SECTION 3

BASE CASE I

MOBIL METHANOL-TO-GASOLINE TECHNOLOGY

3.1 MATERIAL BALANCE

The overall material balance is shown below:

Input	Mlb/hr
Coal, as mined	2,227.8(1)
Air	5,733.8
Water	4,157.4
	12,169.0

Output	Mlb/hr
Coal fines	102.5(2)
Ash	140.1
Products	530.9(3)
Byproducts	13.7
Blowdown water	508.8
Stack and vent losses	10,873.0
	12,169.0

(1) 27,334 T/SD

(2) 1,230 T/SD

(3) 50,075 Bbl/SD

Overall plant consumptions per barrel of product, converting SNG into a FOE barrel, are:

Coal:	0.521	T
Water:	5.69	Bbl
Air:	1.37	T

Stack and vent losses amount to about 2.6 tons per barrel of product. The C_3 plus hydrocarbon yield (85.4% 10 RVP gasoline) is 0.509 Bbl/Bbl of converted methanol.

Appendix A contains the complete, detailed material balance for Base Case I.

3.2 PRODUCT YIELDS AND QUALITY

Stream numbers are given below for reference to the material balance sheets in Appendix A and process diagrams in Sub-Section 3.4.

3.2.1 SNG (49)

Quantity

16,306.3 lb-mol/hr
265.4 Mlb/hr
148.5 MMSCF/SD

Composition (Only compounds greater than 0.1% are listed: see Appendix A for detailed composition.)

	Percent
Hydrogen	1.7
Methane	95.5
Ethane	0.2
Propane	0.1
Butane	0.1
Carbon dioxide	0.5
Inerts (N_2 + Ar)	1.9
	100.0

Other

Heat of combustion (HHV)	980 Btu/SCF
Carbon monoxide (0.1% max.)	0.02%
Water	0.01%
Sulfur	None

Compatibility Indexes (versus pure methane)

Index	Calculated	Preferable	Objectionable
Lifting, I_l	1.03	under 1.0	above 1.06
Flash-back, I_f	1.02	under 1.15	above 1.2
Yellow-tip, I_y	1.05	above 1.0	under 0.8

The SNG product is of satisfactory quality and is compatible with pure methane. The inerts from the oxygen stream for gasification, however, give rise to a lifting index value between the preferable and objectionable values. From a processing standpoint, there is little that can be done to reduce this value. The selection of a more expensive oxygen plant yielding a 99+% pure product, however, would alleviate this problem. (The SNG product, on the other hand, has a lifting index value better than the preferable value when compared with the high methane natural gas standard cited in the A.G.A. Research Bulletin Number 36. This gas has a 5.0% inerts content.)

3.2.2 Gasoline (50)

Quantity — 22,045 Bbl/SD, 235.7 Mlb/hr

Blending

Component	Wt. %
Mixed butanes	2.4
Alkylate	3.2
Stabilized gasoline	87.8
Hydrotreated gasifier naphtha	6.6
	100.0

Properties

Estimated properties and a comparison with unleaded gasoline specifications are presented in Table 3.2.1. Table 3.2.2 gives a more detailed listing of the principal unleaded gasoline specifications.

The 10 RVP gasoline is of excellent quality and meets all specifications. Its octane rating is estimated to be about one above the specification number. Volatility and composition are similar to present-day gasolines. Although the content of the troublesome durene is below the target maximum of 5.0 wt. %, it would be preferable if it were below 4.0 wt. %. (2)

3.2.3 Mixed Butanes (103)

Quantity — 2,205 Bbl/SD, 18.3 Mlb/hr

Properties

Estimated properties and a comparison with LPG specifications are shown in Table 3.2.3.

This product is a satisfactory commercial butane fuel. Because of the high iso-butane content of 76 vol. %, it has, however, a higher potential economic value as an alkylation unit feedstock.

3.2.4 Propane LPG (102)

Quantity	1,555 Bbl/SD 11.5 Mlb/hr

Properties

Estimated properties and a comparison with LPG specifications are shown in Table 3.2.3.

This product is a satisfactory commercial propane fuel.

3.2.5 Byproducts

Sulfur (29)

Quantity	61 T/SD
Impurities	0.5 wt. %

Anhydrous Ammonia (17)

Quantity	103 T/SD
Impurities (mainly water)	0.5 wt. % max.
Grade	agricultural

Excess Power (6,000 volts)	5.96 MW(e)

3.2.6 Coal Fines (2.1)

Quantity	102.5 Mlb/hr

The thermal requirements do not require the use of all the fines produced in the coal preparation unit.

TABLE 3.2.1

COMPARISON OF PRINCIPAL UNLEADED GASOLINE SPECIFICATIONS WITH ESTIMATED METHANOL-TO-GASOLINE GASOLINE PROPERTIES- CASE I

	Estimated MTG Unleaded Gasoline Properties	Specification
Gravity, °API	61.4	
Octane Numbers		
Research	93	
Motor	83	82 min.
(Research + Motor)/2	88	87 min.
Volatility		
Reid Vapor Pressure, lb	10.0	
Distillation, °F		
IBP	85.5	
10%	110.5	158 max.
30%	146.1	
50%	200.0	170/250 min./max.
70%	262.8	
90%	336.9	374 max.
EP	388.6	437 max.
V/L Ratio (=20), °F	@ 129.5	@ 140 max.
Sulfur, wt. %	Nil	0.10 max.
Composition, vol. %		
Paraffins	51.3	
Olefins	11.3	20 max. (target)
Naphthenes	8.7	
Aromatics	28.7	
Durene Content, wt. %	4.6	5 max. (target)
Molecular Weight	94.3	

TABLE 3.2.2
PRINCIPAL UNLEADED GASOLINE SPECIFICATIONS

	ASTM D439[1]	OTHER	POSSIBLE WAIVERS
Octane Numbers			
(Research + Motor)/2, min. (D2699 and D2700)	87		
Motor, min. (D2700)	82		
Volatility			
Reid Vapor Pressure, max. (D323)	15[2]		15.5-16.0 (in winter)
Distillation, °F (D-86)			
10% Evap. max. temp.	158[2] (140 avg.)		
50% Evap. min./max. temp.	170/250[2] (avg. 240 max.)		
90% Evap. max. temp.	374[2] (370 avg.)		383[6]
End Point, max. temp.	437		446[6]
% Recovered, min.	-	95[3]	No Spec.
% Residue, max.	-	2[3]	
V/L Ratio, max. °F @ 20 (D2533)	140[2]		
Existent Gum, max. mg/100 mls (D381)	5		
Sulfur, max. wt. % (D1266)	0.10	0.05[4]	0.15[6]
Benzene, max. wt. %		5[7]	
Bromine Number, max. (D1159)	-	30[4]	
Induction Period, min. (D525)	-	240[5]	
Corrosion, max. (D130)	No. 1		
Lead Content, max. g/USG (D2547 or D2599)	0.05		

(1) 1976 Annual Book of ASTM Standards
(2) Lower max. limits apply according to season, geographical location, and individual state specification.
(3) Applicable in several states.
(4) California
(5) Recommended
(6) ASTM ES-1-74 (Emergency) specifications for conventional (not unleaded) gasoline.
(7) Federal specification.

TABLE 3.2.3

COMPARISON OF PRINCIPAL LPG SPECIFICATIONS WITH ESTIMATED METHANOL-TO-GASOLINE LPG PROPERTIES- CASE I

	Commercial Propane ASTM D1835*	Est. MTG C_3 LPG Properties	Commercial Butane ASTM D1835*	Est. MTG C_4 LPG Properties
Vapor Pressure at 100°F, max. psig (D1267)	208	171	70	52
Volatile Residue				
Butane and Heavier, max. vol. %	2.5	1.9	-	-
Pentane and Heavier, max. vol. %	-	-	2.0	0.7
Corrosion, max. (D1838)	No. 1	No. 1	No. 1	No. 1
Sulfur, grains (D2784)	15	None	15	None

* 1976 Annual Book of ASTM Standards

BASE CASE I
3.3 THERMAL EFFICIENCY

Table 3.3.1 is a summary of the overall plant thermal efficiency, which is defined as the combustion heat of the products, byproducts and excess power divided by the combustion heat of the total coal feed. The efficiency has been calculated using both the high and low heating values.

TABLE 3.3.1

METHANOL-TO-GASOLINE CASE I - THERMAL EFFICIENCY

	Quantity, Unit/SD	High Heating, Value (HHV)	Total HHV, MMBtu/hr	Percent of Input	Low Heating, Value (LHV)	Total LHV MMBtu/hr	Percent of Net Input
Input							
Coal, DAF	18,286 T	12,720Btu/lb	19,383	-	12,236Btu/lb	18,646(1)	-
Fines(excess)	(823 T)	"	(872)	-	"	(840)	-
Net Coal	17,463		18,511			17,806	
Output							
SNG	148.52MMSCF	980.4Btu/SCF	6,067	32.8	882.6Btu/SCF	5,462	30.7
C_3LPG	1,555 Bbl	3.816MMBtu/Bbl	247	1.3	3.509MMBtu/Bbl	227	1.3
C_4LPG	2,205 Bbl	4.191MMBtu/Bbl	385	2.1	3.865MMBtu/Bbl	355	2.0
10 RVP Gasoline	22,045 Bbl	5.105MMBtu/Bbl	4,689	25.3	4.771MMBtu/Bbl	4,382	24.6
Sub-Total	-	-	11,388	61.5		10,426	58.6
Sulfur	61 T	3,780 Btu/lb	19	0.1	3,780 Btu/lb	19	0.1
Ammonia	103 T	9,693 Btu/lb	83	0.5	8,020 Btu/lb	69	0.4
Power(excess)	5.96 MW(e)	3,415 Btu/kWH	20(2)	0.1	3,415 Btu/kWH	20(2)	0.1
Total			11,510	62.2		10,534	59.2

(1) If LHV of as mined coal used (7,893 Btu/lb), overall LHV thermal efficiency becomes 61.3%.

(2) Direct thermal conversion used.