwh	0.43
Total utilities			1.01

Table 7.6 (Concluded)

CARBON MONOXIDE BY COSORB® SEPARATION OF SYNGAS (H_2:CO RATIO = 3:1) FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)[*]	75		150[†]		300
Investment ($ million)					
Battery limits	5.5		8.6		13.5
Off-sites	0.8		1.3		2.0
Total fixed capital	6.3		9.9		15.5
Scaling exponents		0.65		0.65	
Production costs (¢/lb)					
Raw materials	13.60		13.60		13.60
By-products	-10.57		-10.57		-10.57
Utilities	1.01		1.01		1.01
Variable costs	4.04		4.04		4.04
Operating labor, 2/shift[§], $17.50/hr	0.41		0.20		0.10
Maintenance labor, 2%/yr of BL inv	0.15		0.11		0.09
Control lab labor, 20% of op labor	0.08		0.04		0.01
Labor costs	0.64		0.35		0.21
Maintenance materials, 2%/yr of BL inv	0.15		0.11		0.09
Operating supplies, 10% of op labor	0.04		0.02		0.01
TOTAL DIRECT COSTS	4.87		4.52		4.35
Plant overhead, 80% of labor costs	0.51		0.29		0.17
Taxes and insurance, 2%/yr of TFC	0.17		0.13		0.10
Depreciation, 10%/yr of TFC	0.84		0.66		0.52
Plant gate cost	6.39		5.60		5.14
G&A, sales, research	0.50		0.50		0.50
NET PRODUCTION COST	6.89		6.10		5.64
ROI before taxes, 25%/yr of TFC	2.10		1.65		1.29
PRODUCT VALUE	8.99		7.75		6.93

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[*] Of carbon monoxide.

[†] Base case.

[§] For base case; may be different for other capacities.

Table 7.7

CARBON MONOXIDE BY CRYOGENIC SEPARATION OF SYNGAS (H_2:CO RATIO = 3:1) FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Syngas (3/1 ratio)	246¢/mscf	0.0551 mscf	13.56
Misc. chemicals			0.05
Gross raw materials			13.60
By-products			
Hydrogen (98.5%)	50¢/lb	-0.207 lb	-10.35
Fuel gas	0.417¢/1,000 Btu	-49.1 Btu	-0.20
Total by-products			-10.55
Utilities			
Cooling water	5.4¢/1,000 gal	1.2 gal	0.01
Electricity	3.6 ¢/kwh	0.195 kwh	0.70
Total utilities			0.71

Table 7.7 (Concluded)

CARBON MONOXIDE BY CRYOGENIC SEPARATION OF SYNGAS (H_2:CO RATIO = 3:1) FROM NATURAL GAS

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)[*]	75		150[†]		300
Investment ($ million)					
Battery limits	3.2		4.8		7.3
Off-sites	0.4		0.7		1.0
Total fixed capital	3.6		5.5		8.3
Scaling exponents		0.60		0.60	
Production costs (¢/lb)					
Raw materials	13.60		13.60		13.60
By-products	-10.55		-10.55		-10.55
Utilities	0.71		0.71		0.71
Variable costs	3.76		3.76		3.76
Operating labor, 2/shift[§], $17.50/hr	0.41		0.20		0.10
Maintenance labor, 2%/yr of BL inv	0.08		0.06		0.05
Control lab labor, 20% of op labor	0.08		0.04		0.02
Labor costs	0.57		0.30		0.17
Maintenance materials, 2%/yr of BL inv	0.08		0.06		0.05
Operating supplies, 10% of op labor	0.04		0.02		0.01
TOTAL DIRECT COSTS	4.45		4.14		3.99
Plant overhead, 80% of labor costs	0.46		0.25		0.14
Taxes and insurance, 2%/yr of TFC	0.10		0.07		0.06
Depreciation, 10%/yr of TFC	0.48		0.37		0.28
Plant gate cost	5.49		4.83		4.47
G&A, sales, research	0.50		0.50		0.50
NET PRODUCTION COST	5.99		5.33		4.97
ROI before taxes, 25%/yr of TFC	1.20		0.92		0.69
PRODUCT VALUE	7.19		6.25		5.66

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[*] Of carbon monoxide.

[†] Base case.

[§] For base case; may be different for other capacities.

Table 7.8

CARBON MONOXIDE BY CRYOGENIC SEPARATION OF SYNGAS (H_2:CO RATIO = 2:1) FROM PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs

	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Syngas (2/1 ratio)	278¢/mscf	0.0425 mscf	11.82
Misc. chemicals			0.04
Gross raw materials			11.86
By-products			
Hydrogen (99.4%)	50¢/lb	-0.143 lb	-7.15
Fuel gas	0.417¢/1,000 Btu	-368 Btu	-0.15
Total by-products			-7.30
Utilities			
Cooling water	5.4¢/1,000 gal	1.2 gal	0.01
Electricity	3.6 ¢/kwh	0.158 kwh	0.57
Total utilities			0.58

Table 7.8 (Concluded)

CARBON MONOXIDE BY CRYOGENIC SEPARATION OF SYNGAS (H_2:CO RATIO = 2:1) FROM PARTIAL OXIDATION OF VACUUM RESIDUE

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lbf/yr)[*]	75	150[†]	300
Investment ($ million)			
Battery limits	3.4	5.2	7.9
Off-sites	0.6	0.8	1.2
Total fixed capital	4.0	6.0	9.1
Scaling exponents		0.60	0.60
Production costs (¢/lb)			
Raw materials	11.86	11.86	11.86
By-products	-7.30	-7.30	-7.30
Utilities	0.58	0.58	0.58
Variable costs	5.14	5.14	5.14
Operating labor, 2/shift[§], $17.50/hr	0.41	0.20	0.10
Maintenance labor, 2%/yr of BL inv	0.09	0.07	0.05
Control lab labor, 20% of op labor	0.08	0.04	0.02
Labor costs	0.58	0.31	0.17
Maintenance materials, 2%/yr of BL inv	0.09	0.07	0.05
Operating supplies, 10% of op labor	0.04	0.02	0.01
TOTAL DIRECT COSTS	5.85	5.54	5.37
Plant overhead, 80% of labor costs	0.47	0.25	0.14
Taxes and insurance, 2%/yr of TFC	0.11	0.08	0.06
Depreciation, 10%/yr of TFC	0.53	0.40	0.30
Plant gate cost	6.96	6.27	5.87
G&A, sales, research	0.50	0.50	0.50
NET PRODUCTION COST	7.46	6.77	6.37
ROI before taxes, 25%/yr of TFC	1.33	1.00	0.76
PRODUCT VALUE	8.79	7.77	7.13

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[*] Of carbon monoxide.

[†] Base case.

[§] For base case; may be different for other capacities.

Table 7.9

CARBON MONOXIDE BY COSORB® SEPARATION OF METHANOL SYNGAS FROM COAL

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Variable costs	Unit Cost	Consumption/lb	¢/lb
Raw materials			
Syngas (as for MeOH)	264¢/mscf*	0.0468 mscf	12.36
Misc. chemicals	1¢	0.13	0.13
Gross raw materials			13.14
By-product			
Hydrogen-rich stream	258¢/mscf*	-0.0332 mscf	-8.57
Utilities			
Cooling water	5.4¢/1,000 gal	3 gal	0.02
Steam	$6.40/1,000 lb	1.03 lb	0.66
Electricity	3.6¢/kwh	0.12 kwh	0.43
Total utilities			1.11

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*Unit values refer to 278¢/mscf on a (CO + H_2) contained basis.

Table 7.9 (Concluded)

CARBON MONOXIDE BY COSORB® SEPARATION OF METHANOL SYNGAS FROM COAL

PRODUCTION COSTS

Location: U.S. Gulf Coast
PEP Cost Index: 400

Capacity (million lb/yr)[*]	75		150[†]		300
Investment ($ million)					
Battery limits	5.4		8.4		13.2
Off-sites	0.8		1.3		2.0
Total fixed capital	6.2		9.7		15.2
Scaling exponents		0.65		0.65	
Production costs (¢/lb)					
Raw materials	12.49		12.49		12.49
By-products	8.56		8.56		8.56
Utilities	1.11		1.11		1.11
Variable costs	5.04		5.04		5.04
Operating labor, 2/shift[§], $17.50/hr	0.41		0.20		0.10
Maintenance labor, 2%/yr of BL inv	0.14		0.11		0.09
Control lab labor, 20% of op labor	0.08		0.04		0.02
Labor costs	0.63		0.35		0.21
Maintenance materials, 2%/yr of BL inv	0.14		0.11		0.09
Operating supplies, 10% of op labor	0.04		0.02		0.01
TOTAL DIRECT COSTS	5.85		5.52		5.35
Plant overhead, 80% of labor costs	0.51		0.29		0.17
Taxes and insurance, 2%/yr of TFC	0.16		0.13		0.10
Depreciation, 10%/yr of TFC	0.82		0.65		0.51
Plant gate cost	7.34		6.59		6.13
G&A, sales, research	0.50		0.50		0.50
NET PRODUCTION COST	7.84		7.09		6.63
ROI before taxes, 25%/yr of TFC	2.07		1.62		1.27
PRODUCT VALUE	9.91		8.71		7.90

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[*] Of carbon monoxide.

[†] Base case.

[§] For base case; may be different for other capacities.

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Acc. No.	Chapter	Company
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58074	4	ICI
58097	4	ICI
431024	4	LINDE
431036	4	TENNECO CHEMICALS
472172	4	UNION CARBIDE

Figure 4.7

SYNGAS (H_2:CO RATIO = 3:1)
BY STEAM REFORMING OF NATURAL GAS

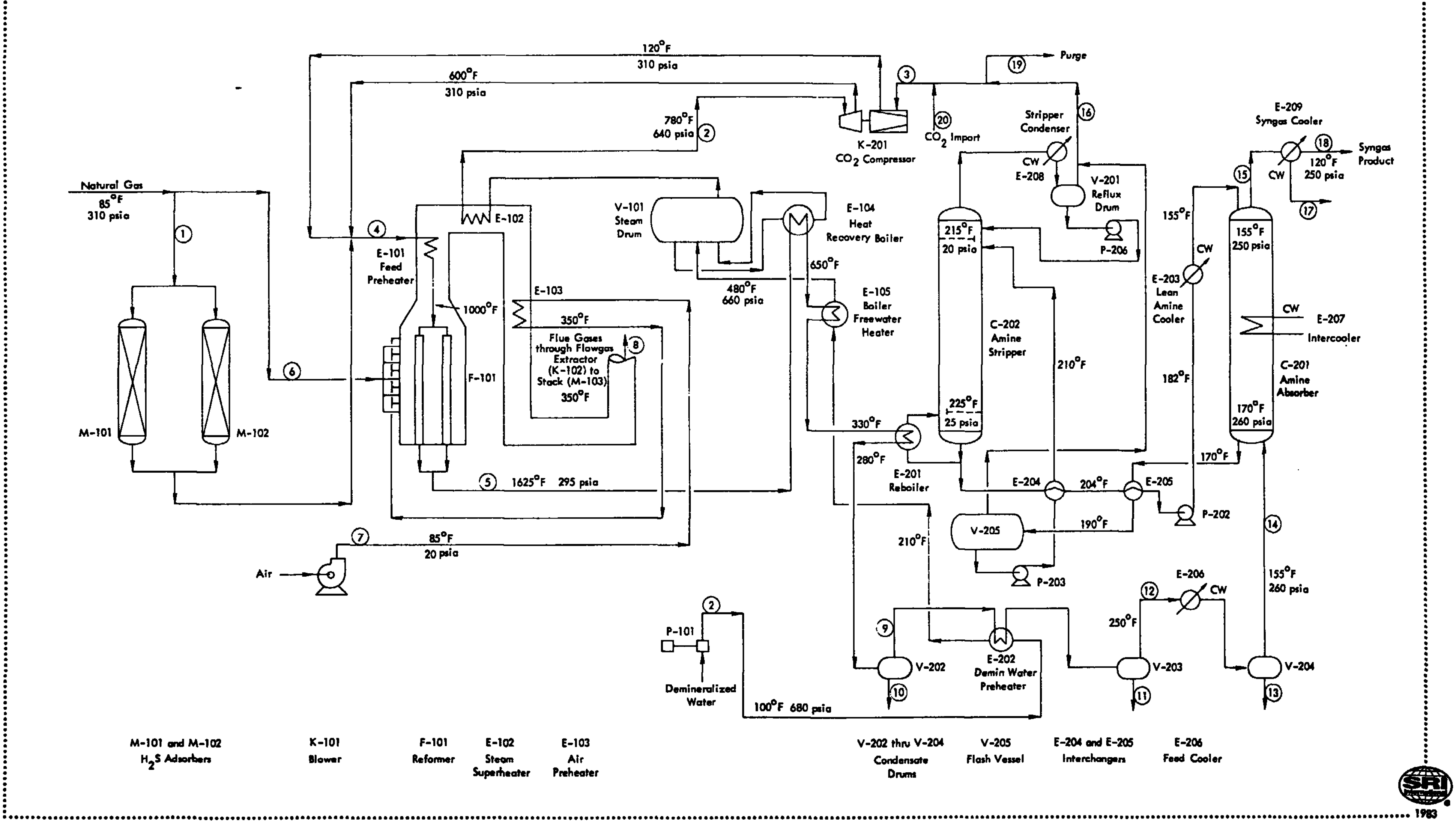


Figure 4.8

SYNGAS (H_2:CO RATIO = 2:1)
BY STEAM REFORMING OF NATURAL GAS

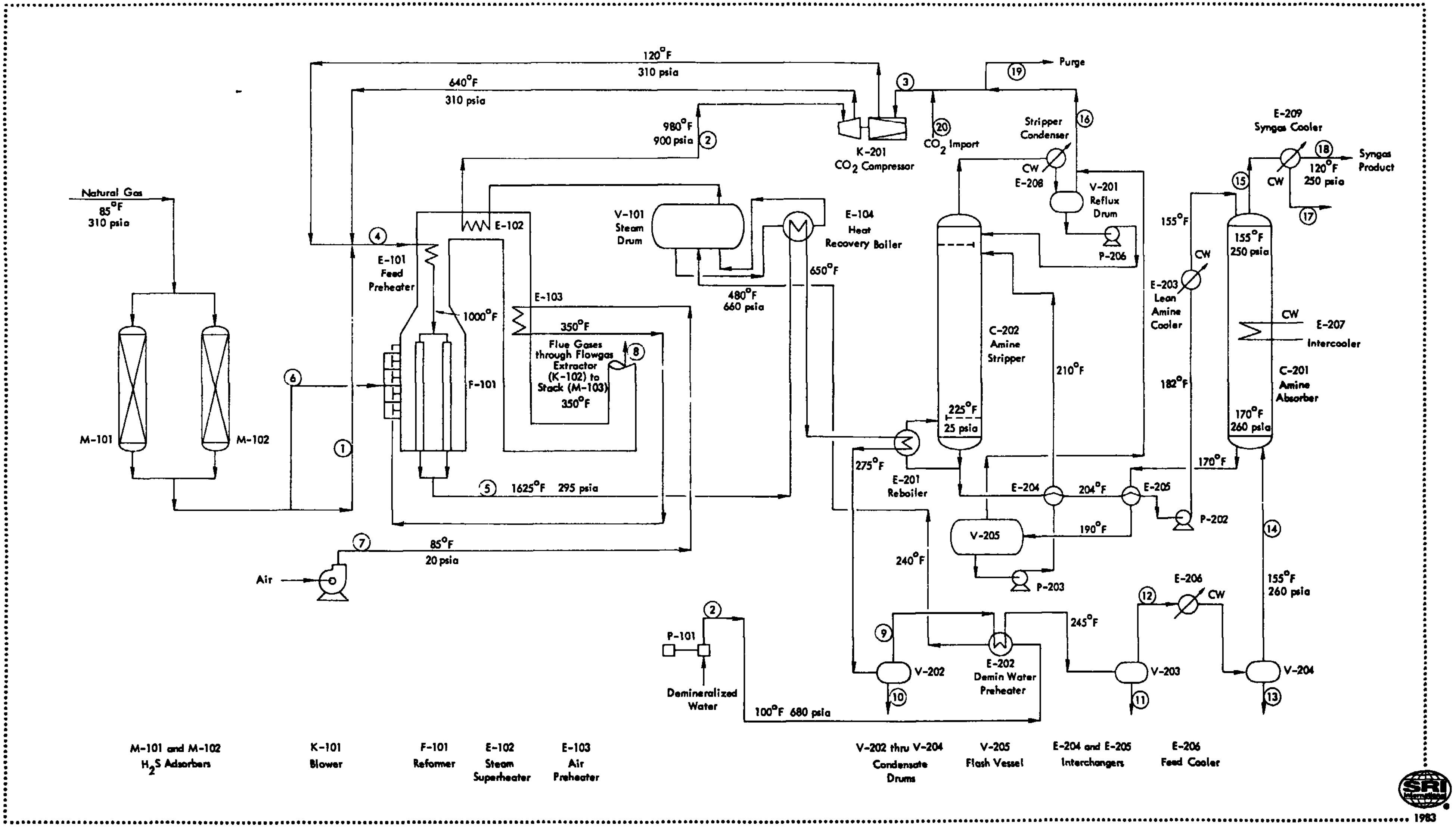


Figure 4.9

HYDROGEN FROM STEAM REFORMING OF NATURAL GAS

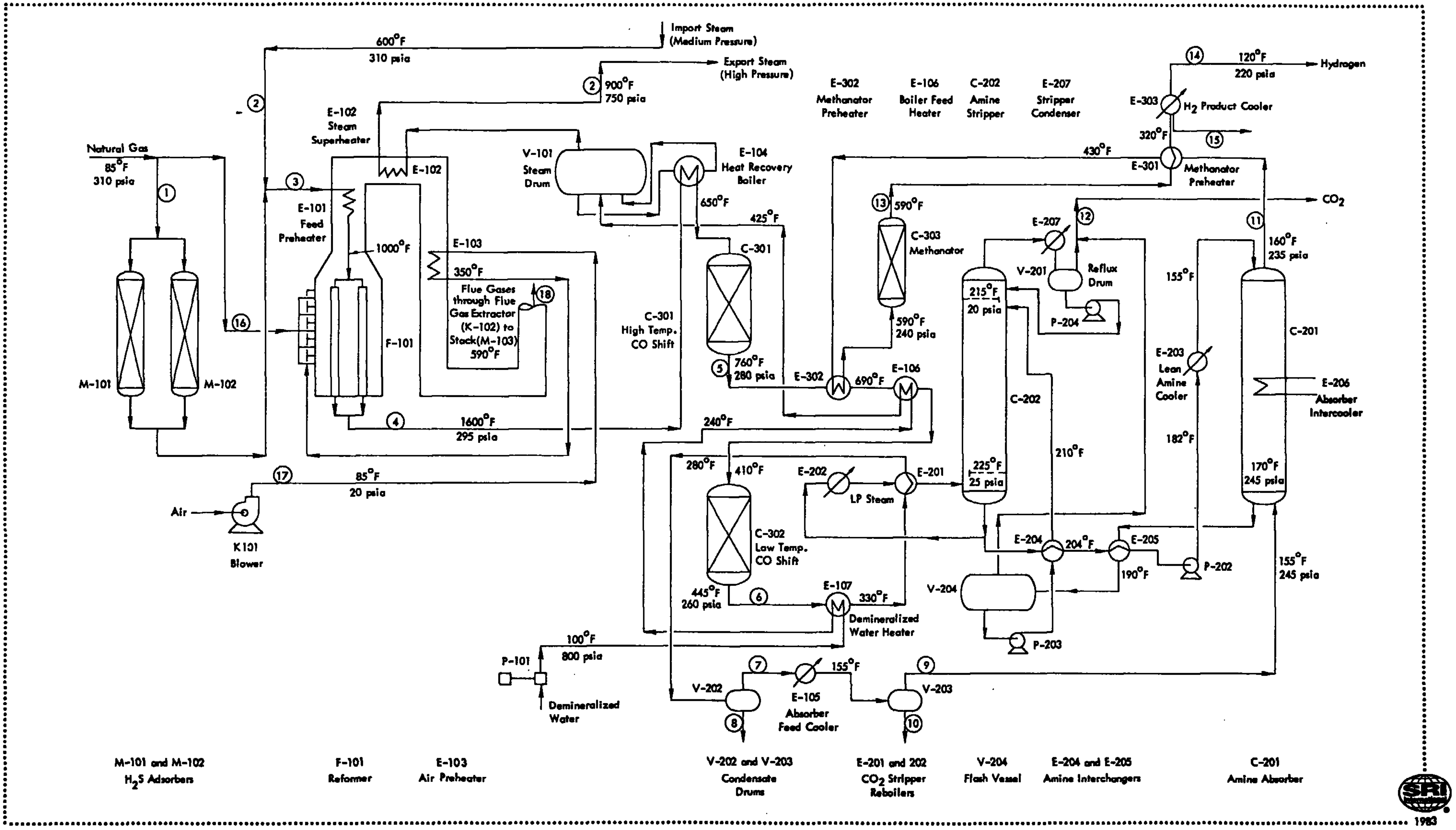
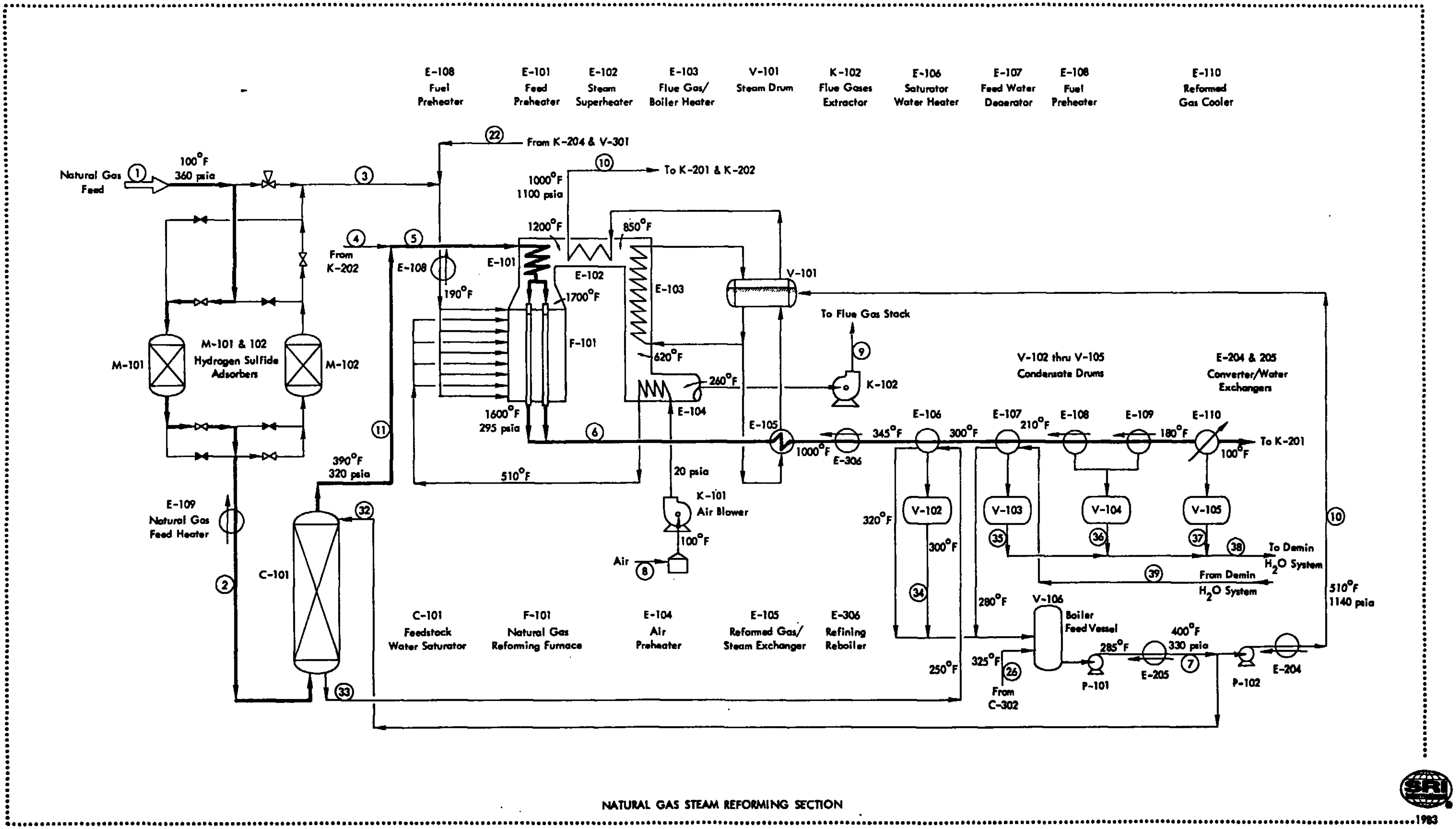


Figure 4.10 (Sheet 1 of 2)

METHANOL FROM NATURAL GAS BY ICI LP PROCESS (HIGH EFFICIENCY DESIGN)



NATURAL GAS STEAM REFORMING SECTION

Figure 4.10 (Sheet 2 of 2)

METHANOL FROM NATURAL GAS BY
ICI LP PROCESS (HIGH EFFICIENCY DESIGN)

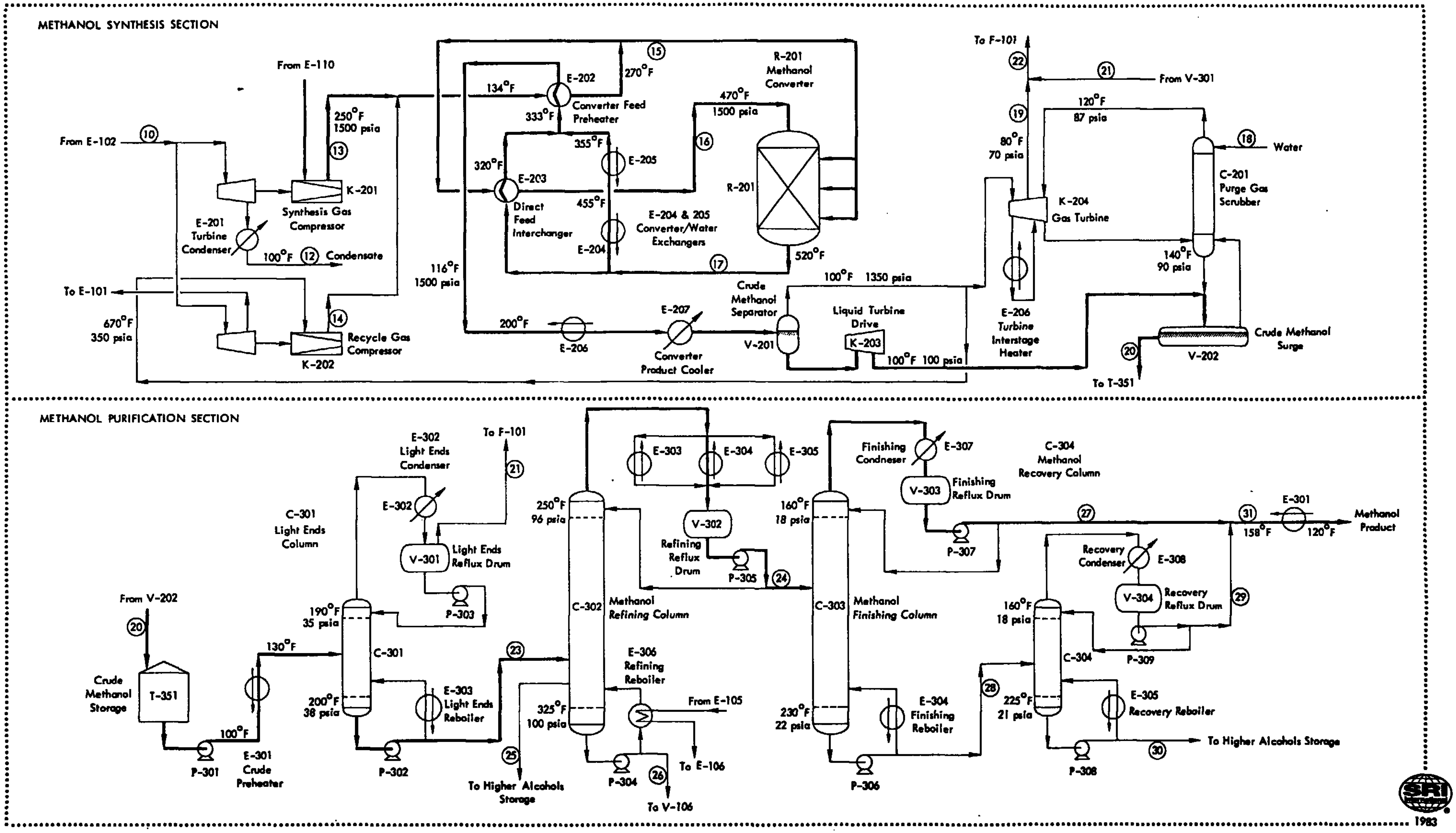
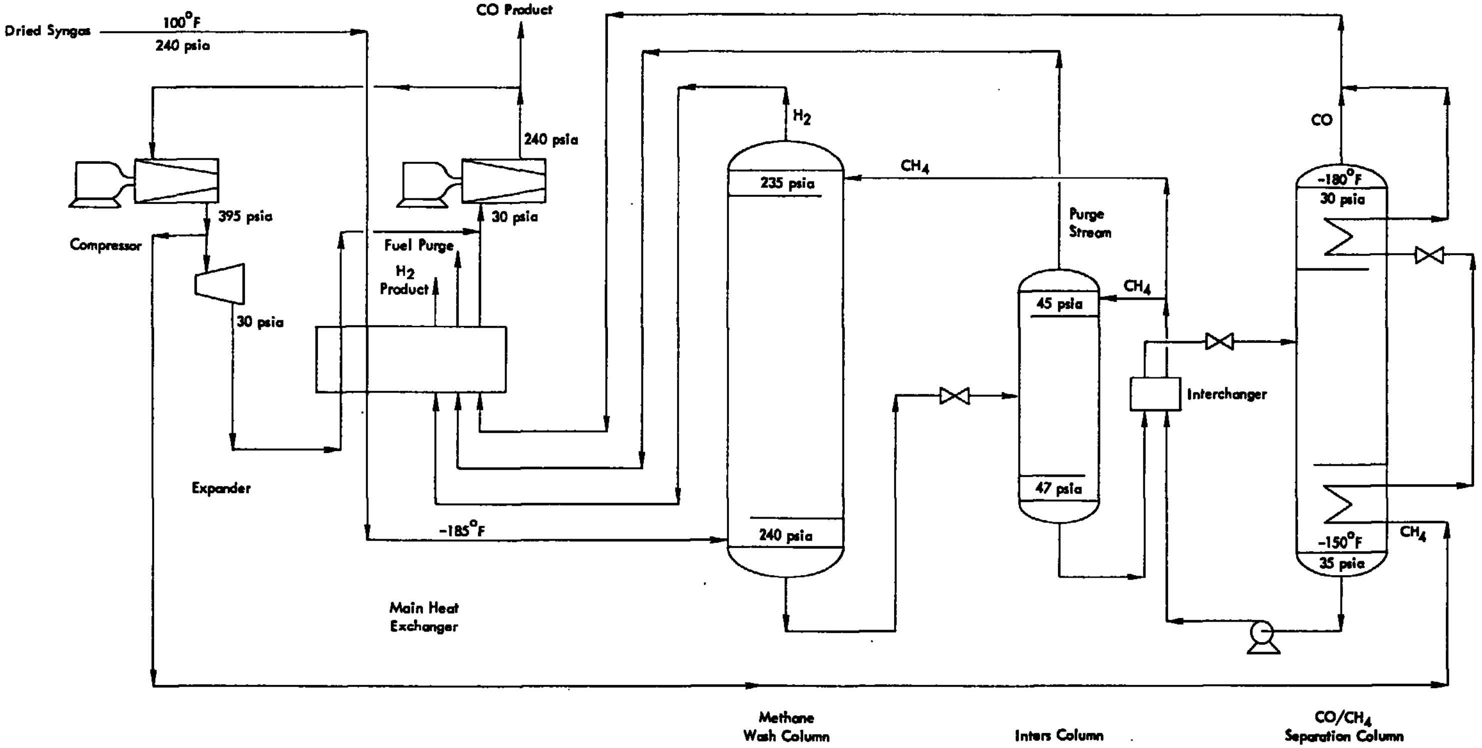


Figure 4.11

H_2/CO SEPARATION BY METHANE WASH



1983

Figure 4.12

TENNECO'S COSORB® PROCESS

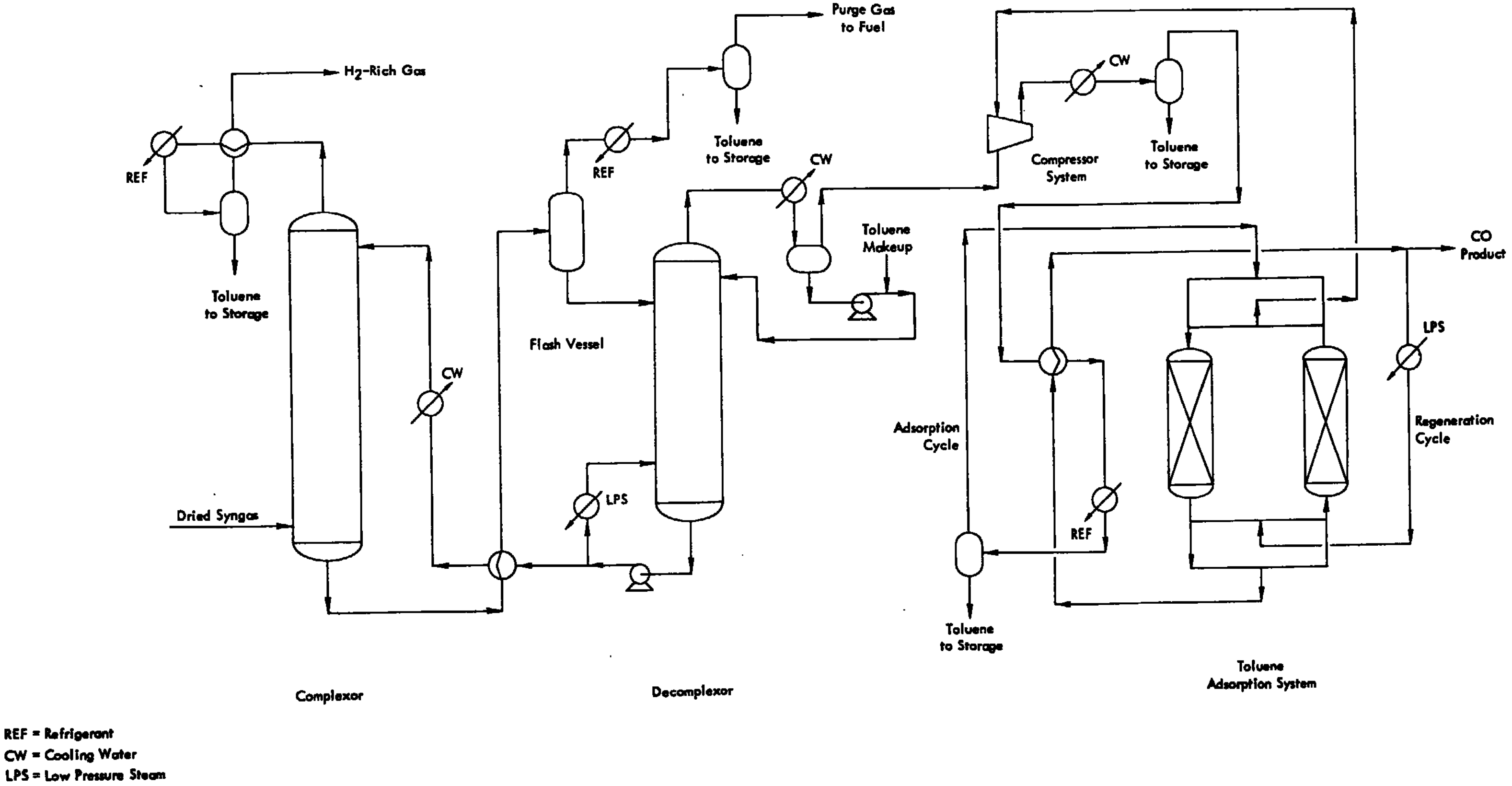


Figure 4.13

FLUE GAS SCRUBBING SYSTEM

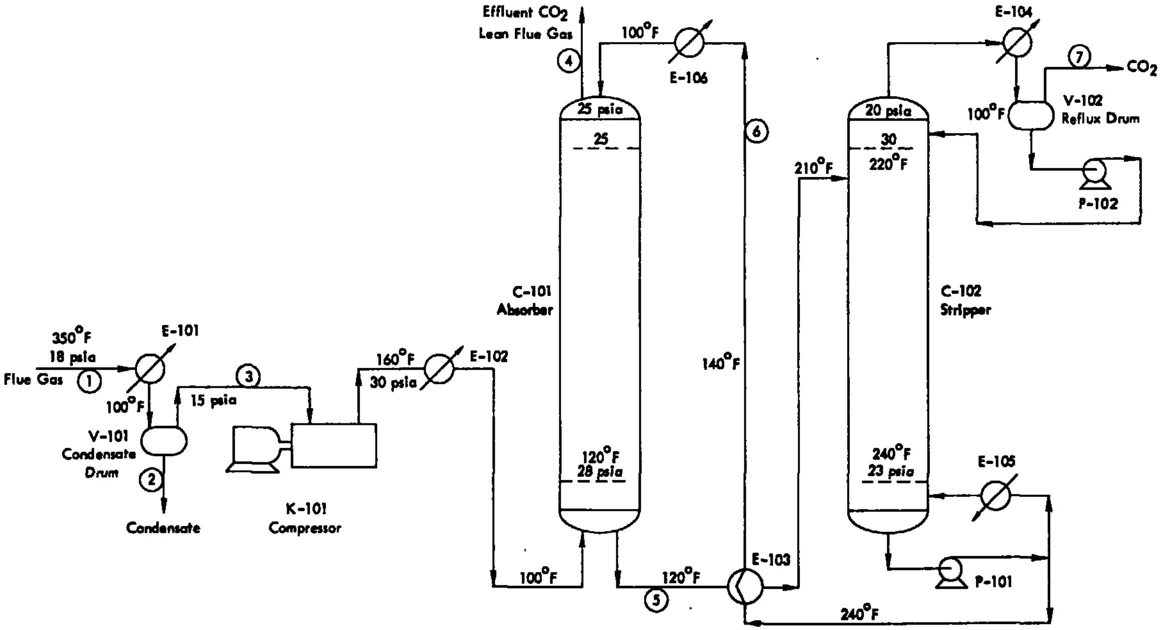


Figure 4.14

FLOWSHEET FOR HYDROGEN PRODUCTION USING P.S.A.

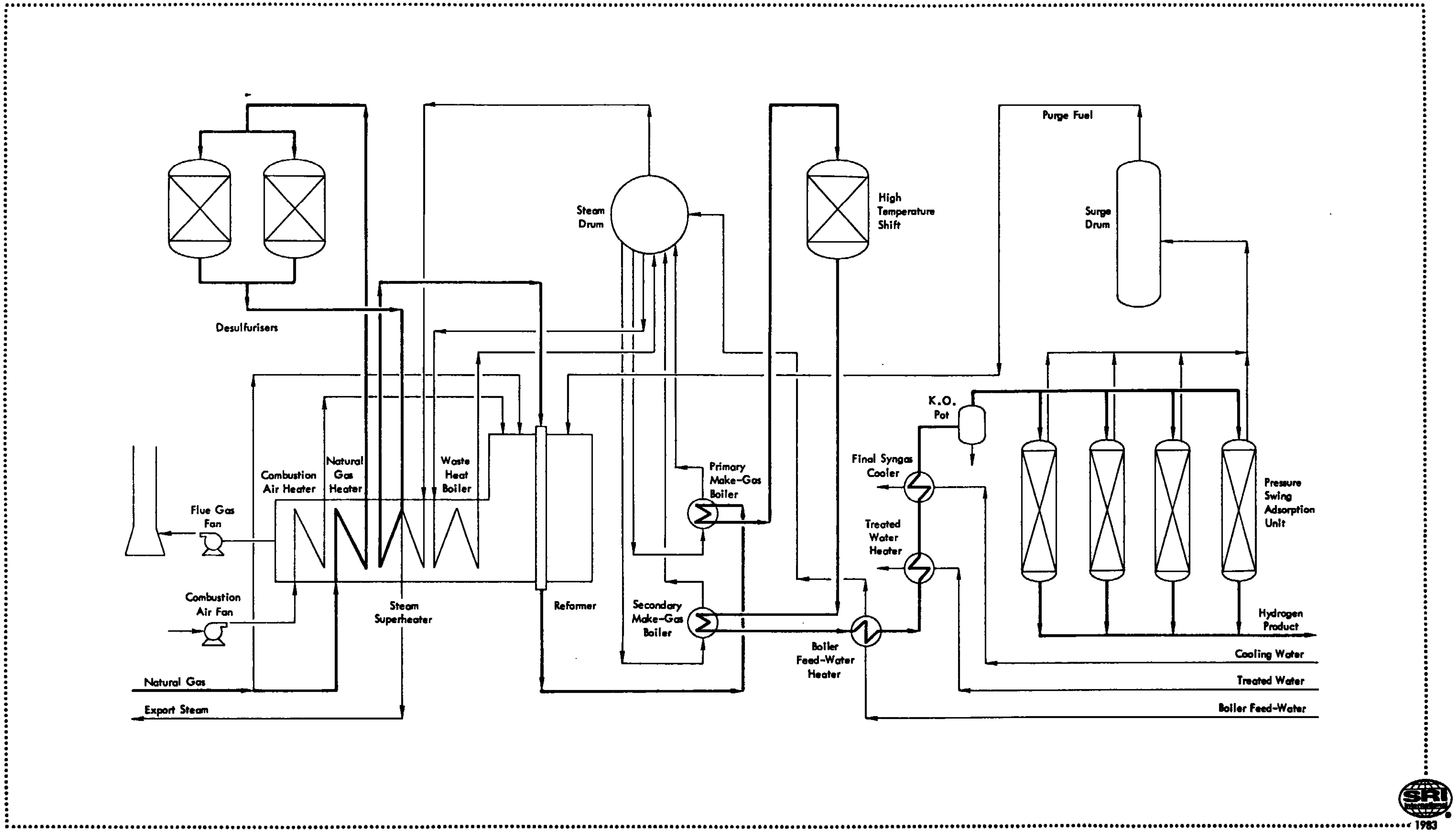


Figure 6.7

METHANOL FROM COAL
SCHEMATIC FLOW DIAGRAM

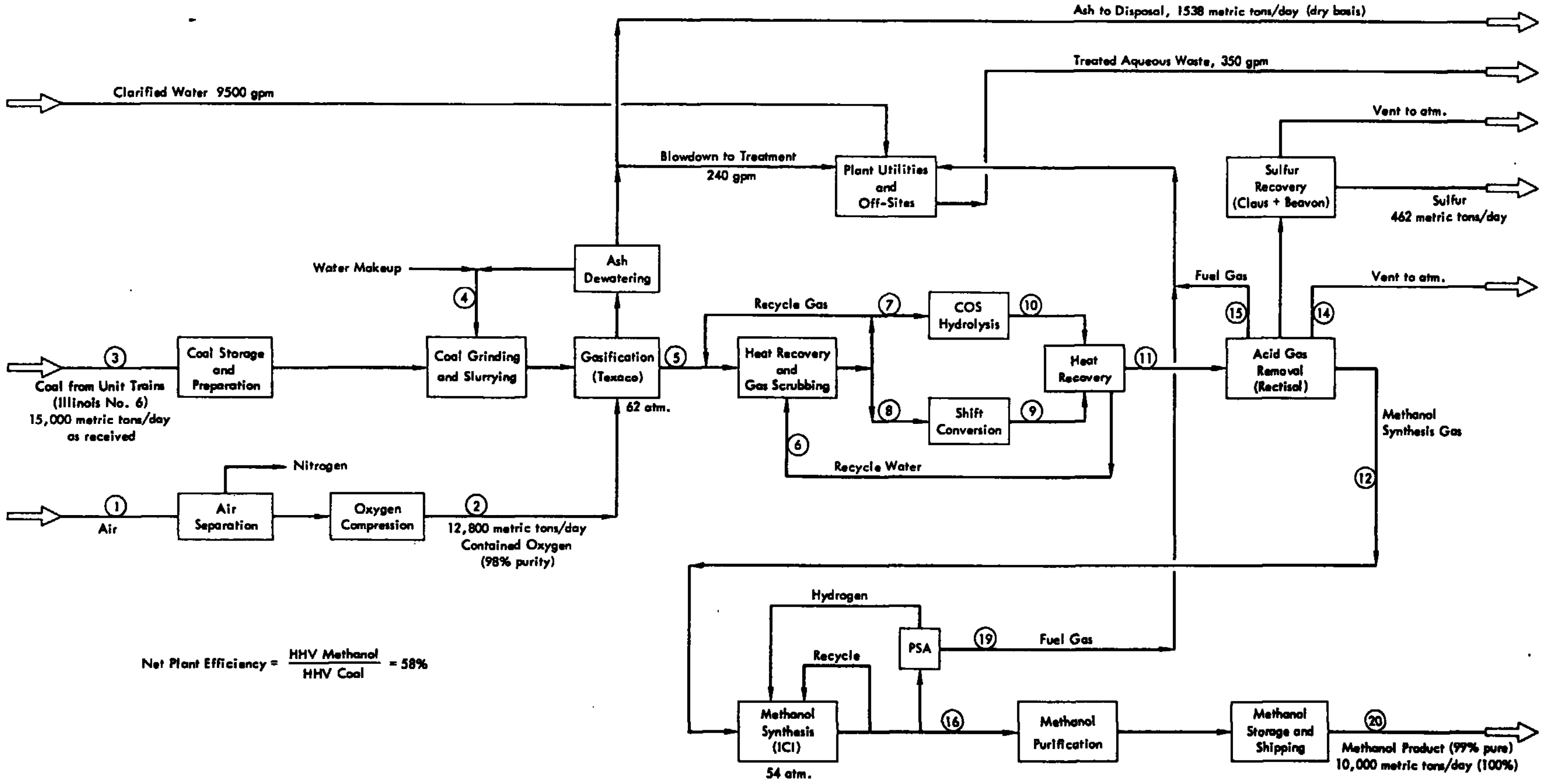


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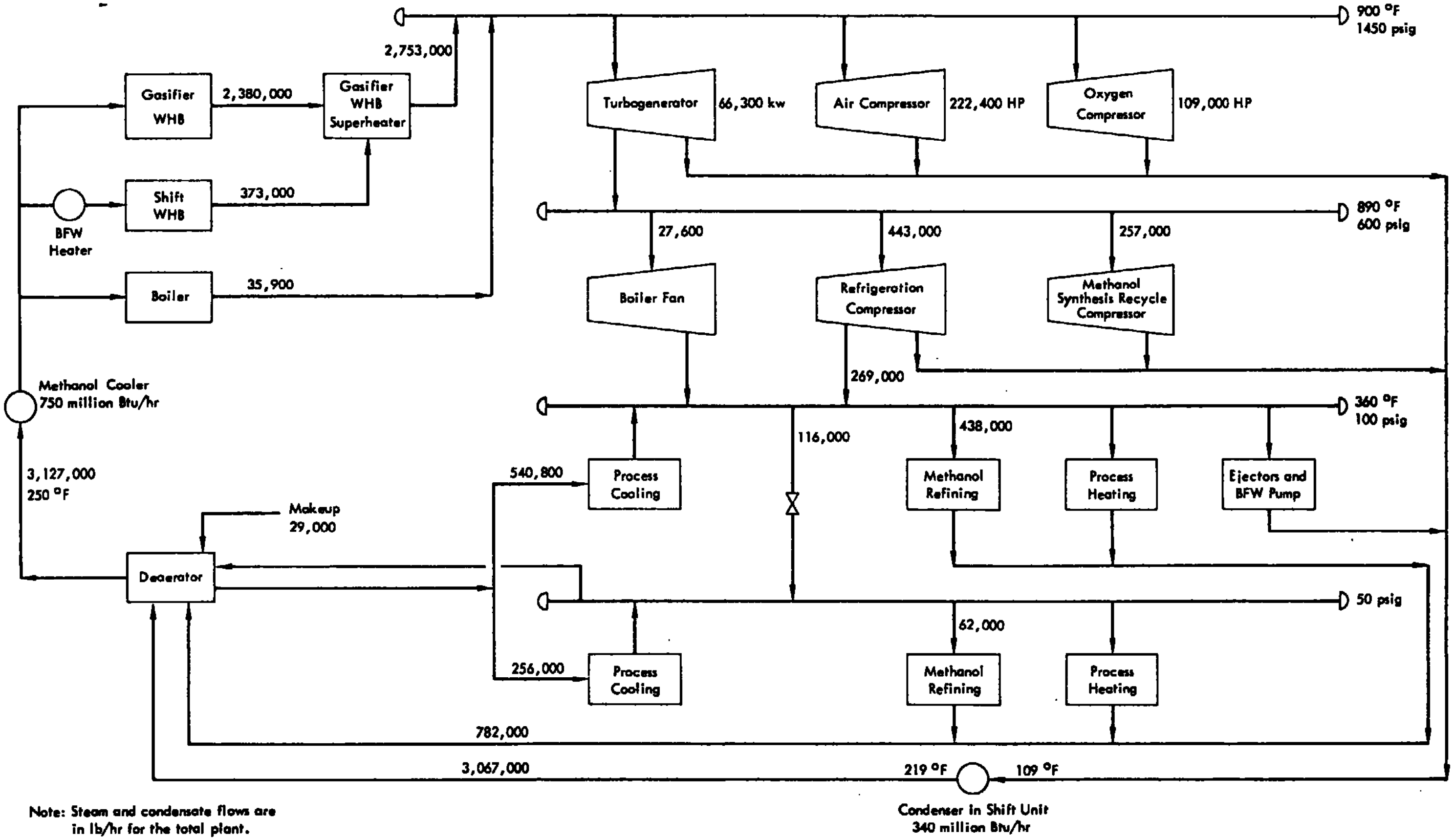
Figure 6.8

METHANOL FROM COAL
MAIN STEAM AND POWER SOURCES
AND USES



Note: Steam and condensate flows are in lb/hr for the total plant.