4.1 Background

The scenario for Case 3, a standalone LPMAS plant, was chosen because of the potential for low cost natural gas feedstock and it is less expensive to produce syngas from natural gas than from coal or coke.

4.2 Study Basis

Figure 4-1 shows the key components for the standalone plant. Natural gas is partially oxidized with steam and oxygen. CO_2 is recovered from the syngas and recycled back to the POX plant to reduce the H₂/CO ratio. Syngas is sent to the LPMAS plant. The balance of the system is similar to Case 1.

Syngas generation via partial oxidation was chosen because it generates a syngas with a low H_2/CO ratio and a low methane content. The methane slippage is significantly higher with authermal reforming (which would result high unconverted syngas flows). Steam reforming produces a syngas with too high a H_2/CO ratio.

4.2.1 Partial Oxidation

The partial oxidation plant consists of twelve trains processing a total of 228 MMSCFD of natural gas. With CO₂ recovery and recycle, the syngas has a H_2/CO ratio of 1.54. The composition of the syngas is provided in Table 4-1.

4.2.2 Syngas Conversion

As in Case 2, a single syngas conversion level was studied. The level, approximately 98%, was based on the assumption that a true standalone plant must be in fuel balance and that any unconverted syngas is consumed in the plant.

4.2.3 LPMAS Recycling

A recycle LPMAS system is required to achieve the high conversion level since a single pass system is limited by methanol equilibrium (see Figure 4-2). The minimum recycle ratio needed to avoid methanol equilibrium constraints is 2.4. The effect of recycling was examined by varying the recycle ratio between 2.4 and 5.7. At the higher ratios, the methanol equilibrium is not restricting. Figure 4-3 shows that the per pass syngas conversion decreases as the recycle ratio increases.

4.3 Economic Analysis

Table 4-2 summarizes the key operating conditions and production rates for each of the four different recycle ratio cases.

The following basis was used for the economic analysis:

- \$1/MMBtu natural gas feed price
- 4-year construction period
- 100% equity
- Gulf Coast location
- 25-year plant life

At each recycle ratio, the required value of the ether product was determined to achieve a 13 percent rate of return based on discounted cash flow analysis. That is, the revenue from the ether product was adjusted to achieve the target rate of return.

4.4 Results

The effect of the recycle ratio/per pass conversion on the required ether price is shown in Figure 4-4. The lowest required ether price is at the methanol equilibrium limit (highest per pass conversion/lowest recycle ratio).

Figure 4-5 shows that the required catalyst productivity declines as the recycle ratio increases. At the minimum recycle ratio, the required productivity is 285 g isobutanol/Kg-hr.

Table 4-3 summarizes the economics for the four cases.

4.5 Sensitivity study - Natural Gas Feedstock Price

As noted in Section 4.3, the study basis price for natural gas was \$1/MMBtu. Figure 4-6 show the effect of the natural gas feedstock cost on the required ether price. The two solid curves correspond to natural gas prices of \$0.5/MMBtu and \$2/MMBtu

4.6 Sensitivity study - Location Factor

Location factor is a term used by cost estimators to adjust the plant costs from a location where the captial and construction costs are known, to another site where the costs may be different. As noted in Section 4.3, the study basis for Case 3 is for a Gulf Coast location and the location factor is 1.0. To show the effect of location, the required ether price was calculated at two other location factors, 0.8 and 1.2. The results of this study are presented in Figure 4-7.

4.7 Sensitivity Study - Elimination of CO₂ Recovery System

The CO₂ recovery system shown in Figure 4-1 represents about 25% of the capital cost of producing the syngas. A sensitivity study was conducted where the CO₂ system was deleted. A block flow diagram of the modified system is shown in Figure 4-8. As shown in Table 4-4, the H₂/CO ratio increases from 1.54 to 2.02.

With this syngas, it was immediately apparent that the methanol equilibrium limitation dictates a high recycle ratio (5.7) to achieve the 98% conversion requirement. Since this is a H₂-rich syngas, it was decided to investigate the effect of increasing the methanol/isobutanol selectivity ratio. It was assumed that excess methanol is sold at the current market price of 35 cents per gallon. The results are shown in Figure 4-9.

At higher selectivity ratios, overall capital costs are lower because of lower recycle ratios. However, as the selectivity ratio increases, more low-value methanol is produced and less high-value MTBE is produced and the overall revenues decrease. The minimum required ether price is reached at a selectivity ratio of 4.0 when the capital savings from the decline in recycle requirements is offset by decreases in revenues because of higher methanol (lower MTBE) production.

4.8 Conclusions

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- Within the study basis parameters, a natural gas-based standalone LPMAS plant could be economically developed.
- A catalyst productivity of 285 g isobutanol/Kg-hr is required to achieve a 13% rate of return (1.03 mole methanol / mole isobutanol). The required ether price at this condition is 68 cents/gallon (\$1/MMBtu natural gas).
- The required ether price is very sensitive to the cost of the feedstock natural gas and the location of the plant.

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Case 3 - Standalone LPMAS

4.9 Tables and Figures

	Study Basis		
Natural gas feed, 10 ⁶ SCFD	228		
Syngas H_2/CO ratio	1.54		
CO ₂ /Feed C, mol/mol	0.28		
Steam/Feed C, mol/mol	1.0		
Syngas production, 10 ⁶ SCFD	587		
Syngas composition, mol%			
co	38.9		
H ₂	59.9		
CO ₂	0.0		
H ₂ O	0.4		
ĊH₄	0.5		
N ₂	0.2		
Ar	0.1		

Table 4-1Syngas Production from Partial Oxidation

Table 4-2 Case 3 - Standalone LPMAS Operating Summary

Case	3 - 1	3 - 2	3-3	3-4
Case Conditions				
Natural gas feed, MMSCFD	228	228	228	228
No of LPMAS trains	3	3	4	5
LPMAS fresh feed, MMSCFD	587	587	587	587
LPMAS reactor feed, MMSCFD	1928	2297	2821	3976
LPMAS recycle ratio, recycle mol/feed mol	2.284	2.913	3.806	5.773
No. of reactors per train	2	2	2	2
Overall syngas conversion	99%	99%	99%	99%
Overall CO conversion	99%	99%	98%	98%
Overall H2 conversion	98%	98%	99%	99%
Per pass syngas conversion	52%	45%	38%	29%
Per pass CO conversion	57%	47%	35%	24%
Per pass H2 conversion	48%	44%	40%	35%
LPMAS reactor inlet molar composition				
со	20.43%	20.66%	22.43%	23.86%
H2	36.93%	34.32%	30.57%	25.23%
CO2	30.26%	31.83%	32.53%	35.44%
H2O	0.16%	0.14%	0.12%	0.10%
Methanol	0.25%	0.27%	0.29%	0.31%
Isobutanol	0.01%	0.01%	0.02%	0.02%
N2, Ar	7.38%	8.07%	8.89%	9.55%
CH4	4.57%	4.69%	5.15%	5.50%
LPMAS reactor outlet molar composition				
со	10.90%	13.02%	16.74%	20.16%
H2	23.71%	23.11%	21.16%	18.25%
CO2	39.97%	39.96%	39.00%	40.12%
H2O	5.44%	4.42%	3.51%	2.41%
Methanol	2.64%	2.20%	1.81%	1.34%
Isobutanol	2.29%	1.85%	1.46%	1.00%
Other alcohols	0.17%	0.14%	0.11%	0.07%
N2, Ar	9.20%	9.67%	10.28%	10.56%
CH4	5.69%	5.62%	5.95%	6.08%
Total alcohol production, stpd	5265	5266	5267	5268
g i-methanol/kg-catalyst-hr	127	106	87	61
g i-Butanol/kg-catalyst-hr	285	239	195	138
Ether production, bpd	32144	32147	32153	32158

Case				
<u>First year revenue, MM\$/yr</u>				
Ether	356.7	366.2	385.8	421.7
Unconverted olefin value @ \$10/bbl	5.5	5.5	5.5	5.5
First year operating costs, MM\$/yr				
Natural gas feed	83.1	83.1	83.1	83.1
Operations and maintenance labor	11.4	11.4	11.4	11.4
Maintenance, taxes and insurance	58.7	60.9	65.5	73.8
Catalyst and chemical costs	13.6	13.6	13.6	13.6
Capital costs.MM\$				
POX plant	213.3	213.3	213.3	213.3
AGR	95.4	95.4	95.4	95.4
Air separation	81.0	81.0	81.0	81.0
Mixed alcohol synthesis	183.5	206.7	254.1	340.5
Alcohol separation	4.7	4.7	4.7	4.7
Alcohol dehydration	4.9	4.9	4.9	4.9
Ether production	28.6	28.6	28.6	28.6
Offsites	122.3	126.9	136.4	153.7
Total	733.8	761.5	818.4	922.2
Field indirect costs and HO eng. costs	110.1	114.2	122.8	138.3
Contingency	168.8	175.1	188.2	212.1
Total plant costs	1012.6	1050.9	1129.4	1272.6
Required ether value for 13% IRR cents per				
gallon	67.7	69.5	73.2	80.0

Table 4-3 Case 3 - Standalone LPMAS Economic Summary

Case 3 - Standalone LPMAS

	No CO ₂ Recovery
Natural gas feed, 10 ⁶ SCFD	268
Syngas H_2/CO ratio	2.02
CO ₂ /Feed C, mol/mol	0.0
Steam/Feed C, mol/mol	1.0
Syngas production, 10 ⁶ SCFD	747
Syngas composition, mol%	
CO	30.5
H_2	61.7
CO ₂	6.7
H ₂ O	0.4
CH ₄	0.4
N ₂	0.2
Ar	0.1

Table 4-4Modified Syngas Production - No CO2 Recovery

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REARIES IN SUCCESSION



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Figure 4-8 Case 3S - Standalone LPMAS Modified Syngas Production Block Flow Diagram

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Summary and Conclusions

5.0 Summary

This study has examined a number of factors that had significant bearing on the results of the study:

- Methanol/isobutanol selectivity
- Syngas H₂/CO ratio
- Syngas conversion/disposition of unconverted syngas
- Recycling syngas to LPMAS reactor
- Methanol equilibrium limitation
- LPMAS reactor space velocity
- CO₂ removal
- Steam addition
- Base load vs. load following operation
- Plant location
- Feedstock costs

In using this study, it is important to bear in mind that the results (i.e. catalyst productivities) are very specific to the study basis and operating conditions.

Table 5-1 summarizes the operating conditions for the most economic scenario for each case. Also included is the Case 3 sensitivity study (Case 3S) where the methanol/isobutanol selectivity ratio was raised from 1.03 to 4.0.

For Case 1, to produce a ether product that is at or below the current MTBE market price of 85 cents per gallon with a once-through LPMAS system, the required catalyst productivity would need to be in the range of 370-460 g iBuOH/Kg-hr (methanol/isobutanol ratio - 1.03).

For Case 2, the most economical case is when the LPMAS reaction is at methanol equilibrium. The internal rate of return is 13.9% and the required catalyst productivity is 265 g iBuOH/Kg-hr.

For Case 3, the most economical case is also when the LPMAS reaction is at methanol equilibrium. For \$1/MMBtu natural gas feedstock, the required ether price is 68 cents/gallon. For \$2/MMBtu natural gas feedstock, the required ether price is 84 cents/gallon.

As shown in Case 3S, there is potential for higher returns if coproduction of methanol and ethers is an option.

5.1 Conclusions

For all three scenarios, economical LPMAS plants are possible, even at current ether market prices. However, large improvements in catalyst productivity and alcohol selectivity must be achieved prior to commercialization of this process.

If inexpensive natural gas feedstock is available, because of the less demanding catalyst productivity and selectivity requirements, coproduction of methanol and ethers looks attractive.

Summary and Conclusions

5.2 Tables and Figures

Case	1	2	3	3S
Feed	Coal	Coke	NG @ \$1	NG @ \$1
Syngas H ₂ /CO ratio	0.5	0.4	1.54	2.02
LPMAS reactor feed H ₂ /CO ratio	0.5	0.5	1.8	3.3
MeOH/iBuOH ratio	1.03	1.03	1.03	4.0
LPMAS syngas recycle ratio	0	2.0	2.3	1.9
Per pass conversion, %	38-49	48	52	45
Overall conversion, %	38-49	95	98	98
Productivity, g iBuOH/Kg-hr	370-460	265	285	181
g MeOH/Kg-hr	165-205	118	126	314
Req'd ether price @13% ROR, cents/gal	85-76		68	53
ROR at 85 cents/gal ether, %		13.9		

Table 5-1 Summary of Conditions
