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THE ECONOMICAL PRODUCTION OF ALCOHOL FUELS FROM COAL-DERIVED SYNTHESIS GAS

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The Economical Production of Alcohol Fuels from Coal Derived Synthesis Gas

CONTRACTOR NAME:
West Virginia University Research Corporation
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213 Glennlock Hall
Morgantown, WV 26506

Report No.: TPR4
Reporting Period: 7/1/92 to 9/30/92
Due Date: 10/20/92

TASK 1. REACTION STUDIES

The objective of Task 1 is to prepare and evaluate catalysts and to develop efficient reactor systems for the selective conversion of hydrogen-lean synthesis gas to alcohol fuel extenders and octane enhancers.

Task 1 has focused on reaction modeling studies, designing equipment, and staffing the project. Modeling studies have begun, preliminary designs for two laboratory scale reactors were completed, and materials and equipment for construction are being ordered. Procurement will be slow since bids must be obtained on nearly every item purchased.

One postdoctoral fellow has been hired to synthesize catalyst. He arrived at the end of the reporting period and is beginning experimental research. In an effort to prepare ultra-fine particles, a visiting scientist has started preparing carbon supported molybdenum sulfide materials using supercritical fluid techniques. Results from this work will be available for the next quarterly technical report. A new graduate student has been added to the project to develop methods of titrating the number of active sites on metal sulfide catalysts.

Two postdoctoral fellows have been hired for reaction engineering work. One started in July, the other will begin November 15. A new graduate student has also been added to the project who will contribute to the reaction modeling studies. A detailed report on our modeling work is provided in section 1.1.

Research at UCC&P has not yet begun. We expect the subcontract with UCC&P to be put in place during the next quarter.

1.1 Results From Modeling Studies

Reaction of CO and H_2 over an appropriate catalyst produces not only alcohols but also a broad spectrum of other products. Methanol, C_2 to

C_x linear and branched alcohols, hydrocarbons, water and carbon dioxide are major reaction products. Describing production of each individual product through a network of rate equations is too massive a task to be considered in a modeling study. Moreover, this kind of kinetic modeling would be of little use for process design and reaction system optimization, since the main effects associated with operating variables could not be isolated. For our purposes, the key products are methanol and higher alcohols, which determine the properties and value of the end product; water, which affects separation costs of the end product; and hydrocarbons, which are an undesirable product.

In this study, we are developing an isothermal kinetic model based on lumping alcohols with more than one carbon as a single product, considering methane production as the only side reaction producing hydrocarbons, and using alcohol dehydration as the reaction consuming higher alcohols. This simplified reaction scheme is listed below:

$$(1) \qquad CO + H_2 \rightleftharpoons CH_3OH$$

$$(2) \qquad CH_3OH + (N_C\text{-}1)\,CO + 2\,(N_C\text{-}1)\,H_2 \longrightarrow HA + (N_C\text{-}1)\,H_2O$$

$$(3) \qquad CO + H_2O \rightleftharpoons CO_2 + H_2$$

$$(4) \qquad CO + 3\,H_2 \longrightarrow CH_4 + H_2O$$

$$(5) \qquad HA \longrightarrow OL + H_2O$$

Reaction (1) is methanol synthesis; reaction (2) is higher alcohol [HA] synthesis proceding through a methanol intermediate; reaction (3) is water-gas shift, necessary for reaction at low hydrogen to carbon monoxide ratio; reaction (4) is methane production; and reaction (5) is dehydration of higher alcohol [HA] to produce olefin [OL]. These five reactions provide an overall reaction scheme involving only six products.

Kinetic expressions for these five reactions have been assumed to have the following form:

(6) $$r_1 = k_1\left[p_{CO}\,p_{H_2}^2 - \frac{p_{CH_3OH}}{K_1}\right]$$

(7) $$r_2 = \frac{k_2\,p_{CH_3OH}}{(1 + k_W\,p_{H_2O})}$$

(8) $$r_3 = k_3\left[p_{CO}\,p_{H_2O} - \frac{p_{CO_2}\,p_{H_2}}{K_3}\right]$$

(9) $$r_4 = k_4\,p_{H_2}$$

(10) $$r_5 = k_5\left[p_{HA}\right]^{\frac{1}{2}}$$

These equations use standard notation where r_1 is the rate of reaction for equation (1); k_1 is the rate constant for reaction (1); p_{CO} is the partial pressure of carbon monoxide at reaction conditions; and K_1 is the equilibrium constant for reaction (1), which is reversible. These rate expressions will be refined for our catalyst systems when experimental data become available.

Rate equations (6) through (10) may be used in standard reaction engineering models for a batch reactor and a dynamic continuous stirred tank reactor [CSTR]. Material balances on each reaction product in the dynamic CSTR model are listed below:

(11) $$CH_3OH: \quad V\frac{dC_{CH_3OH}}{dt} = F^o_{CH_3OH} - F_{CH_3OH} - W(r_1 - r_2)$$

(12) $$HA: \quad V\frac{dC_{HA}}{dt} = F^o_{HA} - F_{HA} - W(r_2 - r_5)$$

(13) $$CO_2: \quad V\frac{dC_{CO_2}}{dt} = F^o_{CO_2} - F_{CO_2} - W\,r_3$$

(14) $$CH_4: \quad V\frac{dC_{CH_4}}{dt} = F^o_{CH_4} - F_{CH_4} - W\,r_4$$

(15) $$OL: \quad V\frac{dC_{OL}}{dt} = F^o_{OL} - F_{OL} - W\,r_5$$

In these equations, V is the volume of the reactor, C_{CH3OH} is the molar concentration of methanol, F^{o}_{CH3OH} is the inlet molar flow rate of methanol, F_{CH3OH} is the outlet molar flow rate of methanol, W is the weight of the catalyst, r_1 is the rate for reaction (1) and r_2 is the rate of reaction 2.

Material balances for each individual reaction product in the batch reactor are listed below:

$$(16) \quad CH_3OH : \quad V\frac{dC_{CH_3OH}}{dt} = - W(r_1 - r_2)$$

$$(17) \quad HA : \quad V\frac{dC_{HA}}{dt} = - W(r_2 - r_5)$$

$$(18) \quad CO_2 : \quad V\frac{dC_{CO_2}}{dt} = - W r_3$$

$$(19) \quad CH_4 : \quad V\frac{dC_{CH_4}}{dt} = - W r_4$$

$$(20) \quad OL : \quad V\frac{dC_{OL}}{dt} = - W r_5$$

The terms in equations (16) through (20) are defined as in the previous set of equations, with the difference being that a batch reactor does not have flow into and out of the reactor.

The compositions of the products from the CSTR and batch reactor may be calculated by numerical integration of the above sets of ordinary differential equations. Development of a computer program for these calculations is in progress. This program will be used to study the yield of higher alcohols as a function of catalyst and reaction conditions.

Task 1 Coordinator: E. Kugler

TECHNICAL PROGRESS REPORT

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TASK 2. PROCESS SYNTHESIS AND FUEL EVALUATION

The objective of Task 2 is to use process synthesis and fuel evaluation studies to optimize the overall conversion process from choice of raw material feed stocks to final product slate.

This report is organized into an executive summary and four appendices which provide more detail on the ideas outlined in the executive summary. The appendices are as follows:

1. Base Case Description
2. Joint Products in the Production of Coal-Derived Alcohol Fuels
3. Literature Review (Alcohol as an Alternative Fuel)
4. Methanol Plus Higher Order Alcohol (Characteristics as a Fuel)

EXECUTIVE SUMMARY

A base case flow sheet for the production of higher alcohols from coal derived synthesis gas has been completed, including an economic analysis. The details of the flow sheet and economics are in Appendix 1. The pay back period for the capital investment for the plant has been calculated as a function of the market price of the product, and this figure is also shown as Figure 1 in Appendix 1. The estimated installed cost is almost $500 MM, and the estimated annual operating cost is $64 MM. At a price in the vicinity of $1.00/gal for the alcohol product, the pay back period for construction of the plant is four years. These values should be considered preliminary, since many of the capital costs were obtained from other paper studies sponsored by DOE and TVA and very few values could be found from actual plants which were built. This issue is currently being addressed. The most expensive capital costs were found to be the gasifier, the cryogenic air separation plant, the steam/power generation plant and the acid gas/sulfur removal processes taken as a whole.

It is planned to focus attention on alternatives to the base case. The problem is that it is less expensive to make syngas from natural gas. Therefore, it is essential to reduce the cost of syngas from coal. This is where the energy park concept becomes important. In order for this process to be economical (at current market and political conditions) a method must be found to reduce the cost of syngas manufacture either by producing energy or by-products. Energy is produced in the base case, but the amount and method has not been optimized. The economic arguments for this concept are detailed in Appendix 2.

Some of the alternatives which will be considered are as follows. A sour gas shift converter will be investigated as an alternative method to natural gas for increasing the H_2/CO ratio. Another alternative is to use natural gas but to do a partial oxidation rather than steam reforming. This could be advantageous since steam reforming is endothermic and partial oxidation is exothermic. Therefore, more energy could be recovered for profit. Of course, the advantage of partial oxidation will depend upon its cost relative to steam reforming. Alternatives to the Texaco gasifier will also be investigated. The advantage of the Texaco gasifier is that at its high operating temperature, no dangerous coal liquids and other toxic chemicals are formed, except for the sulfur gases. Other gasifiers which operate at lower temperatures produce these but also produce the raw materials for value added by-products, such as coal tar pitch. If by-products are the answer to making syngas production more economical, perhaps an optimal situation will be required between production of dangerous intermediates which lead to value added products and the "clean" gasification at high temperatures. Another expensive component of syngas production is oxygen separation from air. It has been reported that alternatives to cryogenics are becoming more economical. We plan to investigate this more fully. Finally, the base case involves use of the Rectisol process for acid gas treatment. We plan to investigate the economics of alternative processes such as Selexol and MEA or Exxon hindered amines. Economics for Selexol are difficult to locate, however, Union Carbide can provide estimates for capital and operating costs based upon proprietary information. Another alternative acid gas treatment process is called hot gas clean up. There is some literature, but no evidence of pilot or other tests. We plan to investigate further.

From the literature, it was found that most studies of the performance of alcohol fuel additives involved at most 25% additive, and at least 70% of the additive was methanol with the remainder higher alcohols. It was also learned that higher alcohols increase water tolerance. Union Carbide has investigated molecular sieves and related adsorption technology for water removal from the final product. The inescapable conclusion is that these processes are very expensive. However, based upon the water tolerance information obtained, the water present in the final product should not be a problem. Details of previous studies, the characteristics, and performance of methanol and higher alcohol fuels can be found in Appendix 3 and Appendix 4. Because there does not appear to be enough information on the performance of fuel additives comprised largely of higher alcohols, the fuels testing group plans to do engine tests in order to determine the performance of different higher alcohol mixtures. These results will be used to determine the types and cost of separation steps needed after the alcohol synthesis reactor.

Task 2 Coordinator: J. Shaeiwitz

Appendix 1

BASE CASE 1 DESCRIPTION

9/16/92

The following report gives a brief description of each of the units in the block flow diagram. All capital cost data in this report, except where otherwise specified, has been estimated from similar installations described in the *Houston Area Medium-BTU Coal Gasification Project Final Report*, published in June 1982 by Union Carbide (1). (All references to material in this report will be referred to as *Houston.*) A factor of 0.65 was used for exponential scaling of the cost of a single train with a different capacity. Linear scaling was used when costing a number of identical trains. The base case is approximately 0.25 times the size of the facility described in the *Houston* report.

SYNGAS PRODUCTION FROM NATURAL GAS

Compressed natural gas (stream 14) and steam (stream 15) are heated in the Steam reformation block. The output gas (stream 17) goes to the Rectisol block. The cost for this unit was estimated from data found for a hydrogen production facility (2).

Installed Capital Cost (1992 dollars) = $15.1 MM

COAL PREPARATION

Coal (stream 10), limestone (stream 11), and water (stream 12), are sent to the coal preparation block. The coal and limestone are crushed, mixed with the water, and pumped to the gasifier as a 70% solids mixture by weight (stream 13). The coal preparation block is comprised of five plants from the *Houston* report. Plant 01 is the coal slurry preparation plant. The cost of this plant was scaled linearly due to its multiple train format and includes two trains plus one spare compared to eight trains plus two spares for the *Houston* system. Plant 61 is the reclaiming, transfer, and crushing plant. The cost of this plant was scaled exponentially. Plant 22 is the barge terminal. This plant was scaled exponentially. Plant 60 is coal receiving and storage and again the cost for this plant was scaled exponentially. Plant 65 is the limestone handling facility. The cost of this plant is assumed to be the same as the *Houston* report for the base case.

Power needs = 1.5 MW
Installed Capital Cost (1992 dollars) = $41.1 MM

CRYOGENIC OXYGEN PLANT

Compressed air (stream 1) is sent to the cryogenic oxygen plant block, and is separated into high purity oxygen (stream 2), nitrogen (stream 3), argon (stream 6), other rare gases (stream 7), and a water and carbon dioxide waste mixture (stream 28). A small quantity of nitrogen (stream 4) is sent to the Rectisol block. The cryogenic oxygen plant block does not include the inlet air compressors or the outlet oxygen compressors, but it does include a refrigeration system that serves the needs of the entire base case. The *Houston* system uses four trains of cryogenic oxygen production and two trains plus one spare of refrigeration. In the cryogenic system, there are provisions for gaseous and liquid oxygen backups sufficient to maintain downstream plant operation in the event of a shutdown in the cryogenic facility. Since our needs are approximately 25% that of the *Houston* system, we assume that only one cryogenic train will be necessary. As for the refrigeration system, we assume that one train plus one spare will be sufficient. We also assume that some scale down is possible for this system, so the capital investment has been calculated linearly for the reduction in trains, and exponentially for throughput reduction per train. The *Houston* plants which comprise the cryoplant block are 02 and 08.

Power needs = 0.0
Steam needs = 1300 lbs/hr 250 psig, 530°F
Installed Capital Cost (1992 dollars) = $66.1 MM

RECTISOL

The raw gas streams (streams 17 and 18) , nitrogen gas (stream 19) for methanol regeneration, and methanol make–up (stream 20) for vapor loss all enter the Rectisol block. H_2S levels are reduced to the ppb range and CO_2 levels to the ppm range. The bulk of the clean syngas (stream 22) is sent to the alcohol synthesis loop while 1% (stream 25) is sent to the COS hydrolysis block. A $CO_2 - N_2$ mixture (stream 24) and a CO_2 rich stream (stream 23) are produced as byproducts. This block is the same as *Houston* plant 05. The cost for this plant was estimated by using linear and exponential scaling.

Power needs = 0.8 MW
Steam needs = 2500 lbs/hr saturated 100 psig
18000 lbs/hr 50 psig at 300°F
Installed Capital Cost (1992 dollars) = $32.9 MM

TEXACO GASIFIER

The coal slurry (stream 13) is mixed with compressed oxygen (stream 9) and burned at 2300–2800°F and 1180 psi in the Texaco gasifier block. The hot, raw gas (stream 8) is sent to the Syngas heat recovery block, and the slag (stream 33) is sent to the slag handling block. The *Houston* system uses ten trains of gasifiers with two of the ten as spares. Our base case calls for a coal feed approximately one quarter that of the *Houston* plant. Thus, we assume that our plant will require two trains plus one spare train, and the capital cost will be thirty percent that of the *Houston* system. The equivalent of the Texaco Gasifier Block is Plant 03 in the *Houston* report.

Power needs = 0.4 MW
Steam needs = 9100 lbs/hr 50 psig, 300°F
Installed Capital Cost (1992 dollars) = $141.1 MM

SLAG HANDLING

Molten slag from the Texaco gasifier block (stream 33) is direct quenched with water and sent to slag disposal (stream 37). A small amount of water (stream 36) is purged from the closed loop and is replaced by water make–up (stream 34). This block is the same as *Houston* plant 63. The cost for this plant was estimated by exponential scaling.

Power needs = 0.0
Installed Capital Cost (1992 dollars) = $2.6 MM

COS HYDROLYSIS

The sulfide rich stream from the Rectisol block (stream 25), a small stream of clean syngas (stream 38), and air (stream 39) are sent to the COS hydrolosysis block where COS is converted to H_2S. The product gas (stream 41) is sent to the Claus sulfur recovery block. The COS hydrolysis block may actually be part of the Rectisol block, but in any case, its cost is assumed to be negligible.

SYNGAS HEAT RECOVERY

The raw gas stream from the Texaco gasifier block (stream 8) at 2300°F and 1180 psi enters the Syngas heat recovery block and is cooled against process boiler feed water at 60°F (stream 71). The raw gas stream exits at 630°F (stream 18), and the boiler feed exits as steam at 1500 psig and 900°F (stream 68). It is assumed that the raw gas stream is cooled further prior to entering the Rectisol block. This block is part of *Houston* plant 04, which includes heat recovery and gas shifting for part of the feed. It was assumed that one syngas cooling train was approximately equal to one–sixth of the total cost of *Houston* plant 04. The cost of the two cooling trains was then scaled exponentially.

Heat removed = 3.36×10^8 Btu/hr
Power needs = 0.3 MW
Installed Capital Cost (1992 dollars) = $6.7 MM

CLAUS PLANT

Hydrogen sulfide rich gas (stream 41) is mixed with air (stream 42) and converted in a two step reaction to elemental sulfur (stream 46). The unreacted hydrogen sulfide (stream 45) is then sent to the Beavon plant for furthur treatment. This block is the same as *Houston* plant 06. The cost for this plant was estimated by exponential scaling.

Power needs = 0.2 MW
Steam needs = 10000 lbs/hr saturated 700 psig
7500 lbs/hr 250 psig at 530°F
Installed Capital Cost (1992 dollars) = $9.6 MM

BEAVON PLANT

The Claus tail gas (stream 45), air (stream 47), and water (stream 48) all go to the Beavon block. Additional sulfur is made (stream 51), and the gas leaving (stream 50) is sufficiently free from sulfides that it can be vented to the atmosphere. A sour water stream (stream 54) is sent from the plant for treatment. The cost of this block was estimated from data collected from various sources (3).

Installed Capital Cost (1992 dollars) = $3.6 MM

MoS_2 ALCOHOL SYNTHESIS LOOP

Clean syngas (stream 26) at 140 atmospheres enters the catalytic reactor along with the syngas recycle (stream 56B). The products (stream 26A) are taken to the separations block where the unreacted syngas is removed (stream 59). Part of this stream (stream 27) is sent to power generation while the rest (stream 56) is sent to CO_2 removal. The cost of this block was estimated from the cost of a methanol synthesis loop (4).

Installed Capital Cost (1992 dollars) = $40.0 MM

CO_2 REMOVAL

This block is very similar to the Rectisol block. Recycled gas from the alcohol separation block (stream 56) is the only feed. CO_2 free syngas (stream 56A) is then recompressed and sent back to the reactor. CO_2 is taken off as a product (stream 57). The cost of this block is assumed to be an exponential function of the Rectisol block.

Installed Capital Cost (1992 dollars) = $15.6 MM

STEAM/POWER GENERATION

10% of the unreacted syngas from the alcohol synthesis loop (stream 27) is mixed with water and heated in the Syngas saturation block. This mixture (stream 66) is then letdown in a turbine, and (stream 70) is then burned with air (stream 67) to provide heat for 1500 psig, 900°F steam production. This steam (stream 74) is mixed with steam of the same type from the Syngas heat recovery block and let down in the steam turbines for power production. As a gross estimate, the four blocks, Syngas saturation, gas turbine, combuster, and steam turbines, as well as other needs in this category not shown on the flowsheet, are assumed to fall within *Houston* plant 31. The power rating on the *Houston* steam turbines is 60 MW, and the load on our turbines is slightly above 50 MW. Therefore, it is assumed that the cost for these blocks will be roughly equivalent to that for *Houston* plant 31.

Power production = 54.6 MW
Installed Capital Cost (1992 dollars) = $65.8 MM

STAND ALONE COMPRESSORS AND POWER SUMMARY

There are 5 compressors which are not included in any of the blocks. Their inlet, outlet, pressure change, power rating, and installed capital cost are listed below. Following this is a summary of the total plant power output/input (5).

FUNCTION	INLET STREAM	P (atm)	OUTLET STREAM	P (atm)	POWER (MW)	COST (MM$)
Air Prep	–	1	1	5	–24.0	0.7
O_2 Prep	2	1	9	80	– 8.8	14.7
CH_4 Prep	–	2	14	80	– 2.4	5.1
Rxtr Prep	22	80	26	140	– 5.2	9.7
Recy Comp	56A	125	56B	140	– 0.7	2.0
Total compressor needs					–41.1	
Other inplant needs					– 6.6	
Total produced in steam and gas turbines					+54.6	
Net power output					+ 6.9	
Total installed compressor costs (1992 dollars)						32.2

TOTAL ESTIMATED CAPITAL INVESTMENT (MM$)

Synthesis Gas via Methane	15.1
Coal Preparation	41.1
Texaco Gasifier	141.1
Slag Handling	2.6
Steam/Power Generation	65.8
Synthesis Gas Heat Recovery	6.7
Cryogenic Oxygen Production	66.1
Rectisol (Acid Gas Separation)	32.9
COS Hydrolysis	
Claus (Sulfur Recovery)	9.6
Beavon	3.6
MoS_2 Alcohol Synthesis Loop	40.0
CO_2 Removal in Alcohol Synthesis Loop	15.6
Other Compressors	32.2
TOTAL	472.4

OVERALL ECONOMIC EVALUATION

The following table gives the totals and breakdowns for the yearly operating costs as well as the total installed cost for the plant. Figure 1 is a graph of the payback period for the plant versus the value of the mixed alcohol product.

TOTAL ESTIMATED INSTALLED CAPITAL COST (MM$)			472.4
TOTAL ESTIMATED OPERATING COSTS (MM$/YR)		64.5	
Coal ($30/ton deivered)		21.2	
Natural Gas ($3/MSCF)		11.3	
Other Expenses		32.0	
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS) (MM$/YR)			8.7
Power	($0.05/kW--hr)	2.8	
Slag	($5/ton) (6)	0.4	
Sulfur	($13.60/100 lbs.) (7)	5.5	

Credits for nitrogen, argon, and other rare gases have not been included because prices were not availible and potential markets have not yet been identified.

Figure 2 is flow chart for Base Case 1
Table 1 is flow table for Base Case 1

IMPORTANT POINTS OF INFORMATION

Several decisions were made for the creation of this base case which should be outlined. Also, there are alternatives which have not been fully considered which will be considered more detail later. They are listed below along with the reasons behind them.

- Catalytic steam/methane reformation used to adjust the H_2:CO ratio upwards. The ratio from coal gasification is less than 1. Since the optimal ratio for higher alcohol synthesis is approximately 1.2, an additional source of hydrogen was required. The reformer was assumed to operate at equilibrium, as suggested in the literature (8). Other alternatives to this block are available and will be considered.

- The traditional method for purifying high quantities of pure oxygen is by cryogenics, which is used for the base case. However, recent reports suggest that membrane and catalytic processes are becoming economically competitive with cryogenics. Therefore, we will examine these alternatives, especially since oxygen production is the second most costly block in the base case.

- The Rectisol system was chosen as the base case system for H_2S and COS removal. The major alternative to Rectisol is Selexol. The literature indicates that Rectisol has a higher installed capital cost, but a lower fixed operating cost than Selexol. Both of these systems are capable of removing H_2S to the ppm level and beyond. However, there is some evidence that quantities of H_2S are beneficial if the reaction involves the MoS2 catalyst. If this is so, then a system such as the Benfield acid gas removal process might be more suitable. The Benfield system does not remove as much H_2S and has lower capital and operating costs.

- The operating pressure for the Texaco gasifiers has been set at 80 atmospheres. This is the highest pressure indicated in the literature at which a Texaco gasifier has been run. Since the pressure required at the reactor is 140 atmospheres, we would of course like to run the gasifiers at as high a pressure as possible. Another limiting factor is the oxygen feed pressure. According to various sources, the highest pressure available with conventional centrifugal compressors is around 60 atmospheres. It is assumed that, because of the size of the base case, a higher cost for the oxygen compressor would be acceptable in return for savings on feed gas compression. In addition, other gasification systems will also be investigated.

- As a place to start, approximately 7% of the total clean syngas is diverted for steam generation and power production, resulting in an overall net power surplus of approximately 7 MW. Factors such as the demand for mixed alcohols or the price of electricity will be considered in order to determine suitable splits.

REFERENCES FOR BASE CASE 1

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4. Frank, Marshall E. "Methanol: Emerging Uses, New Synthesis," *Chemtech,* June 1982.

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8. Rase, Howard F., *Chemical Reactor Design for Process Plants, Volume 2,* John Wiley & Sons, New York, 1977, pp.133–138.

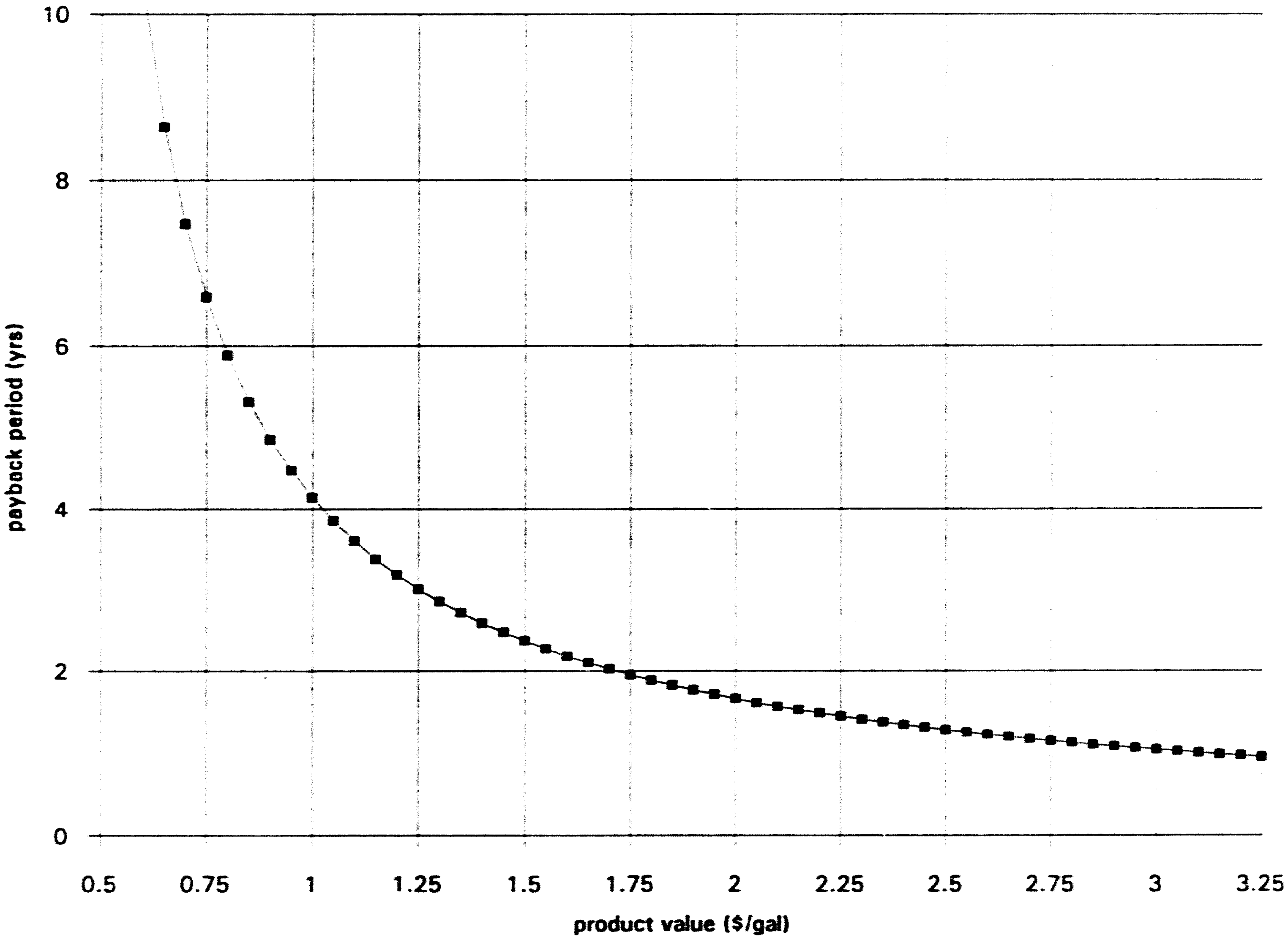


Figure 1
Profitability of Mixed Alcohols from Coal in Base Case 1

Rev 1 7/2/92 Rev 2 8/5/92 Rev 3 8/19/92

RECTISOL) IS MISSING FROM THIS FLOWSHEET BUT IS INCLUDED IN FLOW SUMMARY TABLE

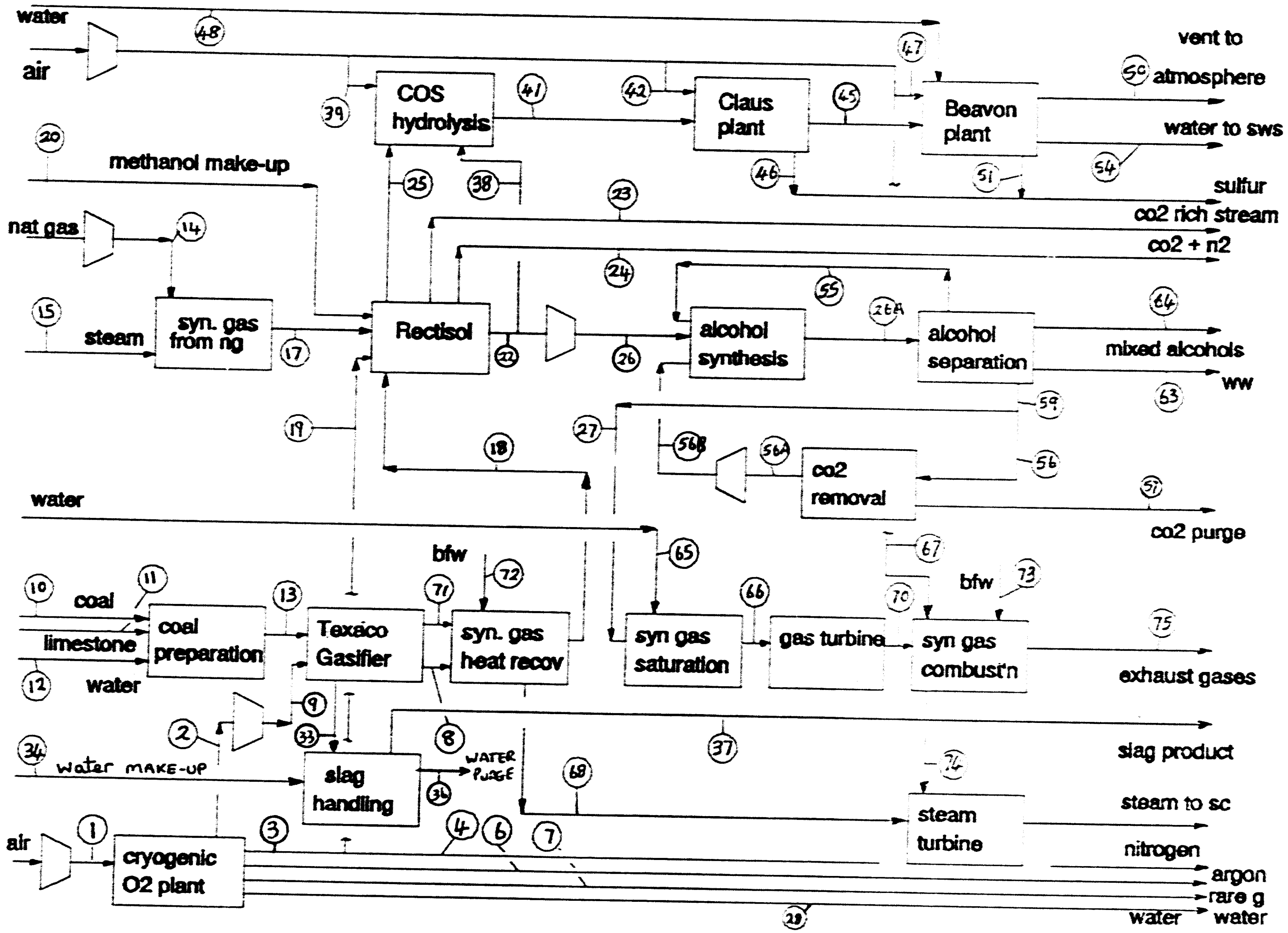


Figure 2
Base Case 1

FLOW TABLE FOR BASE CASE 1

9-26RWM2	001	001A	002	003	004	006	007	008	009	010
Ar	94.1	94.1	0.0	0.0	0.0	94.1		0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	4524.3
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0		21.2	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0		3269.0	0.0	0.0
CO2	3.3	3.3	0.0	0.0	0.0	0.0		1245.3	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0		2.9	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0		2398.8	0.0	1838.8
H2O	243.3	243.3	0.0	0.0	0.0	0.0		3100.0	0.0	51.5
H2S	0.0	0.0	0.0	0.0	0.0	0.0		58.0	0.0	0.0
N2	7882.0	7882.0	0.0	7882.0	7161.4	0.0		33.0	0.0	39.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0		14.2	0.0	0.0
O2	2119.0	2119.0	2119.0	0.0	0.0	0.0		0.0	2119.0	264.0
S	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	60.1
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0		0.0	0.0	83.8
kmol/hr	10341.7	10341.7	2119.0	7882.0	7161.4	94.1	3.1	10142.4	2119.0	6862.0
kg/hr	296792.1	296792.1	67808.0	220695.7	200518.9	3763.2		210399.3	67808.0	78924.1
Temp.(C)	25.0	25.0	25.0	25.0	25.0	25.0	25.0	1300.0	50.0	25.0
Press.(psi)	75.0	15.0	30.0	30.0	30.0	30.0	30.0	1180.0	1180.0	15.0

Table 1

FLOW TABLE FOR BASE CASE 1

	011	012	013	014	14A	015	017	017A	018	019
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	4524.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	595.2	595.2	0.0	4.8	0.0	21.2	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	194.9	0.0	3269.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	395.4	0.0	1245.3	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.9	0.0
CaCO3	3.7	0.0	3.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	1838.8	0.0	0.0	0.0	2166.6	0.0	2398.8	0.0
H2O	0.0	3740.0	3791.5	0.0	0.0	7907.5	6921.7	10021.7	3100.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	58.0	0.0
N2	0.0	0.0	39.6	0.0	0.0	0.0	0.0	0.0	33.0	720.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	14.2	0.0
O2	0.0	0.0	264.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	60.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	83.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	3.7	3740.0	10605.7	595.2	595.2	7907.5	9683.4	10021.7	10142.4	720.6
kg/hr	370.0	67320.0	146614.1	9523.2	9523.2	142335.0	151855.5	180390.6	210399.3	20176.8
Temp.(C)	25.0	25.0	25.0	25.0	25.0	300.0	700.0	50.0	332.0	25.0
Press.(p	15.0	15.0	1180.0	1180.0	29.0	1180.0	1180.0	1180.0	1180.0	15.0

Table 1 (Continued)

FLOW TABLE FOR BASE CASE 1

	020	022	023	024	025	026	026A	027	028	029
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	18.0	0.0	0.0	0.0	18.0	0.0	319.0	0.0	0.0	0.0
CH4	0.0	26.0	0.0	0.0	0.0	25.8	257.7	25.8	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	693.8	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	250.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	83.6	0.0	0.0	0.0
CO	0.0	3463.9	0.0	0.0	0.0	3429.3	2939.3	293.9	0.0	0.0
CO2	0.0	0.0	984.5	574.3	82.0	0.0	346.9	34.7	0.0	2.8
COS	0.0	2.5 ppm	0.0	0.0	TRACE	2.5 ppm	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	4565.3	0.0	0.0	0.0	4519.7	3418.2	341.8	0.0	0.0
H2O	0.0	0.0	0.0	0.0	0.0	0.0	41.8	0.0	243.3	0.0
H2S	0.0	50ppm	0.0	0.0	70.8	50ppm	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	753.6	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	14.2	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	18.0	8055.3	984.5	1327.9	185.0	7974.7	8350.2	696.2	243.3	2.8
kg/hr	576.0	106536.1	43315.8	46368.2	6833.0	105470.7	172582.4	10851.9	4378.7	123.2
Temp.(C)	25.0	25.0	25.0	25.0	25.0	310.0	310.0	50.0	25.0	25.0
Press.(p	15.0	1180.0	15.0	15.0	15.0	2060.0	2060.0	2060.0	15.0	15.0

Table 1 (Continued)

FLOW TABLE FOR BASE CASE 1

	033	034	036	037	038	039	041	042	045	046	047
Ar	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0		18.0	0.0	18.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.3		0.3	0.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	34.6		34.6	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0		82.0	0.0	82.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	0.0	0.0
CaCO3	3.0	0.0	0.0	3.0	0.0		0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	45.7		45.7	0.0	0.0	0.0	0.0
H2O	0.0	200.0	200.0	0.0	0.0		0.0	0.0	64.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0		70.8	0.0	6.8	0.0	0.0
N2	0.0	0.0	0.0	0.0	0.0		0.0	89.2	89.2	0.0	12.8
NH3	0.0	0.0	0.0	0.0	0.0		14.2	0.0	14.2	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0		0.0	32.0	0.0	0.0	3.4
S	0.0	0.0	0.0	0.0	0.0		0.0	0.0	0.0	64.0	0.0
Al2O3	83.8	0.0	0.0	83.8	0.0		0.0	0.0	0.0	0.0	0.0
kmol/hr	86.8	200.0	200.0	86.8	80.6	0.0	265.6	121.2	274.2	64.0	16.2
kg/hr	8849.6	3600.0	3600.0	8849.6	1065.4	0.0	7898.4	3520.4	8306.2	2048.0	466.9
Temp.(C)	1300.0	25.0	50.0	50.0	25.0	25.0	25.0	25.0	370.0	25.0	25.0
Press.(p	1180.0	500.0	15.0	15.0	1050.0	15.0	15.0	15.0	15.0	15.0	15.0

Table 1 (Continued)

FLOW TABLE FOR BASE CASE 1

	048	050	051	054	055	056	056A	056B	057	059	063
Ar		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH		18.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4		0.0	0.0	0.0	0.0	231.9	231.9	231.9	0.0	257.6	0.0
C2H6O		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO		0.0	0.0	0.0	0.0	2645.3	2645.3	2645.3	0.0	2939.2	0.0
CO2		82.0	0.0	0.0	0.0	312.2	0.0	0.0	312.2	346.9	0.0
COS		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2		0.0	0.0	0.0	0.0	3076.4	3076.4	3076.4	0.0	3418.2	0.0
H2O		0.0	0.0	70.8	0.0	0.0	0.0	0.0	0.0	0.0	41.8
H2S		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2		12.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3		14.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S		0.0	6.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	0.0	127.0	6.8	70.8	0.0	6265.8	5953.6	5953.6	312.2	6961.9	41.8
kg/hr	0.0	4783.5	217.6	1274.4	0.0	97667.6	83930.8	83930.8	13736.8	108519.5	752.0
Temp.(C)		370.0	25.0	370.0	310.0	310.0	310.0	310.0	25.0	310.0	25.0
Press.(psi)		15.0	15.0	15.0	2060.0	1840.0	1840.0	2060.0	15.0	1840.0	15.0

Table 1 (Continued)

FLOW TABLE FOR BASE CASE 1

	064	065	066	067	068	070	071	073	074	075
Ar	0.0	0.0	0.0	17.7	0.0	0.0	0.0	0.0	0.0	17.7
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	319.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	25.8	0.0	0.0	25.8	0.0	0.0	0.0	0.0
C2H6O	693.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	250.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	83.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	293.9	0.0	0.0	293.9	0.0	0.0	0.0	0.0
CO2	0.0	0.0	34.7	0.0	0.0	34.7	0.0	0.0	0.0	354.5
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	341.8	0.0	0.0	341.8	0.0	0.0	0.0	0.0
H2O	0.0	241.6	241.6	0.0	6104.0	241.6	6104.0	2611.3	2611.3	635.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	1380.6	0.0	0.0	0.0	0.0	0.0	1380.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	369.5	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	1346.4	241.6	937.8	1767.7	6104.0	937.8	6104.0	2611.3	2611.3	2387.8
kg/hr	63308.2	4348.8	15200.7	51186.6	109871.6	15200.7	109872.0	47003.4	47003.4	66392.2
Temp.(C)	25.0	25.0	600.0	25.0	500.0	25.0	20.0	20.0	500.0	25.0
Press.(p	15.0	15.0	1840.0	15.0	1514.0	15.0	1515.0	1515.0	1515.0	15.0

Table 1 (Continued)

Appendix 2

JOINT PRODUCTS IN THE PRODUCTION OF COAL–DERIVED ALCOHOL FUELS

The production of coal–derived alcohol fuels involves the conversion of coal to syngas (called process A) and the conversion of the syngas to alcohol fuels (called process B). By–products can be obtained from both process A and B. It is also possible to operate A and B jointly. Therefore, the economics of joint product production becomes a consideration in the manufacture of coal–derived alcohol fuels. Production alternatives for the two processes can be analyzed separately and together.

Process A involves the production of syngas with or without the production of by–products such as electrical power, coke, coal tar products, and other coal derived chemicals. By–product production can be in fixed or variable proportions or some combination of both. At the extreme, the proportion of syngas can vary from 0 to 100 percent of the output (not including "waste" products such as slag). When no syngas is produced, all resources are devoted to the production of the by–products. Also, if by–products are manufactured (at the expense of syngas production), the proportions of the various by–products can vary within certain ranges.

Process B involves the conversion of syngas into methanol and waste products (such as sulfur and CO_2) and possibly by–products, such as higher alcohols. Again, by–product production can be in fixed or variable proportions or some combination of both. The proportion of methanol can vary from 0 to 100 percent, just as in the case of process A and the production of syngas. Also, if by–products are manufactured (at the expense of methanol production), the proportions of the various by–products can be varied within certain ranges. Since syngas can be obtained from sources other than coal, such as natural gas, the analysis of process B can be made independently from process A.

Joint product production can also involve both processes as long as syngas consumed in process B is produced from process A. This is the most complicated case and involves varying proportions of by–products from processes A and B and varying the proportions of syngas and methanol production.

The existence of joint product production presents a number of production and marketing difficulties. First, choosing the mix of goods to be produced and their quantities is a constrained optimization problem (not necessarily linear and possibly dynamic). Second, marketing the products in proportion to their production may be difficult and usually requires the cost of stockpiling one or more of the joint products or selling the excess production at a price lower than the anticipated market price. Lastly, couching the production problem in terms of joint product production allows us to determine the necessary conditions for joint production involving both A and B.

An estimate of the required value of by–product credits to make the production of coal–derived methanol economic from process A and B can be obtained by determining the current or anticipated difference between the price of gasoline fuel and the cost of producing methanol from natural gas. This simplified approach ignores all costs due to externalities, such as the reduction of pollution costs, and ignores related costs, such as required modifications of the transportation fuel distribution system or engine modifications.

For example, assume the cost of producing and distributing methanol from syngas costing \$x/Mft^3, without by–product credits, is \$3.00 per gallon gasoline equivalent and the price of oil, with current taxes and crude oil costs, is \$1.25 per gallon. In this case, methanol by–product credits would have to equal \$1.75 per gallon of gasoline equivalent to make the use of methanol economical. The first problem is to find the appropriate by–products from process B that would at least equal \$1.75 per gallon methanol equivalent. Costs or credits due to environmental or engine design differences would then modify the cost differential.

Another factor to consider is the price at which the feedstocks for methanol production can be obtained. For example, methanol can be made from domestic natural gas at a price of \$0.40–0.50/gal and imported methanol made from previously flared natural gas can be purchased at a U.S. port price of about \$0.25/gal. These raw material prices specify the maximum price of syngas that could be obtained from process A or that could be used by process B.

Since methanol can be manufactured from natural gas, process B will be economical only if process costs are decreased or if the value of by–products increase the value of total output.

Likewise, process A would be an uneconomical source of syngas feed for process B unless the production of syngas less by–product credits from process A were less than the equivalent price of feedstocks to produce market priced methanol. If A and B are to be jointly profitable, by–product credits from process A and B must be greater than the difference in costs of obtaining methanol from natural gas or imports.

Joint Product Production Theory

1. Assumptions:

Process A -- coal conversion

$$\text{coal} \longrightarrow \text{processing} \longrightarrow \begin{array}{l}\text{products}\\ \text{syngas}\\ \text{By-products}\end{array}$$

Process B -- syngas conversion, unspecified syngas source

$$\text{syngas} \longrightarrow \text{processing} \longrightarrow \begin{array}{l}\text{products}\\ \text{Methanol}\\ \text{By-products}\end{array}$$

2. The prices of methanol and syngas are determined by the price of methanol obtained from domestic natural gas or the price of imported methanol. The prices of domestic coal and all by-products are assumed to be known and unchangeable.

3. We can optimize A and B separately using an appropriate risk adjusted discount rates. In both cases we can achieve global optimizations through the assumption that joint products for A and B are produced in variable proportions. This is the least constrained case.

$$\max \text{NPV } A = A^* \text{ and } \max \text{NPV } B = B^*$$

4. However, we wish to operate A and B together. To do so economically means we must optimize AB, $A|B$, or $B|A$ by

$$\begin{aligned}\max \text{NPV } (AB) &= A'B' \text{ or}\\ \max \text{NPV } (A|B) &= A'B^* \text{ or}\\ \max \text{NPV } (B|A) &= B'A^*\end{aligned}$$

with appropriate constraints. For $A'B'$ and $A'B^*$ the constraints would be the production of a minimum quantity of one or more of the products. For $B'A^*$, the least binding constraint would be to process a minimum amount of coal. In this case, if $A^* > B^*$, only production from A will be economical.

$A'B'$ is not separable and represents joint product production in A and B in either fixed proportions or variable proportions within certain ranges. If $A'B'$ represents variable proportions over all value ranges, the problem becomes one of two single product productions, not joint product production.

5. The existence of joint product production can (and usually?) reduce the feasible range of solutions for either A or B by the addition of one or more constraints. If this is so, the additional constraints on A or B will result in the following inequality:

$$A'B' < A^* + B^*$$

In this case, joint product production is not economically feasible.

6. Therefore, the necessary conditions for the manufacture of products jointly using A and B are

$$A'B' > A^* + B^* \text{ or}$$
$$B'A^* > A^* + B^* \text{ (means } B' > B^*\text{) or}$$
$$A'B^* > A^* + B^* \text{ (means } A' > A^*\text{)}$$

$$pga < pgb$$
(price of syngas from A < price of gas from natural gas)

7. This means

$$pca > pga - pgb$$

price of by–products from A >
price of syngas from A – price of gas from natural gas

There is no obvious reason for $B' < B^*$.

8. This then raises the question of under what circumstances would $A'B' > A^* + B^*$. The answer depends on the value of the by–products produced from processes A and B relative to the price of syngas and gasoline, and appears to be dependent upon:

A. The by–product credits obtained from A.

B. The by–product credits obtained from B only if there are differences in chemical composition of coal–derived syngas and natural gas so that a higher valued mix of by–products can be produced from process B.

C. The capital and operating costs of AB < A + B. It is not obvious how this could be possible.

D. The sale of the joint products can be made in conjunction with the production schedule, which may involve either fixed or variable production quantities.

Appendix 3

I LITERATURE REVIEW

Methanol can be used in heavy duty diesel engines, e.g., the Detroit Diesel 6V-92 engine runs methanol with a small amount of lubrizol additive as a corrosion inhibitor.

1.1 Alcohol as An Alternative Fuel

Several alcohols have been used as motor fuels. Many studies have been done on the use of methanol and ethanol as blending agents with gasoline for use in internal combustion engines. Ethanol and methanol can be used up to 10% without modifying the engine. Very sparse literature exists,if any, on the use of isobutanol and propanol as fuels. However, Isobutanol and propanol, however, have been used as cosolvents to promote the stability of methanol-gasoline and ethanol-gasoline blends (Lee, 1988 and Wigg, 1974). Since isobutanol has a higher stoichiometric air-fuel ratio than the lighter alcohols, a higher percentage of isobutanol can be used as an extender without requiring significant engine adjustments or redesign (Sanyal, 1991). Table 2 shows the properties of Methanol, Ethanol, N-Propanol and Isobutanol. It should be mentioned at this point that methanol and ethanol have found a fair amount of acceptance as fuels in diesel engines. However, these are dedicated alcohol engines such as DDC 6V-92 TA. The focus of this project is to study the use of higher alcohols as blends in existing engines.

1.1.1 Isobutanol as an alternative fuel

R. M. Bata, A. C. Elrod and Thomas P. Lewandowski (1989) found that the use of isobutanol-gasoline blends results in only a small loss of efficiency relative to gasoline for a given engine. The BSFC (Brake Specific Fuel Consumption) increases about 6.5% (corresponding to about 2.5% reduction of the thermal efficiency) for a 20% reduction of the gasoline consumption in a 2.2 liter, four cylinder automotive spark-ignition engine. It was noted that the loss of efficiency would be less (and possibly reserved) if the engine were designed with a higher compression ratio. The loss of thermal efficiency was less using isobutanol-gasoline blend than using methanol-gasoline and ethanol-gasoline blends since the heating value of isobutanol is closer to that of gasoline. This is due to isobutanol's higher carbon-hydrogen ratio which raises its heating value 70% above that of methanol and 25% above that of ethanol. Butanol is also superior to both methanol and ethanol because it has less affinity for water (Bata, 1989).

Isobutanol emissions characteristics are similar to those of methanol and ethanol (Rice, 1991 and Sanyal, 1991). Carbon monoxide and nitrogen oxides emissions from isobutanol-gasoline blends are lower than those of gasoline, but higher than those from blends of ethanol and methanol for identical engine conditions. Carbon monoxide emissions from alcohol fuels are less as compared to CO emissions from gasoline at a given air-fuel ratio due to the leaning effect related to the lower

Properties	Methanol	Ethanol	N-Propanol	Isobutanol
Formula	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
Molecular Weight	32.04	46.07	60.09	74.12
Composition (Wt%)				
(C)	37.50	52.20	59.90	64.80
(H)	12.60	13.10	13.40	13.60
(O)	49.90	34.70	26.60	21.60
Sp. Gravity 60 F/60 "F	0.793	0.811	0.8045	0.8030
Vapor Density (Air=1)	1.1	1.3	2.1	2.5
Boiling Temp ("F)	147	171.1	207	226.2
Flash Point ("F)	54	54	81	95
Auto Temp ("F)	867	793	750	892
Flammability Limit (upper, lower)	(36,6)	(19,3.3)	(13.7,2.1)	(10.6,1.7)
Energy Content (Btu/g)	64,640	84,160	93,620	100,830
Air/Fuel Ratio	6.463	9.027	10.285	11.126
Heat of combustion (Kcal/mol)				
Liquid	-173.55	-326.85	-482.75	-639.60
Gas	-182.62	-337.02	-494.13	-652.10

Properties of Methanol, Ethanol, Isobutanol and N-Propanol (Ramanathan, 1988).

Table 2

stoichiometric A/F value for alcohols. This effect, together with a lowering of peak combustion temperature for alcohol blends, lowers the nitrogen oxide level for alcohols (Rice, 1991). Unburned fuel emissions (in terms of organic material hydrocarbon equivalent and grams per mile) from Isobutanol-gasoline blend are higher than those from gasoline alone. However, they are lower than the emissions from both ethanol-gasoline and methanol gasoline blends. The above comparisons were made by comparing the emissions from 20% alcohol- 80% gasoline blends (Rice, 1991 and Sanyal, 1991).

1.2 Phase Stability (Susceptibility to Layer Separation)

When small amounts of water are added to blends of alcohol and gasoline, hydrogen bonds form between water and alcohol molecules and the blends separate into two phases. Paraffinic hydrocarbons predominate in the upper phase, while the lower phase consists primarily of alcohols and water (Patel, 1987). The ability of gasoline-alcohol blends to carry water without separation depends on the gasoline temperature, percentage of alcohol in the blend, molecular weight of the alcohol, and on the hydrocarbon composition of the gasoline. More water can be tolerated in higher temperature, higher alcohol percentage, heavier alcohol molecular weight, and higher aromatic content fuels. Methanol blends are the most critical as concerns water tolerance before the phase separation point is reached compared to higher alcohol blends. This is due to the decrease in hydrophylic character of the alcohol as the molecular weight increases. If the water content greatly exceeds the water tolerance level of the alcohol, losses are such as to impair their octane contribution (Pea, 1988).

1.2.1 Methanol

If anhydrous conditions are maintained, 15 % methanol by volume should have no solubility problems. For a typical gasoline, phase separation occurs in the presence of less than 1 % water (Wigg, 1974). In another study, it was mentioned that phase separation begins to occur with 0.1 % water in a blend of 15 % methanol, 85 % unleaded gasoline at ambient temperature (Smith, 1983). In Figure 2, the phase separation occurs with 0.175 % water in 15 % methanol, 85 % gasoline at 70°F. The difference between these data could be caused by the difference in the temperatures and in the water contents in methanol and gasoline.

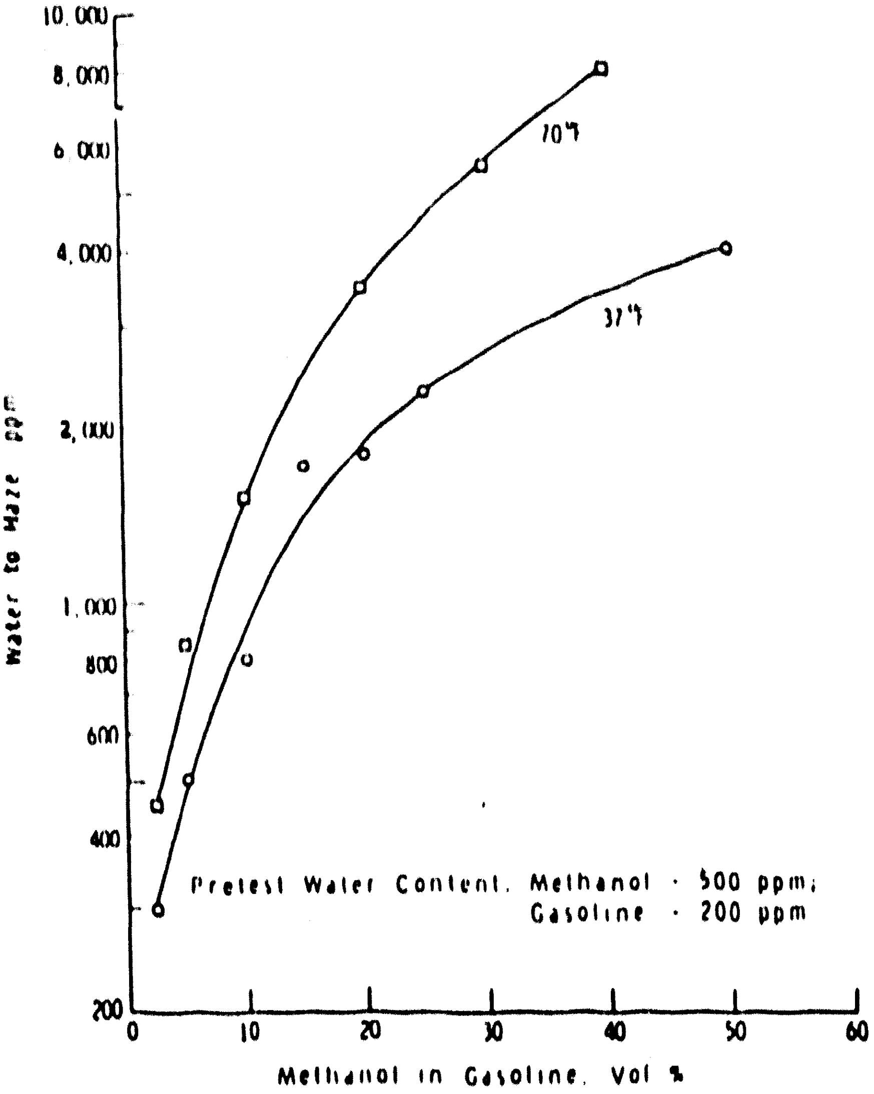


Figure 2 Water Tolerance For Methanol/Gasoline Mixture (Ingamells, 1975)

Figure 3 shows the solubility temperature vs tolerated water for gasoline-methanol blend compared to gasoline-ethanol blend.

1.2.2 Ethanol

Fifteen percent ethanol by volume in 85 % unleaded gasoline at ambient temperature will separate in the presence of 0.65 % water (Smith, 1983). The unleaded gasoline used was purchased from a local service station and there was no information on the initial amount of water in this fuel. Figure 3 shows the solubility temperature vs tolerated water for gasoline-ethanol blends compared to methanol blends. The water tolerance characteristic of ethanol is closer to that of higher alcohols than to methanol. This can be seen from Figures 4 and 5.

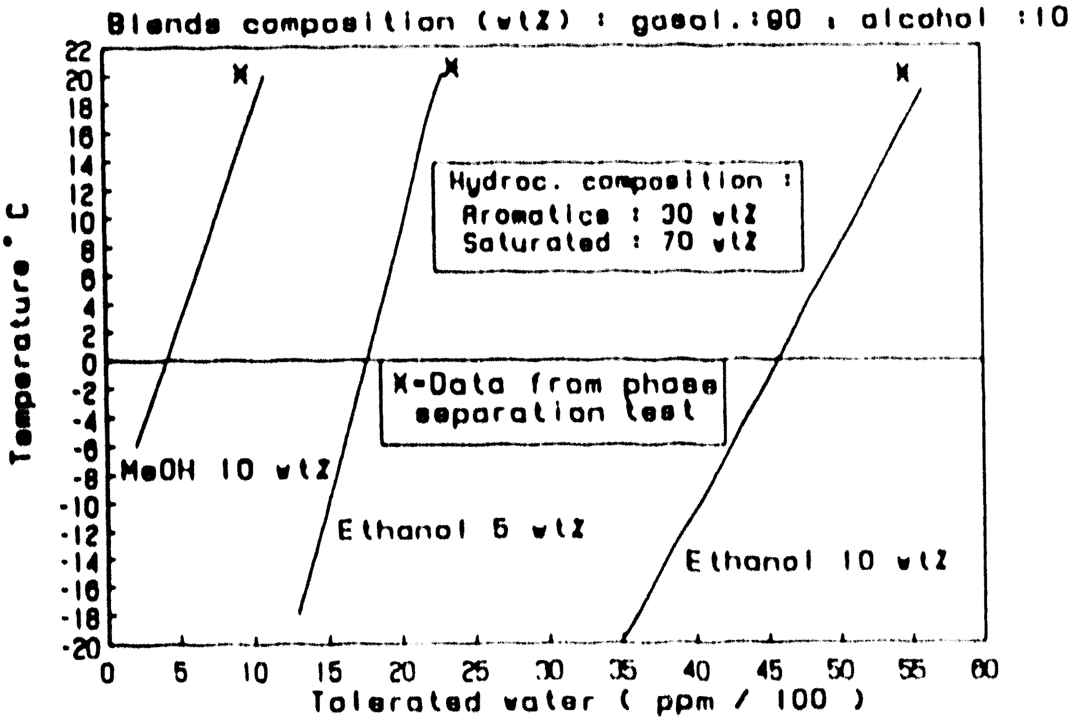


Figure 3. Complete Solubility Temperature vs Tolerated Water for Gasoline-Alcohols Blends (Pea, 1988)

Figures 4 and 5 show the alcohol vs water content in the upper phases at 20°C (68°F). The water present in the upper phase represents the water tolerance limit, since the phases are in equilibrium.

1.2.3 Propanol and Isobutanol

There is a very limited work on the phase stability of propanol-gasoline or isobutanol-gasoline blends. However, there is some data for isopropanol and tertiary butanol. Figures 4 and 5 show the alcohol vs water content for Ethanol, TBA (Tertiary butyl alcohol), and IPA (Isopropanol) at 20 °C (68°F). Propanol

figure 4

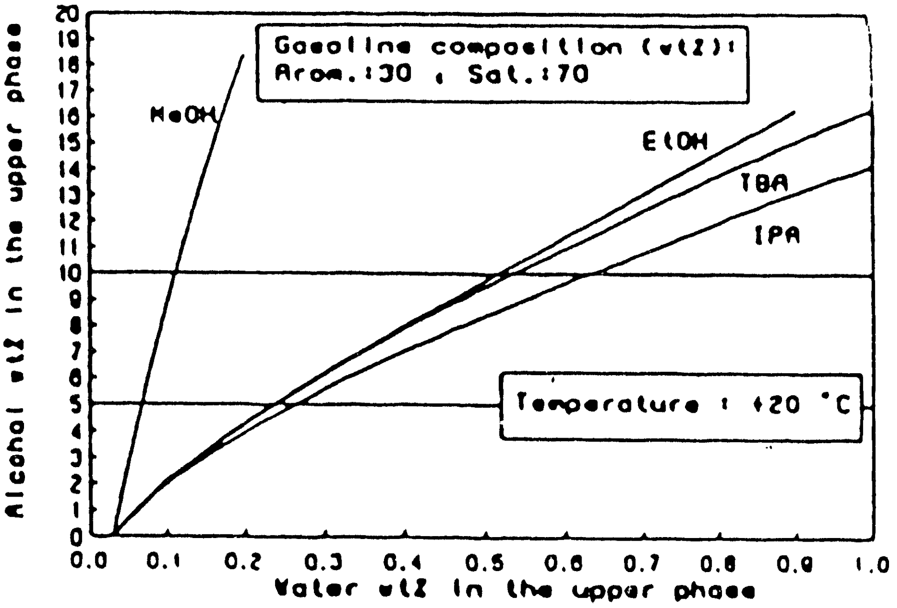


Figure 4. Alcohols vs Water Content in The Upper Phases of Gasoline/Alcohol/Water Systems (Pea, 1988)

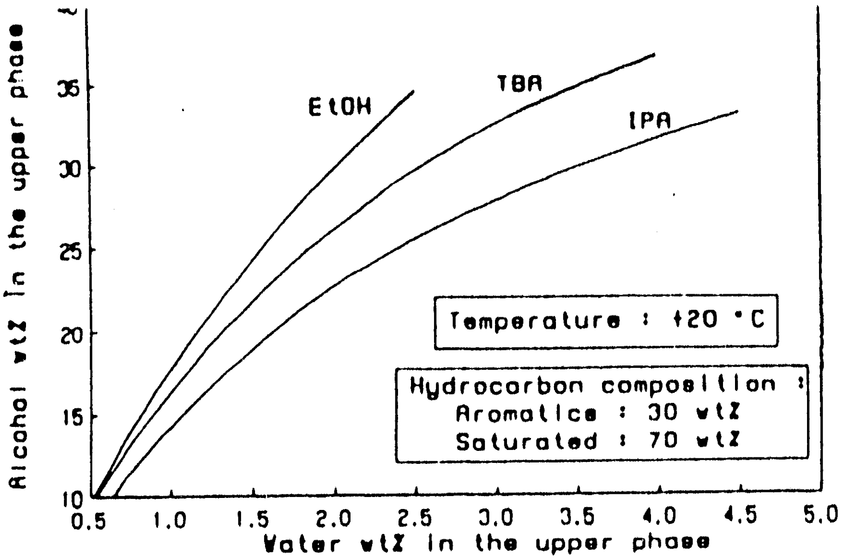


Figure 5. Alcohols vs Water Content in The Upper Phases of Gasoline/Alcohol/Water Systems (Pea, 1988)

and Isobutanol are often used as cosolvents with methanol-gasoline fuels. IPA and TBA have higher water tolerance levels than methanol and ethanol-gasoline blend and can be handled with separated phases without impairing the octane level of the gasoline or without producing lower phases rich in harmful aromatics (Pea, 1988).

1.2.4 Methanol Plus Higher Alcohols

Douthit and Talbot (1984) did a study on the effect of higher alcohols in methanol-gasoline blends. The composition of the higher alcohols composition used was as follows:

Alcohol	vol.%
Ethanol	11.9
1-Propanol	23.0
Isobutanol	43.6
1-Butanol	3.0
2-Butanol	2.2
2-Methyl-1-Butanol	7.3
2-Pentanol	1.7
2-Methyl-1-Pentanol	4.7
4-Methyl-2-Pentanol	2.6

The result on the water tolerance is plotted in Figure 6.

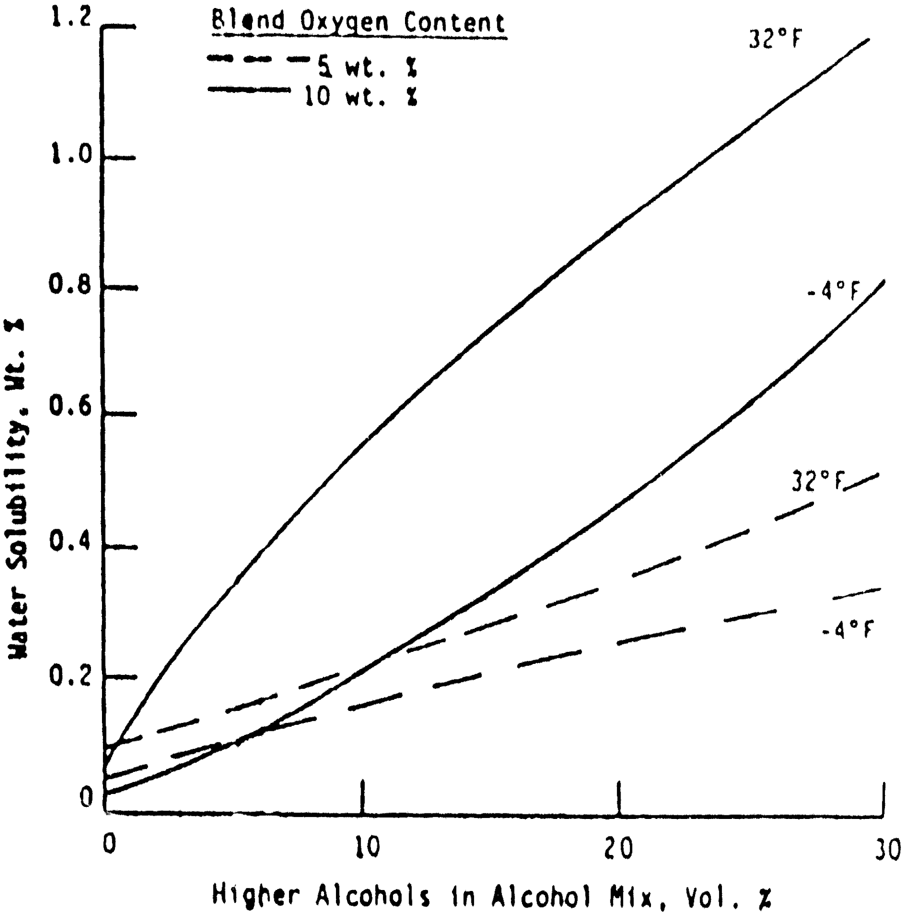


Figure 6 Effect of Higher Alcohols on Water Tolerance of Alcohol/Indolene Blends (Douthit, 1984)

Patel, Kumar, and Kwon did a study on the effect of higher alcohols in methanol-indolene ($C_{7.261}H_{13.87}$)blends. The alcohol (MPHA) composition was as follows: 75% methanol, 5% ethanol, 7.5% 1-propanol, and 12.5% 2-methyl-1propanol (isobutanol). At room temperature, the 90% methanol blend has water tolerance of 8.25 percent by volume and the 90% MPHA blend has about 50% higher water tolerance than 90% methanol blend. At 10% methanol blend the water tolerance is 0.25% (Patel, 1988).

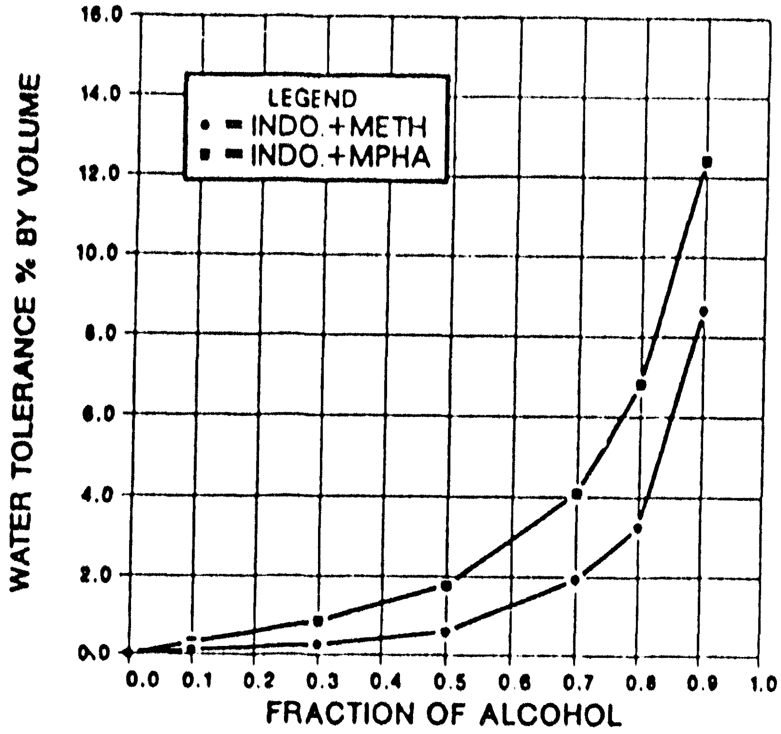


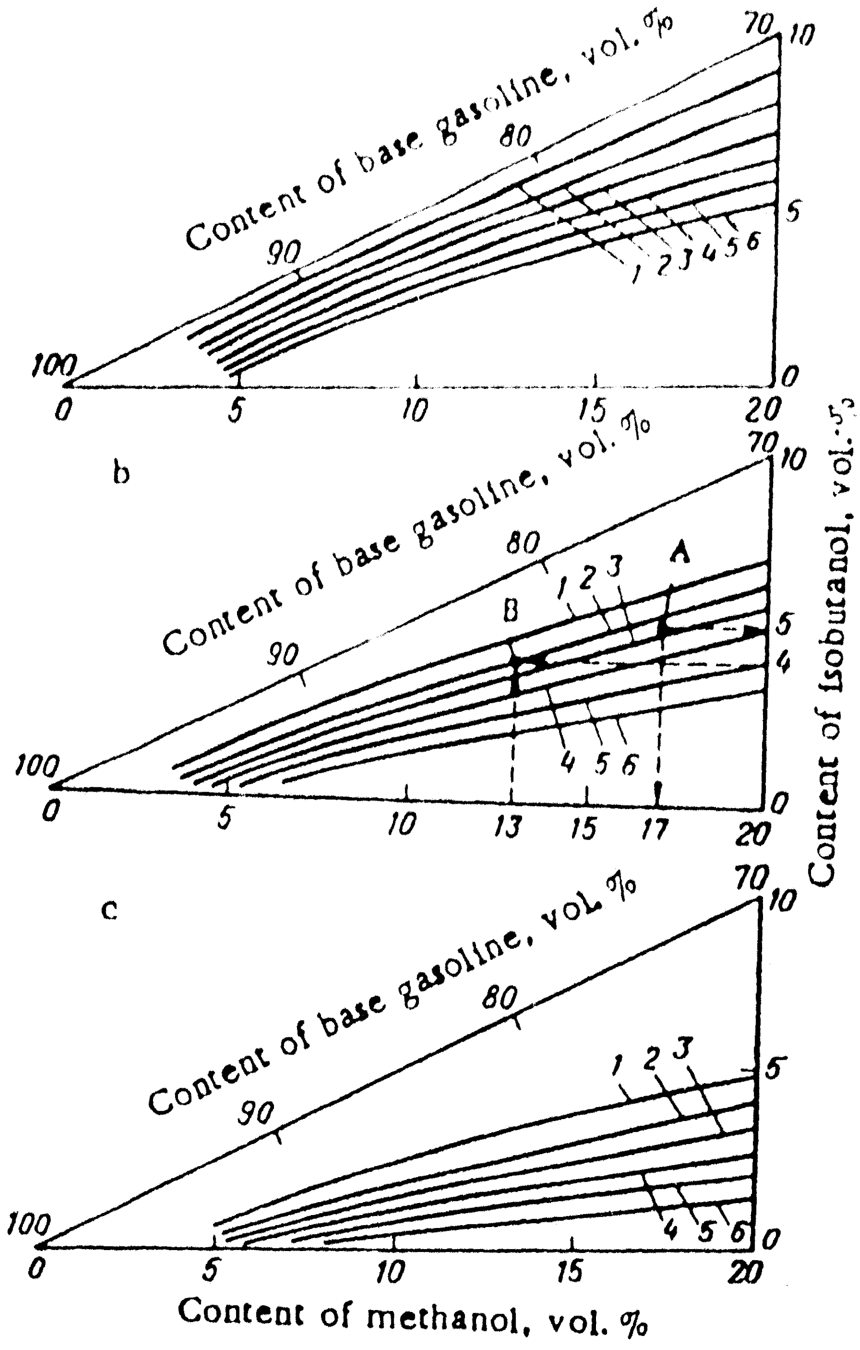
Figure 7. Water Tolerance of Indolene-Alcohol Blends (Patel, 1987)

1.2.5 Ethanol, Isobutanol and Propanol as Cosolvents for Methanol-Gasoline Blends

Since a very small percentage of water can be telerated in the methanol-gasoline blends before phase separation occurs, cosolvents are needed to allow a higher percentage of water.

Lee, Shah, and Brinkman (1988) did a study on the effect of different cosolvents on 50% methanol- 40% isooctane- 10% toluene blend (toluene was used to give the same effect ascommercial gasoline containing about 25% aromatics). The result shows that the minimum concentration of cosolvent in the blend to avoid phase separation was 50 vol.% for ethanol, 9.9 vol.% for propanol and 8.3 vol.% for isobutanol (Lee et al., 1988).

Lebedev, Burmistrov and Pirogov (1984) did a study on the effect of varying composition of isobutanol, methanol and gasoline on the cloud point. Cloud point is the temperature at which the alcohol-gasoline fuel solution becomes opaque. Three gasolines with the following hydrocarbon compositions: aromatics 11%, 15%, and 23% by volume, respectively; paraffins plus naphthenes 38%, 72%, and 71%; olefins 51%, 13%, and 6% were used. Methanol and isobutanol used were first-quality grade, with the respective water contents of 0.08% and 0.09% by weight. The results of this study were plotted in Figure 7. In the region lying above the curve of phase stability at the specific temperature, the gasoline is stable; below the curve, it separates into layers.



(a) A-66 (b) A-72 (c) A-76

1) -35°C 2) -30°C 3) -25°C

4) -20°C 5) -15°C 6) -10°C

Figure 8. Phase Stability Curves for Methanol-Containing Gasoline Based (Lebedev, 1984)

II INSTRUMENTATION

2.1 Engine

A Standard single cylinder CFR spark ignition engine with a variable compression ratio manufactured by Waukesha Motor Company will be used in the experiment. The engine dimensions are given in Table 2.

Table 2. CFR spark ignition engine dimensions

Engine Dimensions	
Compression Ratio Range	4:1 to 18:1
Bore, inches	3.25
Stroke, inches	4.50
Displacement, cubic inches	37.33
Valve Port, diameter, inches	1.187
Connecting rod bearing:	
diameter, inches	2.250
length, inches	1.420
Front main bearing:	
diameter, inches	3.00
length, inches	1.943
Rear main bearing:	
diameter, inches	3.00
length, inches	3.219
Piston pin, floating, diameter, inches	1.25
Connecting rod:	
length, center to center, inches	10.00
width, inches	1.620
Timing gear face, inches	1.00
Exhaust pipe, diameter, inches	1.25
Weight of engine, pounds (approximate)	800

2.2 Spark Plug

Spark Plug that will be used is Champion D16.

2.3 Thermocouple

Thermocouples will be placed at the H2O inlet and outlet, exhaust outlet, air inlet, and cylinder.

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Methanol Plus Higher Order Alcohols

The characteristics of methanol plus higher order alcohols are closer to indolene than those of methanol. Douthit and Talbot (1984) concluded in their paper that blend properties are not uniformly affected by whether the fuel contained methanol or MPHA (Methanol Plus Higher Order Methanol). For example, blend specific gravity increases regularly and the net heat of combustion decreases as the total alcohol content, whether as methanol or as MPHA, of the blend is increased. The composition of MPHA that Douthit and Talbot used is specified in Table 3 . This composition will be referred to as MPHA^1 in the fuel evaluation part of the project.

Base Gasoline - Indolene

Nominal Oxygen Content, Wt.%	Total Alcohol, Vol. %	Alcohol Mixture, Vol. %	
		Methanol	Higher Alcohols(1)
0	0	-	-
5	10.0	100	0
5	10.9	85	15
5	12.2	70	30
10	20.0	100	0
10	22.0	85	15
10	24.4	70	30

	Alcohol	Vol. %
(1) Composition:	Ethyl alcohol	11.9
	1-Propanol	23.0
	Isobutanol	43.6
	1-Butanol	3.0
	2-Butanol	2.2
	2-Methyl-1-butanol	7.3
	2-Pentanol	1.7
	2-Methyl-1-pentanol	4.7
	4-Methyl-2-pentanol	2.6
		100.0

Table 3. Composition of MPHA^1 (Douthit, 1984)

K. S. Patel, S. Kumar and O. Y. Kwon concluded that, in general, MPHA-indolene blends have higher water tolerance, similar specific gravity, similar flash point and different distillation characteristics compared to methanol-indolene-blends (Patel, 1987). The composition of MPHA that they used is 75% methanol, 5% ethanol, 7.5% 1-propanol and 12.5% 2 methyl 1-propanol. This composition is labeled 2 (MPHA') in the fuel evaluation part of the project.

A. Tontodonati, G. Marchesi and M. Bargagna (1984) did research in blending MAS in gasoline. MAS is methanol and higher alcohols from "Syngas." The MAS 70/30 seems to be the best compromise between production cost and behaviour as gasoline component. Mixture containing up to 10% v. MAS is suitable for use in the automotive field. The main characteristics of MAS 70/30 are shown in Table 4 (Tontodonati et al., 1984).

Property	MAS	Methanol
Density at 15 °C(kg/l)	0.804	0.796
R.V.P. (bars)	.230	0.3568
IBP/FBP °C	63/189	65/65
Ev. at 70/100/150 %v	61/85/95	100
Lower Heat Kcal/kg	5870	4767
Flamm. at 50 °C UP/LOW	32.2/3.5	38.5/4.4
Water K.F.	0.1%	
RON Blending	124-130	120-140
MON Blending	93-103	90-100
Composition %V :MeoH	70	100
EtoH	2	
C3	3	
C4	15	
C4+	10	

Table 4. Characteristics of MAS 70/30 vs. Methanol (Tontodonati, 1984)

Stoichiometry

As the alcohol concentration increases, stoichiometric air-fuel ratio decreases. The stoichiometric air-fuel ratio of MPHA[2]-indolene blend is higher than that of methanol-indolene blend (Patel, 1987). Table 5 shows that the stoichiometric A/F ratio increases as the molecular weight increases. Stoichiometric A/F ratio of isobutanol is closer to that of gasoline compared to those of methanol and ethanol.

Property	Gasoline Mixture of HC, unleaded	Methanol CH_3OH	Ethanol C_2H_5OH	Butanol C_4H_9OH ISO
Approximate Specific gravity at 60°F	0.72-0.75	0.79	0.79	0.81
Boiling point				
°F	85-437	149	173	226.6
°C	30-225	65	78.5	108.10
Net Lower Heating Value (mass)				
BTU/lbm	18,700	8,600	11,600	14,280
MJ/kg	43.5	20.1	27	33.0
Net Lower Heating Value (volume)				
BTU/gal	117,000	57,000	76,000	95,880
MJ/l	32	15.9	21.3	26.0
Heat of Vaporization				
BTU/gal	170	500	390	253.7
KJ/kg	400	1,110	900	579
Vapor Pressure at 100°F				
psi	9-13	4.6	2.25	0.62
kPa	62-90	32	17	2.25
Octane Number				
Research	91-100	112	111	113
Motor	82-92	91	92	94
Stoichiometric A/F ratio	14.6	6.4	9	11.1
Vapor Flamability limits, volume	0.6-8	5.5-26	3.5-15	1.8-8.4
Viscosity at 104°F (40°C)				
Centipoise	0.5	0.46	0.83	1.45
Centistokes	0.6	0.58	1.1	1.92
Appearance	Colorless	Colorless	Colorless	Colorless
Vapor Toxicity	M. Irritant	Irritant	Irritant	Irritant

Table 5. Gasoline, Methanol, Ethanol, and Butanol Properties

Octane Value

The octane values of methanol, MPHA'-15 (15% higher alcohol and 85% methanol) and MPHA'-30 (30% higher alcohol and 70% methanol) with nominal oxygen content 5% and 10% (base gasoline is indolene) are illustrated in Figure 9. The (R+M)/2 octane value of the blend increases regularly with alcohol content. In the upper scale, the mixture of higher alcohols has slightly lower anti-knock properties than methanol (Douthit and Talbot, 1984).

Property	Indolene	Methanol	Ethanol	N-Propanol	Isobutanol
Formula	---	CH_3OH	C_2H_5OH	C_3H_7OH	$CH_3CH(CH_3)CH_2OH)$
Specific gravity 60°F/60°F	0.75	0.793	0.8111	0.8045	0.8030
Boiling temp. °F	80-430	147	171.1	207	226.2
Flash point °F	-45	54	54	81	95
Autoignition temp. °F	495	---	---	---	---
Vapor pressure at 68°F, MMHG	---	97.68	48.1	14.9	8
flamability limits					
upper, %	7.6	36	---	13.7	10.6
lower, %	1.3	6.0	3.3	2.1	1.7
Vapor density (air = 1)	3	1.1	1.3	2.1	2.5

Table 6. Properties of Indolene, Methanol, Ethanol, N-propanol, Isobutanol (Patel, 1987).

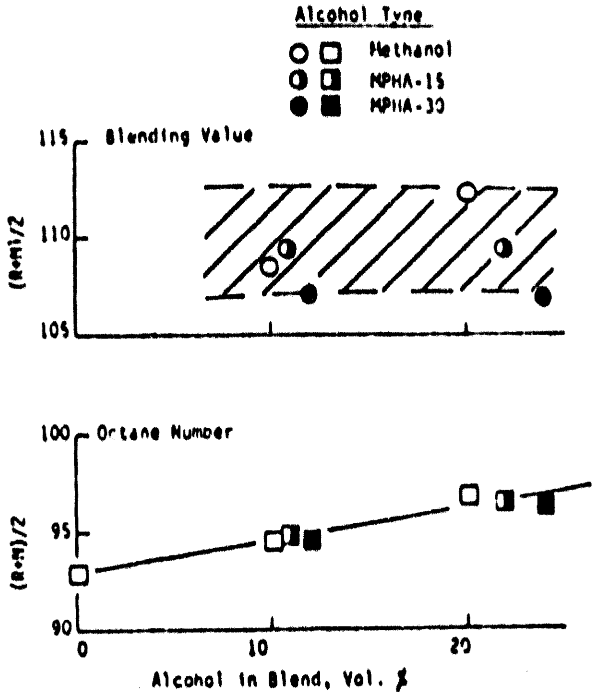

Figure 9. Octane Quality of Alcohol/Indolene Blends (Douthit, 1984)

Distillation Characteristics

Figure 10 shows the distillation characteristics of pure methanol, indolene and MPHA^2. Figures 11 to 14 show the distillation characteristics of indolene, indolene-methanol and indolene-MPHA^2 fuels. At all blend levels, indolene-MPHA blend is closer to indolene compared to indolene-methanol blend (Patel, 1987).

Energy Density

Energy density or heating value of a fuel is a measure of the amount of energy released as a result of the complete combustion of the fuel. The measured heating value decreases as the concentration of alcohol increases in the blend. The heating value of indolene-MPHA^2 blend is higher than indolene-methanol blend at all blend levels (Patel, 1987). Figure 15 shows the heating value of indolene-alcohol blends.

The heating values of the blends are generally predicted using equation 1 (Patel, 1987).

$$HVM = MI * HVI + MA * HVA \qquad (1)$$

where HVM = Heating value of mixture
MI = Mass Fraction of indolene
HVI = Heating Value of indolene
MA = Mass fraction of alcohol
HVA = Heating value of alcohol

Vapor Presure

Higher alcohols in the blend moderate the abrupt increase in Reid Vapor Pressure (RVP) caused by blending methanol to gasoline. The effect of higher alcohols in methanol-gasoline blend varies with the total amount of alcohol present (Figure 8) (Douthit, 1984).

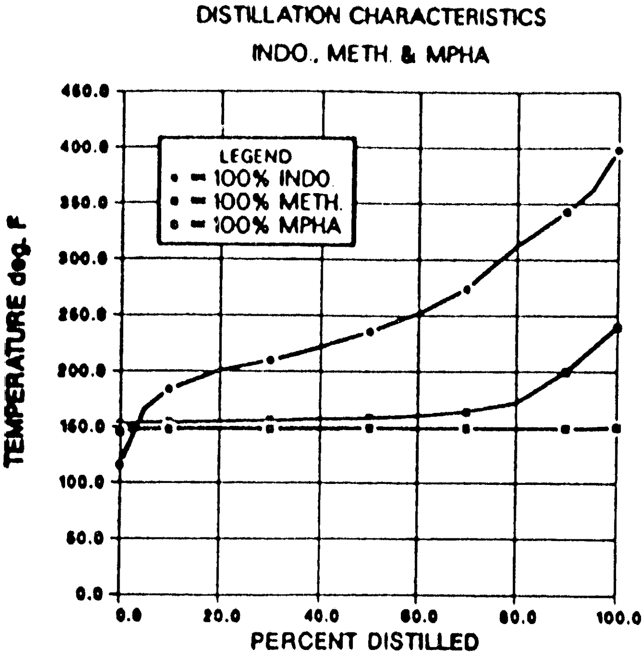

Figure 10Distillation properties of pure fuels (Patel, 1987).

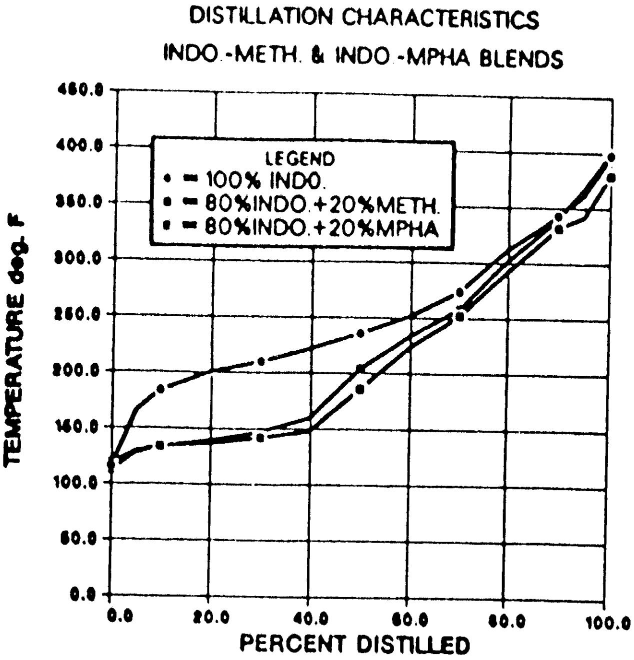

Figure11 Distillation of 20% alcohol blends (Patel, 1987)

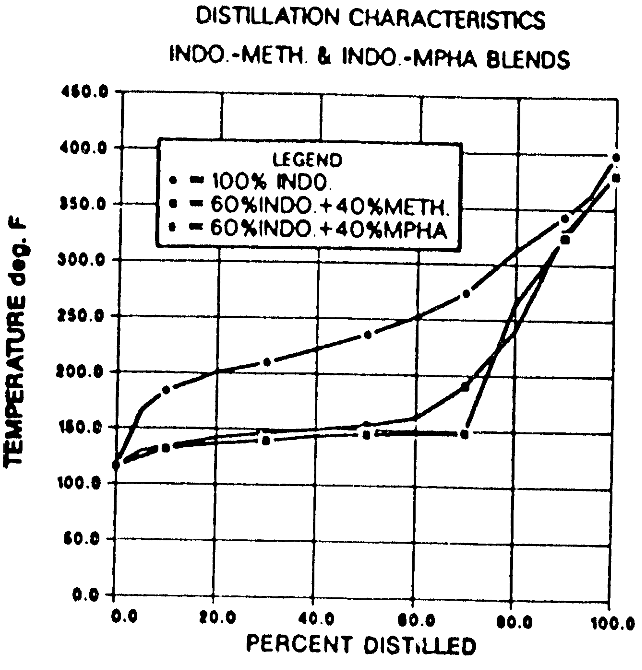

Figure 12Distillation of 40% alcohol blends (Patel, 1987).

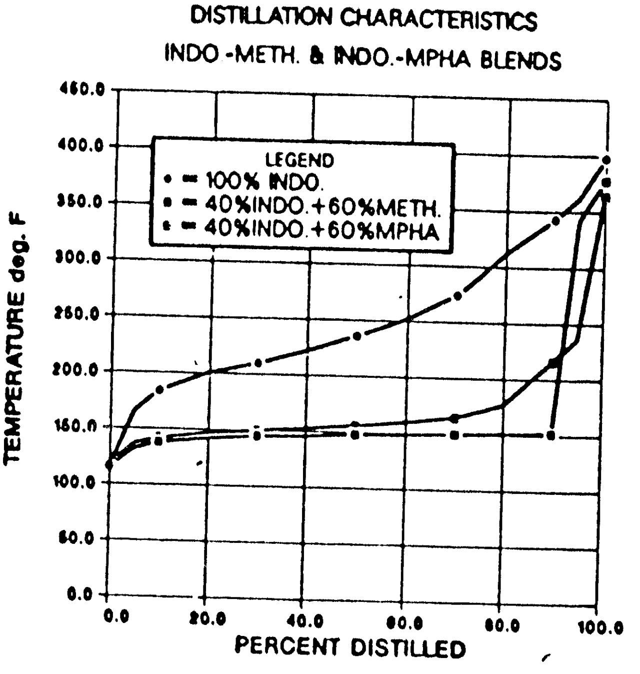

Figure13 Distillation of 60% alcohol blends (Patel, 1987).

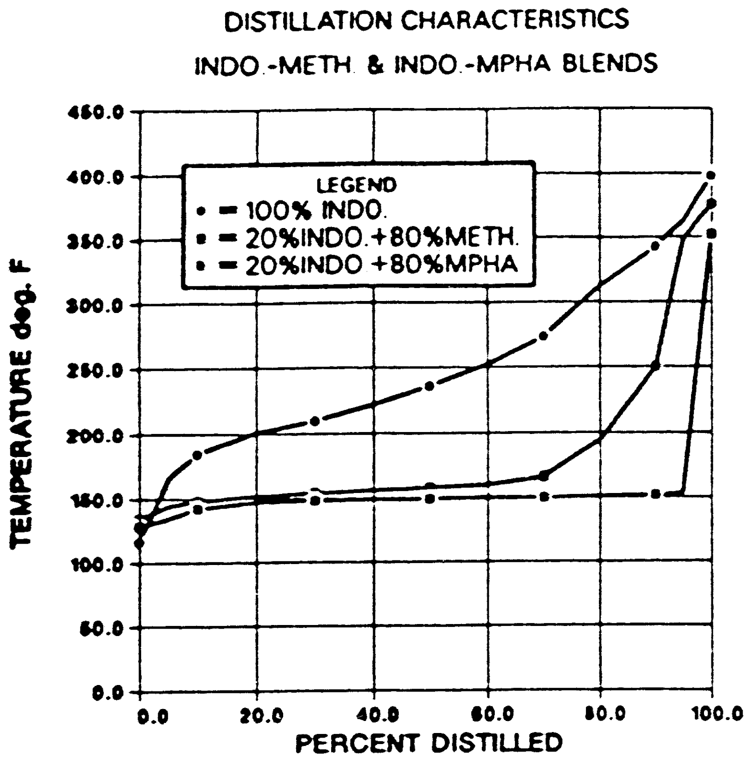

Figure 14 Distillation of 80% alcohol blends (Patel, 1987).

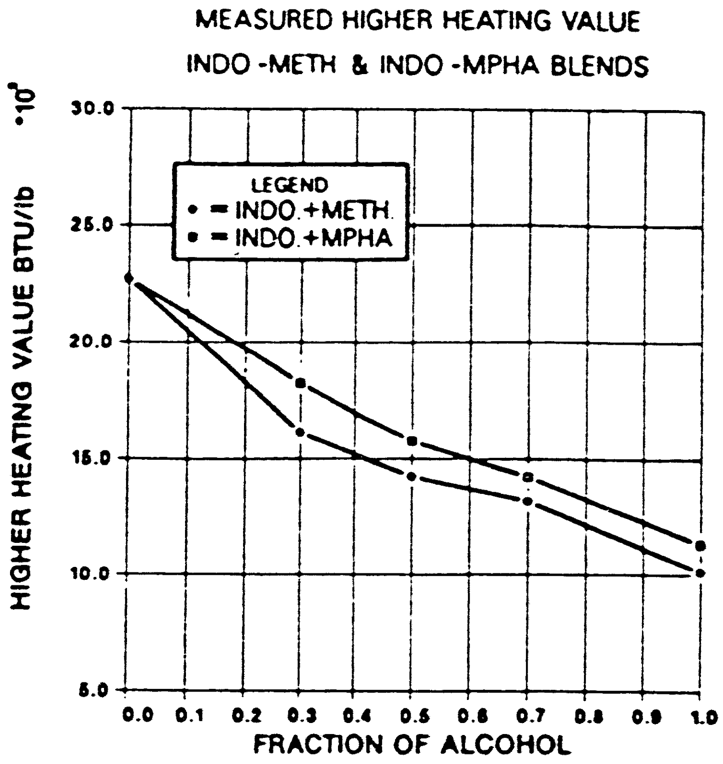

Figure 15 Measured higher heating values indolene-alcohol blends (Patel, 1987)

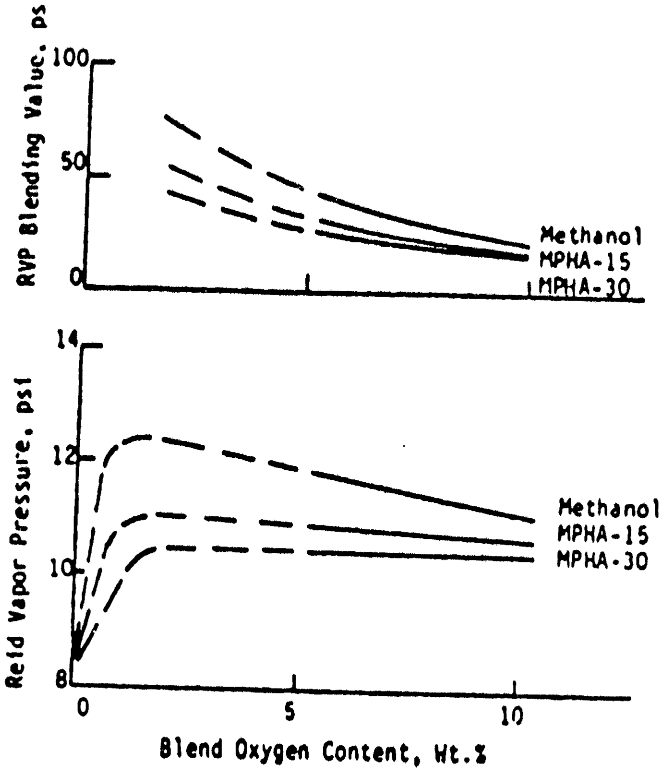

Figure 16 Volatility Effects in Alcohol/Indolene Blends (Douthit, 1984)

MAS blending effect on gasoline's volatility was always markedly lower in comparison to that of methanol, at all concentrations. In comparison to the mixture methanol/TBA (1:1%v), the MAS blending effect is lower at oxygenated concentrations in gasoline up to 5%v and similar at higher concentrations (Tontodonati, 1984).

Water Tolerance

At 5% or 10% total oxygen, addition of the higher alcohols mixture increases fuel blend water tolerance. However, there are indications of a reversal between the 5% and 10 % oxygen blends (Figure 17) (Douthit, 1984).

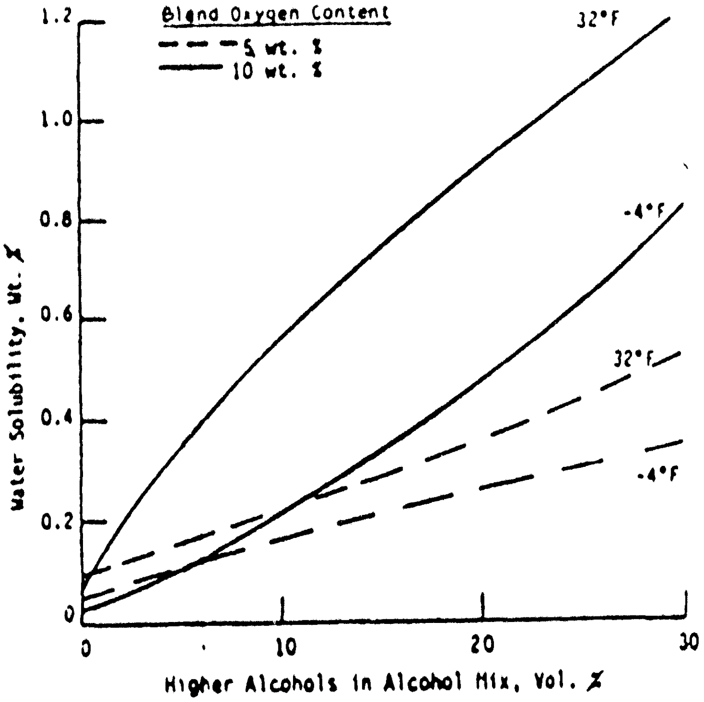

Figure 17 Effect of Higher Alcohols on Water Tolerance of Alcohol/Indolene Blends (Douthit, 1984).

At room temperature, as the alcohol concentration increases, water tolerance increases. The 90% MPHA^2 blend has about 50% higher water tolerance compared to 90% methanol blend at atmospheric temperature (Figure 18). Since MPHA-gasoline blends have higher water tolerance, they may be used without making major modification to the existing fuel distribution and delivery system (Patel, 1987).

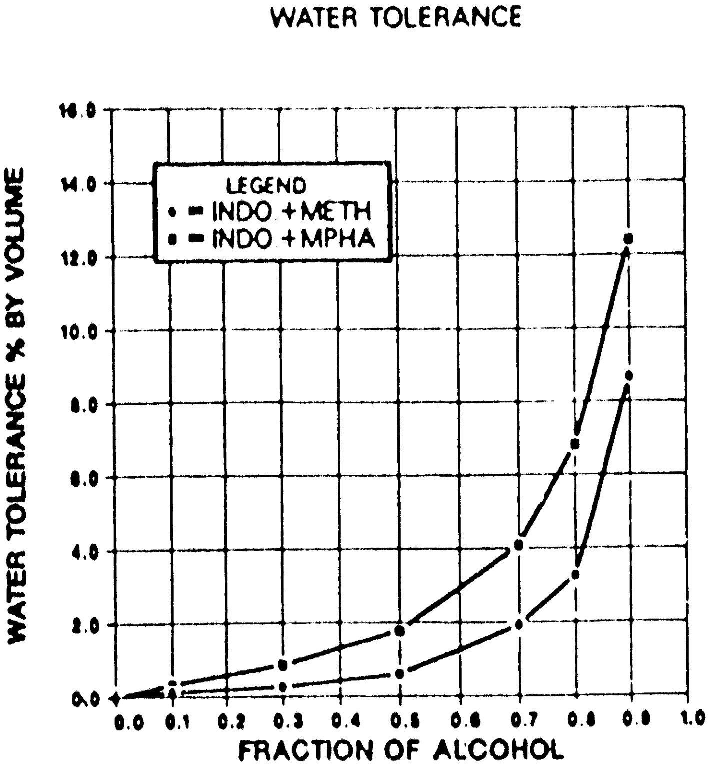

Figure 18. Water tolerance of indolene alcohol blends (Patel, 1987).

Ethanol, Isopropanol, and TBA can tolerate much higher amounts of water than methanol and their behaviour is practically the same. The behaviour of ethanol is closer to that of methanol than to that of the other higher alcohols. Methanol and Ethanol blends in phase separation conditions give lower phases very rich in gasoline if the water added slightly exceeds the water tolerance level. Isopropanol and TBA besides having a higher water tolerance level can be handled with separated phases without impairing the octane level of the gasoline or without producing lower phases rich in

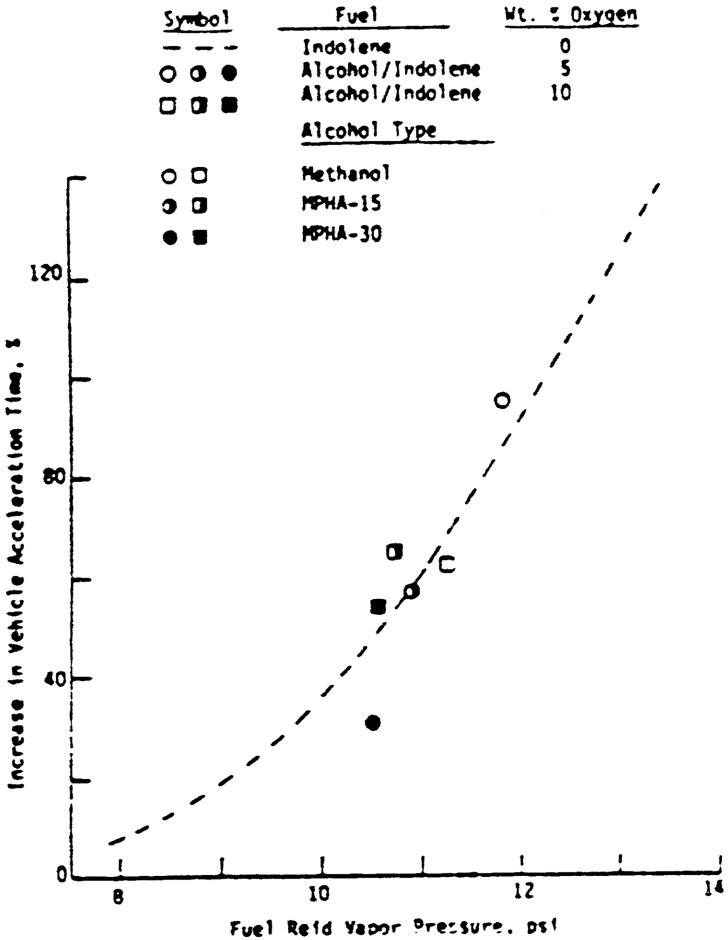

Figure 19 Vehicle Vapor Lock Effects at 90 F with Fuel RVP (Douthit, 1984)

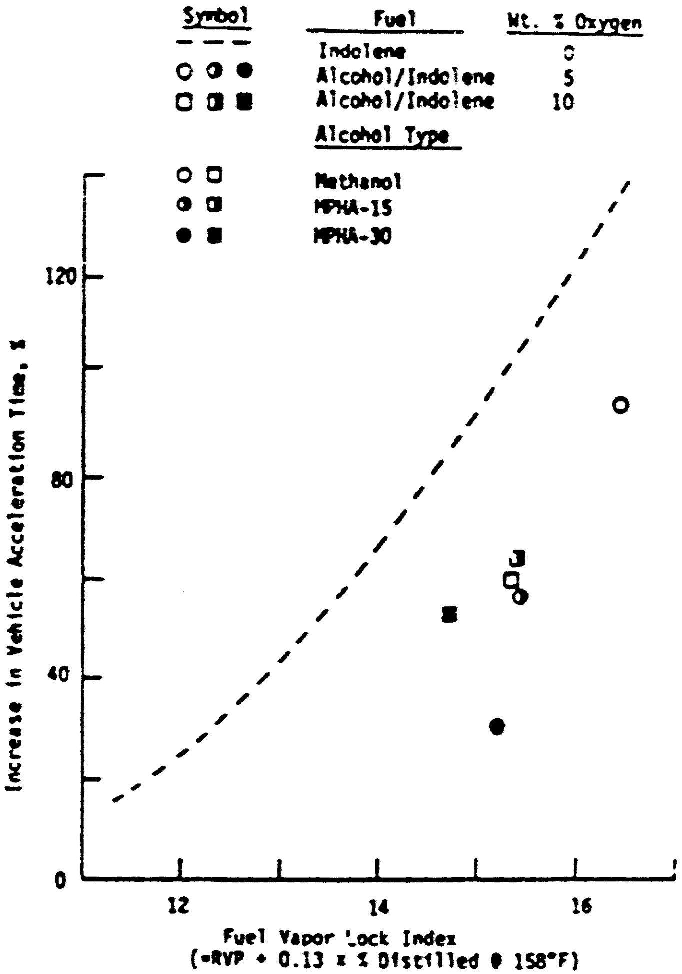

Figure 20 Vehicle Vapor Lock Effects at 90 F with Fuel Vapor Lock Index (Douthit, 1984).

harmful aromatics (Pea, 1988).

Vehicle Acceleration Time

The effect of increased higher alcohol content on acceleration time is very pronounced in the 5% oxygen series. At 10% oxygen, the higher alcohol effect disappears. Figure 19 shows the vehicle vapor lock effects at 90 °F with Fuel RVP and Figure 20 shows the vehicle vapor lock effects at 90 °F with Fuel Vapor Lock Index (Douthit, 1984).

In the 5% oxygen series, the higher alcohol shifts the V/L = 20 temperature time so slightly that vehicle acceleration time appears almost independent of the V/L temperatures (Figure 21) (Douthit, 1984).

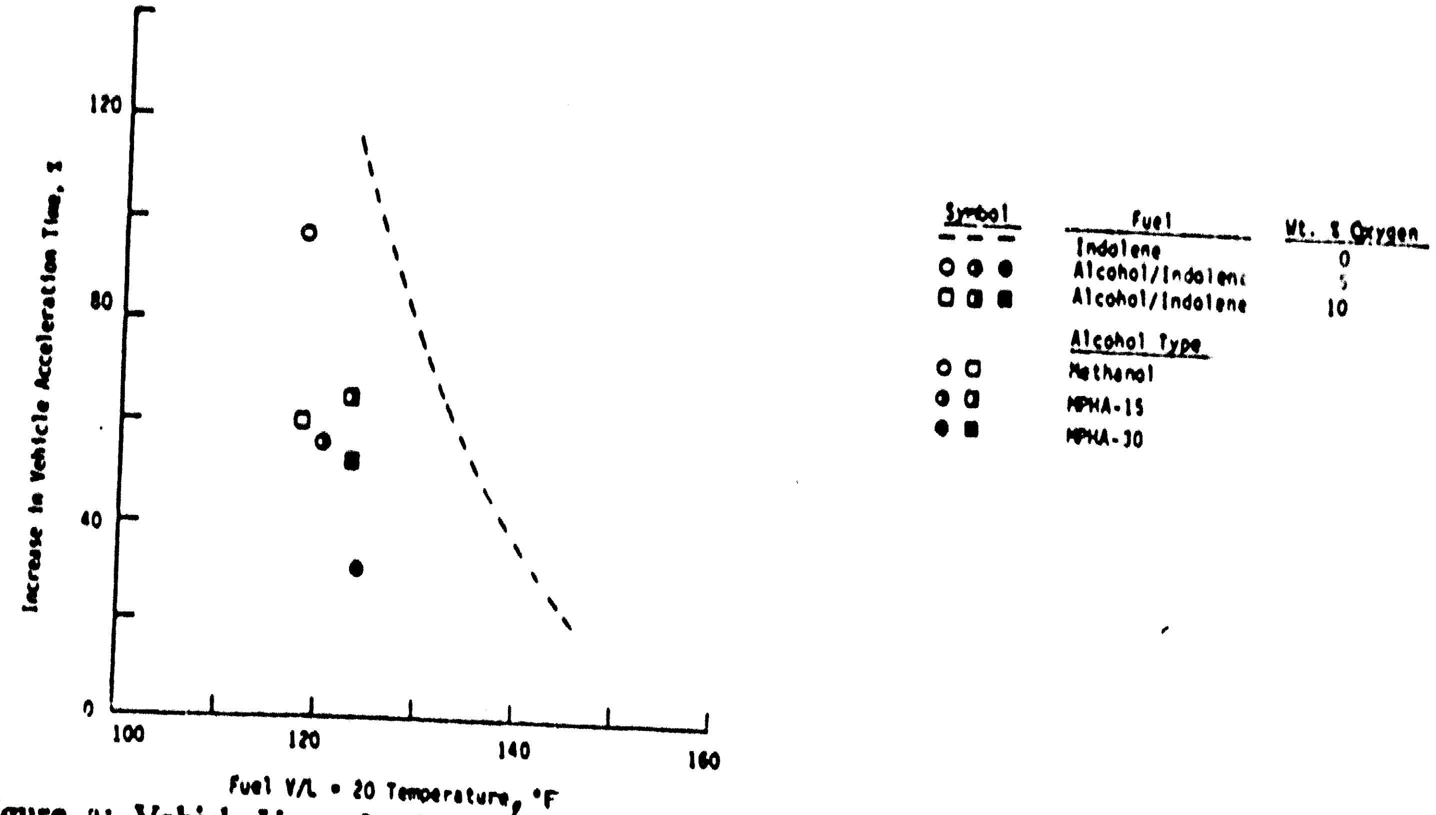

Figure 21 Vehicle Vapor Lock Effects at 90 F with Fuel V/L = 20 Temperature (Douthit, 1987).

Effect of Alcohol on MBT Spark Advance

At any fixed compression ratio, as the alcohol content [MPHA or methanol] increases, the MBT (minimum advance for best torque) spark advance decreases or shifts toward top dead center (Patel, 1987). At any compression ratio, the MBT spark advance of indolene-MPHA blends are higher than indolene methanol blends. With the same intake air temperature, the temperature of air fuel mixture during the compression process is related to the latent heat of the fuel. The MPHA^2 has lower latent heat and lower burning velocity than methanol (Patel, 1987).

Effect of Alcohol on KLCR

As the methanol concentration in the blend increases from 0 to 40%, KLCR increases from 7:1 to 10:1. Further increase in methanol concentration does not cause any further increase in KLCR. The variation of KLCR with MPHA fraction is similar to methanol. The knocking intensity with indolene-MPHA^2 blends is lower than indolene-methanol blends. The KLCR with indolene-MPHA^2 is higher than indolene-methanol blend (Patel, 1987).

Effect of Alcohol on Brake Power

In general, as the alcohol fraction increases, the brake power increases. At any compression ratio or any fraction of alcohol, the brake power of indolene-methanol blend is the same as indolene-MPHA^2 blend (Patel, 1987).

Effect of Alcohol on Brake Specific Fuel Consumption (on a mass basis (Kg/Kw-Hr))

In general, as the alcohol concentration increases, BSFC increases. At any CR, indolene-methanol blend has a higher BSFC than indolene-MPHA^2 blend specifically after 70% blend level. With regard to BSFC, methanol is at a distinct disadvantage compared to MPHA because of its lower heating value (Patel, 1987).

Effect of Alcohol on Brake Thermal Efficiency

At any CR, the thermal efficiency of indolene-alcohol blend is higher than indolene. In general, the indolene-methanol blend has a higher thermal efficiency than indolene-MPHA[2] blend. The brake thermal efficiency depends on combustion period, cooling looses, chemical equilibrium losses, change in specific heat losses and latent heat of vaporization (Patel, 1987).

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