I. Introduction

The work reported herein is an enlargement of Task 13 Preliminary Report (1) and was performed for the Environmental Protection Agency, Office of Research and Development under Task 13, Change No. 2, Contract No. 68-02-1308.

Task 13 Preliminary Report describes the SASOL type process for the production of gasoline-from-coal and presents the approximate capital investment. The evaluation was based on published data on the SASOL plant (2) and costs include the power supply to the nearby village which houses the operating and supervisory personnel. To provide a basis for direct comparision with other coal conversion processes, it was decided to extend the study by modifying the basis such that power requirements for the village were deleted. The modified gasoline-from-coal plant is described in the appropriate sections in this report.

In addition to the modification cited above, the Environmental Protection Agency (EPA) requested that Task 13 be enlarged to include the following:

- Block flow diagrams and cost estimates for the production of methanol, substitute natural gas and low Btu gas via the SASOL-type process.

- Annualized Operating and production costs of the above processes

II. Basis of Evaluation

Basis of the estimates is a mine-mouth plant, Western U.S. coal, with capital investment expressed in 1975 dollars. Flow sheets and cost estimates were to be derived from existing information and no detailed estimates were to be prepared.

The only fuel used in the plant is coal. Part of this coal is used for steam and power generation, both of which are needed to operate the plant and off-site facilities, and the remainder is used for the production of synthesis gas and ultimately from it the desired products.

The Western U.S. coal selected for this study is from a New Mexico source and has properties used by El Paso Natural Gas Company in their feasibility study of Burnham Coal Gasification Complex for the manufacture of substitute natural gas (3). It is fully expected that this coal will gasify well in either air- or oxygen-blown Lurgi gasifiers.

Another assumption made at the outset and incorporated in the block flow diagram was that only limited sulfur and hydrocarbon emissions to the atmosphere would be permitted. Also clean-up of liquid effluents would be required.

The quantity of water required by the plant was not estimated since appropriate site information needed were not available. Items such as wet and dry bulb temperatures, available water quantity and quality, annual rain fall, percent run-off, soil conditions, etc., must be known before estimates of water requirements can be made.

III. Summary

A. Gasoline-From-Coal

Deletion of the power supply to the nearby village reduces the coal feed rate to the fuel gas manufacture (Section 1000) by about 21%. Total coal feed to the plant is revised to 34,249 TPD. The block flow diagram for the gasoline-from-coal plant (MWK Dwg. P3925-D) has been revised accordingly. No excess power production is included and the plant is self-contained in that the only input to the plant is coal, air and water. The revised capital investment is estimated to be $505 million, 1975 dollars. Table 1 presents a complete breakdown of the capital investment by individual sections. These figures, represent the capital investment for a plant which produces 44,500 BPSD (Nominal) gasoline and other hydrocarbon liquids from coal, have been derived from published information (2, 3) and updated to 1975 by means of escalation rates for both labor and material. It should be noted that overnight construction of the plant is assumed. That is, it is assumed that the complete plant can be designed and constructed in such a short period of time that no additional increase in labor or material will be encountered. In short, no forward escalation has been included in the estimated cost of $505 million. In actual practice significant increases in costs probably would be encountered since several years would be required to build the plant.

Production rates of the various products are given in Table 2. Using a modified Panhandle Eastern accounting procedure which is recommended for coal conversion facilities (4), the cost of gasoline for a 20-year average price (excluding escalation) is estimated to be $3.05/MMBtu or $15/barrel assuming all appropriate byproducts are marketable. The price of coal which corresponds to these gasoline costs is $3.60/ton (7). The effect of other coal prices on the gasoline cost is given in Fig. 5. Using a different accounting procedure with a fixed capital charge of 18.22% (6), the gasoline cost for a 15-year average price is estimated to be $4.05/MMBtu or $20/barrel (with by-product credits).

Approximately 80% of the tar, oil and naphtha produced can be further processed into gasoline product. Assuming addition of such a conversion facility does not alter the total plant investment significantly, gasoline cost can be reduced to $2.76/MMBtu or $13.70/barrel using the Panhandle Eastern accounting method. Such a process modification increases the gasoline production rate by about 40%.

It should be pointed out that should the power generation plant for the nearby village (housing the operation and supervisory personnel) be included as an integrated part of the gasoline-from-coal facility, the total coal consumption will be increased to 37,665 TPD (1). Approximately 40% of the coal is used for steam and power generation. The revised total plant investment for the gasoline-from-coal facility including the power plant and other offsites is estimated to be $533 million. 1975 dollars.

B. Methanol-From-Coal

A block flow diagram has been developed and approximate overall material and energy balances calculated for the methanol-from-coal plant. Using the same coal feed rate to the gasification section as used for the gasoline-from-coal plant, the methanol production rate is 11,338 TPD (Table 4). A maximum size train is estimated to produce 2,800 TPD of methanol and the present plant, therefore, consists of four such units in parallel.

Some seventeen sections are required for the methanol-from-coal plant. Most of these sections are similar in design as well as operation to those used in the gasoline-from-coal plant and the costs for these sections are derived from figures given in the gasoline plant. Sections which are different from those in the gasoline plant are the shift conversion, methane reforming, synthesis gas compression and methanol synthesis and recovery. Costs of these sections are derived from in-house information for a smaller size methanol plant. Capital investment for the seventeen sections is estimated to be $472 million (Table 3), 1975 dollars assuming overnight construction of the plant with no forward escalation. Based on this estimate and using the modified Panhandle Eastern accounting procedure, the cost of producing methanol from coal is estimated to be $1.80/MMBtu ($4.90/barrel) assuming all appropriate byproducts are marketable and a coal cost of $3.60/ton. For a 15-year plant life with a fixed capital charge of 18.22%, the methanol cost is estimated to be $2.34/MMBtu or $6.40/barrel. Appendix B presents the operating and annualized production cost for the methanol-from-coal plant.

C. Substitute Natural Gas-From-Coal

A block flow diagram for the substitute natural gas (SNG) from-coal plant have been developed and overall material and energy balances calculated. The SNG-from-coal plant has the same coal feed (21,274 TPD) to the gasification unit (Section 200) as the two previous coal conversion processes. In order for the plant to be self-contained, an additional coal feed rate of 5,435 TPD is required as input to the fuel gas manufacture section for steam and power generation. The corresponding gas production rate is 258 MMSCFD (972 Btu/SCF).

Eighteen sections are required for the SNG-from-coal plants. Most of these sections are similar in design to the two previous coal conversion processes with the exception of the methane synthesis and synthesis gas compression sections. The cost for these two sections are derived from published information (3).

Capital investment for a SNG-from-coal plant producing 258 MMSCFD of gas is estimated to be $365 million, 1975 dollars assuming overnight construction of the plant with no forward escalation. Table 5 presents a detail breakdown of the capital investment for individual sections. Based on this estimate and assuming all by-products are marketable, the gas prices is estimated to be $1.13/MMBtu using the modified Panhandle Eastern accounting procedure and a coal price of $3.60/ton. The SNG cost resulting from an alternative accounting procedure with a 15-year plant life will be $1.50/MMBtu (with by-product credits). Production rates of the various products are listed in Table 6. Appendix C outlines the annualized production and operating costs of the SNG-from-coal plant.

D. Low Btu Gas-From-Coal

A block flow diagram for a comparable low Btu gas-from-coal plant has been developed and overall material and energy balances calculated. The low Btu gas facility has a coal feed rate of 21,274 TPD to the gas manufacture section which is the same rate used in the other three coal conversion processes. In order for the plant to be self-contained, part of the fuel gas manufactured is used in the steam and power generation plant for process consumption. The remainder of the fuel gas (960 MMSCFD @ 230 Btu/SCF) is transmitted as product.

The capital investment for the low Btu gas-from-coal facility is estimated to be $218 million, 1975 dollars and is derived from the fuel gas manufacturing and other corresponding sections of the gasoline-from-coal plant. Table 7 presents a complete breakdown of the capital investment for individual sections of the low Btu-gas-from-coal facility. Based on this estimate and assuming all by-products are marketable, the low Btu gas cost is $0.86/MMBtu using the modified Panhandle Eastern accounting procedure and a coal price of $3.60/ton.

The low Btu gas resulting from the alternative accounting procedure with a 15-year plant life is estimated to be $1.10/MMBtu (with by-product credits). These costs of low Btu gas are derived using an on-stream factor of 0.9. The production costs for 0.7 on-stream factor have also been investigated as typical for hook-up with power plants. The low Btu gas costs for the lower on-stream factor are $1.10/MMBtu using the modified Panhandle accounting procedure and $1.44/MMBtu using the alternative (15-year plant life) accounting procedure and with by-product credits. Figure 5 illustrates graphically the sensitivity of on-stream factors on the low Btu gas cost. Production rates of the various products from the low Btu gas-from-coal plant are listed in Table 8. Annualized production and operating costs of the low Btu gas-from-coal plant are given in Appendix D for two cases: 0.9 and 0.7 on-stream factors.

Table 1

Gasoline-From-Coal Investment Summary

	Section	1975, M$
100	Coal Preparation	38,000
200	Coal Gasification	48,000
300	Gas Purification	41,000
400	Methane Splitting	10,000
500	Synthesis	53,000
600	Product Recovery	28,000
700	Chemical Recovery	8,000
800	Hydrogen & Catalyst Manufacture	8,000
900	Oxygen Production	73,000
1000	Fuel Gas Production	62,000
1100	Steam & Power	42,000
1200	Gas Liquor Treating	13,000
1300	Ash Disposal	8,000
1400	Effluent Water Treating	4,000
1500	Sulfur Recovery	9,000
1600	Raw Water Treating	6,000
1700	Cooling Water	15,000
1800	Offsite & General	39,000
	TOTAL	$505,000

Table 2

Gasoline-From-Coal Production Rate

Product	#/hr	BPD	HHV, 10^9 Btu/hr
Gasoline**	262,353	25,495	5.2654
Diesel Oil	15,121	1,233	0.2913
Waxy Oil	11,847	925	0.2175
Propane LPG	16,056	2,000	0.3412
Acetone	2,650	230	0.0348
Methanol	343	30	0.0033
Propanol	4,832	412	0.0698
i-Butanol	546	46	0.0085
n-Butanol	1,606	136	0.0249
M.E.K.	670	56	0.0097
n-Pentanol	374	32	0.0056
Tar, Oil, Naphtha***	162,074	13,230	3.8804
Phenol	13,665	716	0.0218
Ammonia	28,742	--	0.2763
Sulfur	13,757	--	0.0548
		TOTAL	10.5053

$$\frac{\text{HHV of Products}}{\text{HHV of Coal}} = \frac{10.5053}{25.3209} \times 100\%$$

$$= 41.5\%$$

** Gasoline with research octane number equals 86

***80% of tar, oil, naphtha can be further processed to gasoline product

Table 3

Methanol-From-Coal Investment Summary

	Section	1975, M$
100	Coal Preparation	36,000
200	Coal Gasification	48,000
300	Gas Purification	41,000
400	Shift Conversion	9,000
500	Methane Splitting	32,000
600	Synthesis Gas Compression	19,000
700	Methanol Synthesis & Recovery	65,000
800	Sulfur Recovery	8,000
900	Oxygen Production	43,000
1000	Fuel Gas Manufacture	51,000
1100	Steam & Power Generation	36,000
1200	Gas Liquor Treating	12,000
1300	Ash Disposal	8,000
1400	Effluent Water Treatment	4,000
1500	Raw Water Treatment	6,000
1600	Cooling Water	15,000
1700	Offsites	39,000
TOTAL		472,000

Table 4

Methanol-From-Coal

Production Rate

Product	#/hr	BPD	HHV, 10^9 Btu/hr
Methanol	927,748	81,433	9.2281
Tar, Oil, Naphtha	151,684	12,382	3.6798
Higher Alcohols & Dimethyl Ether	4,452	367	0.0662
Phenols	13,052	684	0.0209
Ammonia	27,453	--	0.2639
Sulfur	11,323	--	0.0451
		TOTAL	13.3040

$$\frac{\text{HHV of Products}}{\text{HHV of Coal}} = \frac{13.3040}{23.4912} \times 100\%$$

$$= 56.6\%$$

Table 5

Substitute Natural Gas-From-Coal Investment Summary

	Section	1975, M$
100	Coal Preparation	32,000
200	Coal Gasification	48,000
300 + 400	Shift Converter & Gas Cooling	15,000
500	Gas Purification	41,000
600	Methane Synthesis	19,000
700	Gas Compression	7,000
800	Gas Liquor Separation	(Included in 300 and 400)
900	Air Separation	43,000
1000	Fuel Gas Manufacture	29,000
1100	Steam & Power Generation	48,000
1200	Phenol Recovery	10,000
1300	Ash Disposal	4,000
1400	Effluent Water Treatment	5,000
1500	Sulfur Plant	8,000
1600	Raw Water Treatment	5,000
1700	Cooling Water	15,000
1800	Offsites	36,000
	TOTAL	365,000

Table 6

Substitute Natural Gas Production Rate

Product	#/hr	Production	HHV, 10^9 Btu/hr
Substitute Natural Gas	474,069	258 MMSCFD	10.4531
Tar, Oil, Naphtha	149,002	12,160 BPD	2.7565
Phenols	10,440	550 BPD	0.0167
Ammonia	17,353	208 STPD	0.1667
Sulfur	12,698	136 LTPD	0.0507
		Total	13.4437

$$\frac{\text{HHV of Products}}{\text{HHV of Coals}} = \frac{13.4437}{19.7462} \times 100\%$$

$$= 68.1\%$$

Table 7

Low Btu Gas-From-Coal Investment Summary

	Section	1975, M$
100	Coal Preparation	25,000
200	Coal Gasification & Gas Purification (Hot Carbonate System)	98,000
300	Ash Disposal	3,000
400	Steam & Power Generation	38,000
500	Gas Liquor Treatment	8,000
600	Effluent Water Treatment	4,000
700	Raw Water Treatment	4,000
800	Sulfur Recovery	7,000
900	Cooling Water	5,000
1000	Offsites	26,000
	TOTAL	218,000

Table 8

Low Btu Gas-From-Coal Production Rate

Product	#/hr	Production	HHV, 10^9 Btu/hr
Low Btu Gas	2,437,756	960 MMSCFD	9,1936
Tar, Oil, Naphtha	88,018	7,185 BPD	1.7247
Phenols	8,320	436 BPD	0.0133
Ammonia	13,780	165 STPD	0.0403
Sulfur	10,114	108 LTPD	0.1325
		Total	11.1044

$$\frac{\text{HHV of Products}}{\text{HHV of Coal}} = \frac{11.1044}{15.728} \times 100\%$$

$$= 70.6\%$$

IV. Process Description

A. Gasoline-From-Coal (MWK Dwg. P3925-D)

a. DESCRIPTION

A block flow diagram for the gasoline-from-coal plant is given in the cited drawing. The process may be divided into following steps:

- Coal Gasification and Raw Gas Purification
- Synthesis Gas Preparation
- Synthesis of Gasoline and Recovery
- Fuel Gas Manufacture - Steam & Power Generation

1. Coal Gasification and Raw Gas Purification

Coal received from the mine at section 100, Coal Preparation, undergoes crushing, screening, stockpiling, reclaiming and briquetting treatment according to needs of the plant. The product from section 100 is conveyed by belt to both section 200, Gasification, and section 1000, Fuel Gas Manufacture. In both areas coal is gasified essentially completely for manufacture of both synthesis gas and fuel gas.

Ash from both sections 200 and 1000 is conveyed either by belt or by water to section 1300, Ash Disposal. This section includes thickeners and screens for the recovery of water for reuse in ash quenching and/or sluicing.

Gasification in section 200 employs steam and oxygen in a mixture introduced under the grates of multiples of Lurgi Gasifiers. Operating under pressure of up to 500 psig, the Lurgi gasifier receives its coal input through a lock hopper pressured by product gas. This lock hopper is periodically filled from an overhead bunker when level indicators show that the hopper has been emptied into the gasifier. The gasifier proper is a water-jacketted pressure vessel equipped with a distributor for the coal feed at the top and a water cooled grate at the bottom which has the dual function of distributing the gasification medium (steam and oxygen or air and steam) and discharging the ash. Ash is discharged to a lock hopper which is periodically emptied when the volume of ash builds to a pre-set level.

In the gasifier, the falling fixed bed of coal supported on the grate moves from coal to ash through stages of devolatilization and combustion. The gas product is principally the result of reaction between hot gases leaving the combustion zone and the devolatilized coal. Gas leaving the relatively cool top outlet of the gasifier is quenched to knock down condensible carbonization products and unconverted steam. Tar is separated from the gas liquor by decanting at about the boiling point of water; oil and naphtha are separated from gas liquor by decanting at essentially room temperature. The gas liquor is principally water but contains both phenols and dissolved gases, e.g., H_2S, CO_2 and NH_3.

Gas released from the feed hopper, as the hopper is depressured for refilling, is collected from a battery of gasifiers and recompressed to gasifier pressure. Little gas is involved in the cycling of the ash hopper as the atmosphere under the grate is steam and oxygen, and the steam is condensed before the vessel is opened for discharge of the ashes.

Cooled raw gas is separated from its condensates and sent to section 300, Gas Purification where it undergoes scrubbing with a chilled polar solvent according to a version of the Rectisol process first employed industrially at SASOL. Stripping of the solvent is achieved both by flashing and also by chilled nitrogen from section 900, Air Separation. Off-gases comprise a hydrogen sulfide concentrate sent to section 1500, Sulfur Recovery, and a mixture of mostly nitrogen and carbon dioxide, sent to the stacks of section 1100, Steam and Power.

2. Synthesis Gas Preparation

Pure gas from section 300 is the net feed to the synthesis section but by virtue of having been generated in a pressure Lurgi gasifier, contains methane which is an unwanted component in the synthesis feed. In section 400, Methane Splitting, methane and other light hydrocarbons produced by the synthesis are split into hydrogen and carbon monoxide which, of course, are the ingredients wanted in the synthesis feed. The splitting is performed catalytically at high temperature with proper additions of steam and oxygen to produce the desired synthesis feed. A small fraction of the split gas is diverted to section 800, Hydrogen Plant, where catalytic treatments of shift and methanation produce a stream of 99% hydrogen for synthesis catalyst reduction and other uses in the plant.

3. Synthesis of Gasoline & Recovery

Synthesis gas from the methane splitting are fed to the synthesis section to make gasoline via the Fischer-Tropsch process. This process involves the catalytic reaction of carbon monoxide with hydrogen according to the following reactions:

$$2nH_2 + n\ CO = (CH_2)_n + n\ H_2O$$

$$nH_2 + 2n\ CO = (CH_2)_n + n\ CO_2$$

Catalyst is made from either millscale or pure magnetite in section 800, Catalyst Plant.

Gas and oil products of the synthesis are washed with water to remove water soluble chemicals. This water plus the reaction water and its dissolved chemicals comprise the feed to section 700, Chemical Recovery. The washed gas and oil become the feed to section 600, Product Recovery. Hydrocarbon products are recovered in section 600 through absorption/stripping operations. Light gases not recovered in the lean oil absorption are:

- vented to the fuel gas system of section 1100 for steam and power generation
- returned to the synthesis as aeration gas
- partly returned to section 400, Methane Splitting, for the conversion of light hydrocarbons to synthesis gas (external recycle stream)

4. <u>Fuel Gas Manufacture - Steam & Power Generation</u>

Fuel gas is manufactured by the pressure gasification of coal in steam-and-air-blown Lurgi gasifiers of section 1000, Fuel Gas Manufacture. Fuel gas manufactured is free of fly ash and is purified in much the same way that the synthesis gas was prepared and purified. Condensation products from synthesis gas and fuel gas manufacture are combined and treated. Section 1000 includes a hot carbonate scrubbing system which removes most of the carbon dioxide and hydrogen sulfide from the fuel gas. Foul gas scrubbed from the fuel gas contains hydrogen sulfide and is treated in section 1500, Sulfur Recovery, along with the hydrogen sulfide concentrate from synthesis gas purification. The sulfides are converted to elemental sulfur and recovered as a solid product. Some of the purified fuel gas is fed to gas turbines for the generation of power; the remainder is burned in process furnaces and in boilers raising steam for process and driver uses. Gas turbines exhaust into the fire box of the boiler and these